Bulk-edge correspondence and dynamics of multiple edge states of a non-unitary three-step quantum walk with $\mathcal{PT}$ symmetry

Makio Kawasaki, Ken Mochizuki, Norio Kawakami, and Hideaki Obuse

Department of Applied Physics, Hokkaido University, Sapporo 060-8628, Japan
Department of Physics, Kyoto University, Kyoto 606-8502, Japan

Topological phases and the associated multiple edge states are studied for $\mathcal{PT}$ symmetric open quantum systems by constructing a non-unitary three-step quantum walk retaining $\mathcal{PT}$ symmetry in one dimension. We show that the non-unitary quantum walk has large topological numbers and numerically confirm that multiple edge states appear as expected from the bulk-edge correspondence. Therefore, the bulk-edge correspondence is valid in the present open quantum system. Toward experimental verifications, we propose a procedure to determine the number of the multiple edge states from time evolution of the probability distribution. Further, we demonstrate that the long time dynamics of the unitary three-step quantum walk can be well simulated on a quantum computer IBM Q.

I. INTRODUCTION

In closed quantum systems, all observables including Hamiltonians are described by Hermitian operators. Hermiticity of an observable ensures that all the eigenvalues are real, and the time-evolution operator generated by a Hamiltonian becomes a unitary operator. In 1998, however, Bender and Boettcher have shown that non-Hermitian Hamiltonians retaining combined parity and time-reversal ($\mathcal{PT}$) symmetry can possess entirely real eigenvalues [1]. Such non-Hermitian Hamiltonians phenomenologically describe open quantum systems where particles flow in and out, corresponding to gain and loss effects, for example. A non-Hermitian Hamiltonian has $\mathcal{PT}$ symmetry if the Hamiltonian commutes with the $\mathcal{PT}$ symmetric operator [1-5]. Systems described by $\mathcal{PT}$ symmetric Hamiltonians are effectively realized in classical optical systems with balanced gain and loss in experiments [6-9]. In these systems, various phenomena that do not occur in closed systems are observed; i.e. unidirectional invisibility [10,12] and sensitivity enhancement of metrology [13-17]. Taking these advantages, the $\mathcal{PT}$ symmetric open systems have attracted great attention to realize novel devices [18-20].

Contrarily, $\mathcal{PT}$ symmetric Hamiltonians in open quantum systems had not been realized in experiments for almost two decades since the first theoretical proposal [1]. Recently, $\mathcal{PT}$ symmetric open quantum systems have been realized in quantum optical systems by adopting postselectors [21-22]. Among them, a quantum walk approach proposed theoretically in Ref. [23] provides a systematic way to incorporate fertile non-unitary dynamics retaining $\mathcal{PT}$ symmetry and extra properties. By using the $\mathcal{PT}$ symmetric non-unitary quantum walk, topological phases and the edge states for open quantum systems have been studied theoretically [24] and experimentally [22]. The topological number is also detected by using non-unitary quantum walks [25-26].

The topological phase for non-Hermitian Hamiltonians (including $\mathcal{PT}$ symmetric one) is one of the rapidly growing research fields in the past couple of years [24-27, 40]. In Hermitian systems, the number of edge states appearing in a band gap near a boundary of two regions is equivalent to the difference of topological numbers in each region. This fundamental principle is called the bulk-edge correspondence and its validity is widely accepted. In non-Hermitian systems, however, the bulk-edge correspondence requires further verifications by the following reasons. First, two kinds of band gaps, point and line gaps, exist for complex energy [32,33,38]. Next, 10 symmetry classes in Hermitian systems are increased to 38 in non-Hermitian systems due to extra symmetries [33]. Furthermore, failures of the conventional bulk-edge correspondence are already reported [34-35,38], though the reason has not yet been fully understood. Since these results strongly depend on the enlarged symmetries and details of systems, the bulk-edge correspondence in non-Hermitian systems should be seriously investigated for various systems.

In this work, we focus on the bulk-edge correspondence of $\mathcal{PT}$ symmetric open quantum systems with large topological numbers by using a non-unitary quantum walk. To this end, we introduce a non-unitary three-step quantum walk with $\mathcal{PT}$ symmetry in one dimension, which can be realized in a quantum optical system. Because of large topological numbers, this quantum walk is expected to exhibit multiple edge states if the bulk-edge correspondence is valid in the open quantum system. We numerically confirm the validity of the bulk-edge correspondence in the $\mathcal{PT}$ symmetric open system by counting the number of eigenvalues corresponding to multiple edge states. Towards experimental verifications showing the existence of multiple edge states, we also propose a procedure to distinguish the number of edge states from time dependences of the probability distribution which is available in the standard experiments of quantum walks. We also demonstrate that long time dynamics of the three-step quantum walk can be well simulated on a quantum computer IBM Q.

This paper is organized as follows. We explain the $\mathcal{PT}$ symmetric non-unitary quantum walks studied in the previous work [22] in Sec. II. In Sec. III we introduce
a non-unitary three-step quantum walk with $\mathcal{PT}$ symmetry. We show that the quantum walk also have extra symmetries which are important for topological phases in open quantum systems. In addition, we show that this quantum walk has large topological numbers and numerically check the validity of the bulk-edge correspondence. Towards future experimental verifications, in Sec. V we introduce a perturbed time-evolution operator and show that we can determine the number of edge states from time dependence of the probability distribution by using this perturbed time-evolution operator. We discuss the realizability of the long-time evolution of the quantum walk on IBM Q in Sec. V. Section VI closes the paper by summarizing our results.

II. $\mathcal{PT}$ SYMMETRIC QUANTUM WALKS

We briefly review the definition of discrete time quantum walks in one dimension [11,13,48]. Quantum walks are defined by a time-evolution operator $U$. The walker’s state is characterized by its position $x \in \mathbb{Z}$ and internal degrees of freedom $L$ and $R$. We describe bases of the internal space as $|L\rangle = (1,0)^T$ and $|R\rangle = (0,1)^T$. For a given initial state $|\psi(0)\rangle$, the state after $t$ time steps is determined by

$$|\psi(t)\rangle = U^t |\psi(0)\rangle. \quad (1)$$

A state of the walker at time $t$ is described as

$$|\psi(t)\rangle = \sum_x [a_x(t) |x\rangle \otimes |L\rangle + b_x(t) |x\rangle \otimes |R\rangle], \quad (2)$$

where $a_x(t)$ and $b_x(t)$ are amplitudes of the states $|x\rangle \otimes |L\rangle$ and $|x\rangle \otimes |R\rangle$, respectively. In most cases, time-evolution operators consist of two kinds of unitary operators, so-called, coin and shift operators:

$$C := \sum_x \left[ |x\rangle \langle x| \otimes \tilde{C}_x \right], \quad (3)$$

$$S := \sum_x \left[ (|x-1\rangle \langle x| \otimes |L\rangle \langle L| + |x+1\rangle \langle x| \otimes |R\rangle \langle R| \right], \quad (4)$$

respectively. $\tilde{C}_x$ is a U(2) matrix acting on the internal states. The shift operator $S$ moves the walker depending on its internal states. Usually, since the time-evolution operator of quantum walks is defined by combining these two unitary operators, the time-evolution operator is also a unitary operator.

Remarkably, quantum walks can further describe non-unitary dynamics by introducing a non-unitary operator to incorporate phenomenological gain and loss of amplitudes. Note that non-unitarity of the time-evolution operator is equivalent to non-Hermiticity of the effective Hamiltonian, where the effective Hamiltonian $H_{\text{eff}}$ is defined as $U = e^{-iH_{\text{eff}}}$. The non-unitary time-evolution operator implemented in Ref. [22] is described as below:

$$U_2 = G\mathcal{S}\mathcal{R}[\theta_2(x)]G^{-1}\mathcal{S}\mathcal{R}[\theta_1(x)], \quad (5)$$

$$\mathcal{R}[\theta(x)] = \sum_x \left[ |x\rangle \langle x| \otimes \begin{pmatrix} \cos \theta(x) & \sin \theta(x) \\ \sin \theta(x) & -\cos \theta(x) \end{pmatrix} \right], \quad (6)$$

$$G = \sum_x |x\rangle \langle x| \otimes \begin{pmatrix} e^\gamma & 0 \\ 0 & e^{-\gamma} \end{pmatrix}. \quad (7)$$

$S$ and $R$ represent the shift operator $[4]$ and the coin operator, respectively. $G$ is a non-unitary operator that describes simultaneous amplification and decay process of walker’s amplitudes. We call $\gamma$ the non-unitarity degree since variations of amplitudes become larger as $\gamma$ increases. Since $U_2$ in Eq. (5) contains two shift operators, $U_2$ is a non-unitary extension of two-step quantum walks. As we will mention later, $U_2$ possesses $\mathcal{PT}$ and other extra symmetries.

We define a quasi-energy $\varepsilon$ by an eigenvalue equation:

$$U |\phi\rangle = \lambda |\phi\rangle, \quad \varepsilon = i \log \lambda. \quad (8)$$

Unitarity of the time-evolution operator ensures $|\lambda| = 1$, and then $\varepsilon$ becomes real. However, $\varepsilon$ becomes a complex number in case of non-unitary time-evolution operators. In both cases, $\varepsilon$ has $2\pi$ periodicity. Two kinds of topological numbers are defined as $\nu_0, \nu_\pi$ when $U$ possesses chiral symmetry since the band gap closes at $\varepsilon = 0, \pi$ because of periodicity of $\varepsilon$.

Here we give a remark on topological phases of the non-unitary time-evolution operator $U_2$. Topological numbers $\nu_0, \nu_\pi$ calculated from the time-evolution operator $U_2$ take the values $\pm 1$ depending on the coin parameters $\theta_1, \theta_2$ in Eq. (4). If we assume that the bulk-edge correspondence still holds in this system, two edge states should emerge when the difference of topological numbers is two. However, the time-evolution operator $U_2$ induces only a single edge state in the standard experimental setup of quantum walks by the following reasons. First, by changing the order of the basis to distinguish even and odd sites, $U_2$ is described by the block diagonal form:

$$U_2 = \begin{pmatrix} U_2^e & 0 \\ 0 & U_2^o \end{pmatrix}, \quad (9)$$

$$|\psi(t)\rangle = \begin{pmatrix} |\psi_e(t)\rangle \\ |\psi_o(t)\rangle \end{pmatrix}, \quad (10)$$

where $U_2^e$ and $U_2^o$ are non-unitary operators and the bases are given by

$$|\psi_e(t)\rangle = \sum_{i \in \mathbb{Z}} [a_{2i}(t) |2i\rangle \otimes |L\rangle + b_{2i}(t) |2i\rangle \otimes |R\rangle], \quad (11)$$

$$|\psi_o(t)\rangle = \sum_{i \in \mathbb{Z}} [a_{2i+1}(t) |2i+1\rangle \otimes |L\rangle + b_{2i+1}(t) |2i+1\rangle \otimes |R\rangle]. \quad (12)$$

Since $U_2^e$ in Eq. (9) has a block diagonal form, the system is decoupled into the two independent subsystems. Second, the initial state is chosen to localize at a single site.
in many experiments of quantum walks. Accordingly, the time-evolution operator $U_2$ realized in experiments is effectively reduced to $U_2^c$ or $U_2^o$ in Eq. (9). Actually, the topological numbers $v_0$ and $v_3$, derived from $U_2^c$ or $U_2^o$, takes $\pm \frac{1}{2}$. Therefore, only a single edge state is realized in the experiment implementing $U_2$ [22]. Hence, it is insufficient to experimentally verify the bulk-edge correspondence of large topological numbers for the non-Hermitian systems.

III. NON-UNITARY THREE-STEP QUANTUM WALKS WITH PT SYMMETRY

In order to overcome the problem that we clarified at the end of the previous section, we define a non-unitary time-evolution operator having large topological numbers and investigate this topological property in this section. We first introduce a time-evolution operator, called non-unitary three-step quantum walk with $\mathcal{PT}$ symmetry in Sec. III A. Then, we study the eigenvalue distribution in homogeneous systems in Sec. III B, and show that the topological numbers are effectively reduced to $\pm \frac{1}{2}$, derived from $U_2$ [22]. We use polarization of a photon as internal states. The coin, shift operators and non-unitary operator $G$ are realized by half wave plates, beam displacers and partially polarizing beam splitters, respectively. (b) Schematic view of the optical system that can realize non-unitary three-step quantum walk $U_3$. $R(\theta)$ and $C(\theta)$ are related via $R(\theta) = C(\theta)\sigma_3$, where we denote the Pauli matrices as $\sigma_1, \sigma_2, \sigma_3$ in this paper. We can convert $R(\theta)$ into $C(\theta)$ by adding an extra half wave plate acting as $\sigma_3$.

A. Non-unitary three-step quantum walk with $\mathcal{PT}$ symmetry

We define the time-evolution operator as

$$U_3 := G^{-1}SC[\theta_2(x)]SC[\theta_2(x)]GSC[\theta_1(x)],$$

(13)

where $G$ and $S$ are defined as Eqs. (4) and (7), and the coin operator is defined as

$$C[\theta(x)] := \sum_x \left| x \right\rangle \langle x | \otimes \left( \cos \theta(x) - \sin \theta(x) \right) \langle \cos \theta(x) \sin \theta(x) \right).$$

(14)

We call the time-evolution operator in Eq. (13) the (non-unitary) three-step quantum walk as Eq. (13) contains three shift operators. Figure 1 (b) shows an optical system that can realize the time-evolution operator $U_3$.

Parameter $\theta$ is effectively reduced to $\pm \frac{1}{2}$, derived from $U_2$ [22]. Hence, it is insufficient to experimentally verify the bulk-edge correspondence of large topological numbers for the non-Hermitian systems.

Next, we consider other symmetries by taking account of a scheme to classify topological phases in non-Hermitian Hamiltonians proposed in Ref. [33]. Here, we show that $U_3'$ (then, $U_3$) has all symmetries of $\mathcal{AZ}^j$ symmetry [33]. In this case, time-reversal, particle-hole, and chiral symmetries are defined for a non-Hermitian Hamiltonian $H$.
\[ TH^T T^{-1} = H, \]  
\[ \Xi H^T \Xi^{-1} = -H, \]  
\[ \Gamma H^T \Gamma^{-1} = -H, \]

respectively. We note that all symmetry operators \( T, \Xi, \Gamma \) are unitary operators. The above relations can be rewritten for a non-unitary operator \( U \) whose effective Hamiltonian satisfies Eqs. (20)-(22) as

\[ TU^T T^{-1} = U, \]  
\[ \Xi U^* \Xi^{-1} = U, \]  
\[ \Gamma U^* \Gamma^{-1} = U. \] 

We find that \( U' \) satisfies the above relations with the following symmetry operators

\[ T = \sum_x |x\rangle \langle x| \otimes \sigma_1, \]  
\[ \Xi = \sum_x |x\rangle \langle x| \otimes \sigma_0, \]  
\[ \Gamma = \sum_x |x\rangle \langle x| \otimes \sigma_1, \]  

where \( \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \). Therefore, \( U_3 \) belongs to the BDI\(^\dagger\) symmetry class in Ref. \[33\]. We, however, remind readers that \( U_3 \) also retain the spatial symmetry originating from \( \mathcal{P}\mathcal{T} \) symmetry in Eq. \[13\]. We can also show that the operator \( U_2 \) implemented in Ref. \[22\] has the same symmetries of \( U_3 \) in the similar way.

We mention that, while a similar non-unitary three-step quantum walk is studied in Ref. \[26\], that quantum walk has completely different symmetries. The non-unitary quantum walk in Ref. \[26\] does not retain \( \mathcal{P}\mathcal{T} \) symmetry, but has pseudo-Hermiticity (or pseudo-unitarity). Moreover, the quantum walk does not retain AZ\(^\dagger\) type time-reversal symmetry, but satisfy AZ type time-reversal symmetry: \( TU^* T^{-1} = U^{-1} \) \[33\], where \( T \) is a unitary operator. Therefore, the non-unitary three-step quantum walk belongs to the different symmetry classes with the present quantum walk \( U_3 \). In addition, based on a time-dependent tight binding model, the bulk-edge correspondence for a non-unitary time-evolution operator with large topological numbers is also studied in Ref. \[29\]. This time-evolution operator also retain AZ type time-reversal symmetry, but no AZ\(^\dagger\) type time-reversal symmetry. Therefore, the symmetry class studied in Ref. \[29\] is also different from the present work. Since topological phases and bulk-edge correspondence in open systems strongly depend on symmetry classes of Hamiltonians or time-evolution operators, it is important to study topological phases of the present quantum walk \( U_3 \).

**B. Eigenvalue distribution in the homogeneous case**

Here we consider the case that parameters of the coin operator \( \theta_1(x) \) and \( \theta_2(x) \) are homogeneous in space and derive the eigenvalue distribution of the time-evolution operator \( U_3' \) \[16\]. We can diagonalize the time-evolution operator \( U_3' \) in Eq. \[16\] in the wave number space by changing the position basis to wave number basis because of the homogeneity:

\[ |x\rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} dk e^{-ikx} |k\rangle. \]  

This procedure results in the diagonal forms of the operators in Eqs. \[1\], \[7\] and \[14\] in the wave number space:

\[ S = \int dk \langle |k| \otimes S_k(k) \rangle, S_k(k) = \begin{pmatrix} e^{ik} & 0 \\ 0 & e^{-ik} \end{pmatrix}, \]  
\[ C(\theta_j) = \int dk \langle |k| \otimes C_k(\theta_j) \rangle, C_k(\theta_j) = \begin{pmatrix} \cos \theta_j & -\sin \theta_j \\ \sin \theta_j & \cos \theta_j \end{pmatrix}, \]  
\[ G = \int dk \langle |k| \otimes G_k \rangle, G_k = \begin{pmatrix} e^{\gamma} & 0 \\ 0 & e^{-\gamma} \end{pmatrix}, \]

where \( j = 1, 2 \). We rewrite the time-evolution operator \( U_3' \) in Eq. \[16\] in the wave number space as

\[ U_3' = \int dk \langle |k| \otimes U_3'(k) \rangle, \]
\[ U_3'(k) = d_0(k)\sigma_0 + d_1(k)\sigma_1 + id_2(k)\sigma_2 + id_3(k)\sigma_3. \]

The coefficients \( d_j (j = 0, 1, 2, 3) \) are given by

\[ d_0(k) = -\left( \cos \theta_1 \sin^2 \theta_2 + \sin \theta_1 \sin 2\theta_2 \cosh 2\gamma \right) \cos k + \cos \theta_1 \cos^2 \theta_2 \cos 3k, \]  
\[ d_1(k) = \sin 2\theta_2 \sin 2\gamma \cos k, \]  
\[ d_2(k) = (\sin \theta_1 \sin^2 \theta_2 - \cos \theta_1 \sin 2\theta_2 \cosh 2\gamma) \cos k - \sin \theta_1 \cos^2 \theta_2 \cos 3k, \]  
\[ d_3(k) = -\sin^2 \theta_2 \sin k + \cos^2 \theta_2 \sin 3k. \]

These coefficients satisfy

\[ d_0(k)^2 - d_1(k)^2 + d_2(k)^2 + d_3(k)^2 = 1. \]  

The eigenvalues of \( U_3'(k) \) are described as

\[ \lambda_{\pm}(k) = \lambda_0(k) \pm i\sqrt{1 - \lambda_0(k)^2}, \]  

hence \( |\lambda_{\pm}(k)| \neq 1 \) is satisfied if there exist \( k \) such that \( |\lambda_0(k)| > 1 \). If \( |\lambda_0(k)| = 1 \), the eigenvalue becomes \( \lambda_0(k) = 1 \) and \(-1\) which corresponds to the quasi-energy \( \varepsilon = 0 \) and \( \pi \), respectively. These points are called exceptional points. We also state that an eigenstate of the \( \mathcal{P}\mathcal{T} \) symmetric time-evolution operator \( U \) breaks \( \mathcal{P}\mathcal{T} \) symmetry if the eigenstate of \( U \) is not the eigenstate of
the symmetry operator $\mathcal{PT}$, or equivalently the corresponding eigenvalue satisfy $|\lambda_\pm(k)| \neq 1$. Figure 2 shows dispersion relations and eigenvalue distributions of the non-unitary three-step quantum walk with homogeneous coin parameters. In Fig. 2 (a)-(c) all eigenvalues satisfy $|\lambda_\pm(k)| = 1$ because none of the eigenstates breaks $\mathcal{PT}$ symmetry. On the other hand, in Fig. 2 (d) eigenvalues not satisfying $|\lambda| = 1$ (or equivalently, complex valued quasi-energies) emerge because several eigenstates break $\mathcal{PT}$ symmetry. As discussed later, the band gap closes at $\varepsilon = 0$ and $\pi$ simultaneously.

## C. Topological numbers

Now we calculate topological numbers of the non-unitary three-step quantum walk. In Hermitian systems, topological numbers of quantum walks with chiral symmetry are given by the formula [44]

$$
\nu_0 = \frac{\nu' + \nu''}{2}, \quad \nu_\pi = \frac{\nu' - \nu''}{2},
$$

(41)

where winding numbers $\nu'$ and $\nu''$ are derived from the time-evolution operator with two different symmetric time frames $U'$ and $U''$. We apply Eq. (41) to the present work.

Since the time-evolution operator $U_3$ changes positions of the walker from odd (even) sites to even (odd) sites at every iteration (this property is called as sublattice structure), we can rewrite the time-evolution operator $U_3$ by changing the order of the basis which is the same in Eqs. (11) and (12)

$$
\tilde{U}_3 = \begin{pmatrix} 0 & U_0^\circ \\ U_0^o & 0 \end{pmatrix},
$$

(42)

where $U_0^o$ and $U_0^e$ are non-unitary operators. We define an operator $\tau_3 := \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$ in this basis, where $I$ denotes an identity operator. Then the relation

$$
\tau_3 \tilde{U}_3 \tau_3 = -\tilde{U}_3
$$

(43)

holds. This relation guarantees that we have the eigenstate with eigenvalue $e^{-i(\nu + \pi)}$ if we have an eigenstate with an eigenvalue $e^{-i\nu}$. Hence the band gap closes at $\varepsilon = \pi$ if the band gap closes at $\varepsilon = 0$ and the two kinds of topological numbers $\nu_0$ and $\nu_\pi$ take the same value. Indeed, one of the winding numbers $\nu''$ becomes zero. Thus we do not distinguish two kinds of the topological numbers and denote them as $\nu$ hereinafter.

Regarding winding numbers, we cannot calculate winding numbers in an ordinally way because the time-evolution operator is a non-unitary operator, i.e. the effective Hamiltonian is non-Hermitian. The method of calculating the winding number in non-Hermitian systems is presented in Ref. [27] and the formula reads

$$
\nu = \frac{1}{2\pi i} \int_{-\pi}^{\pi} dk \frac{1}{q(k)} \frac{d}{dk} q(k).
$$

(44)

Here, $q(k)$ is defined as

$$
\tilde{Q}(k) = \frac{1}{2} \left( |\chi_+\rangle \langle \phi_+| + |\phi_+\rangle \langle \chi_+| - |\chi_-\rangle \langle \phi_-| - |\phi_-\rangle \langle \chi_-| \right) = \begin{pmatrix} 0 & q(k) \\ q^*(k) & 0 \end{pmatrix}.
$$

(45)
In Eq. 45, $|\phi_{\pm}\rangle$ and $|\chi_{\pm}\rangle$ denote right and left eigenvectors of a non-Hermitian Hamiltonian $H(k)$ with the eigenvalues $E_{\pm}$, respectively, and $H(k)$ satisfies chiral symmetry in Eq. 22 with the symmetry operator $\Gamma = \sigma_3$, thus

$$\sigma_3 H^\dagger(k) \sigma_3 = -H(k). \quad (46)$$

We apply the above method to the non-unitary time-evolution operator. The corresponding non-unitary operator $U$ satisfies

$$\sigma_3 U(k) \sigma_3 = U(k). \quad (47)$$

Since $U'_k$ has chiral symmetry with the symmetry operator in Eq. 25, in order to satisfy the condition 47, we perform a unitary transformation:

$$\tilde{U}_k' = e^{-i\frac{\pi}{4} \sigma_3} U'_k e^{i\frac{\pi}{4} \sigma_3}$$

$$= d_0(k) \sigma_0 + id_4(k) \sigma_1 + id_2(k) \sigma_2 - d_1(k) \sigma_3. \quad (48)$$

The eigenvectors of $\tilde{U}_k'$ in Eq. 48 are described as

$$|\phi_{\pm}\rangle = \frac{1}{\sqrt{2 \cos 2\Omega k}} \left( e^{\pm i\Omega x} \right)$$

$$|\chi_{\pm}\rangle = \frac{1}{\sqrt{2 \cos 2\Omega k}} \left( e^{\pm i\Omega x} \pm ie^{i\Omega x} e^{-i\Omega k} \right), \quad (49)$$

$$d_2 + id_3 = |d| e^{i\theta_0}, \quad \sin 2\Omega k = \frac{d_4}{|d|}. \quad (50)$$

From the explicit form of $q(k)$, the winding number is expressed as

$$\nu' = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\theta_k \frac{dk}{dk}. \quad (52)$$

Equation 52 means that $\nu'$ is equal to the winding number of $d_2 + id_3$ around the origin in the complex plane.

Figure 3 shows values of the topological number $\nu$ as function of the coin parameters $\theta_1$ and $\theta_2$. As shown in Fig. 4, the values of the topological numbers do not depend on the non-unitarity degree $\gamma$, unless the band gaps around $\varepsilon = 0$ or $\pi$ close. In contrast to the recent experiment 22, the values of the topological numbers can take 2 or 3.

### D. Bulk-edge correspondence

In order to verify the bulk-edge correspondence, we consider inhomogeneous systems so that the topological number varies in position space by making the coin parameters $\theta_1$ and $\theta_2$ position dependent. We set the parameters satisfying Eq. 19 as

$$\theta_{1(2)}(x) = \begin{cases} \theta_{1(2)}^1 & (|x| < L'), \\ \theta_{1(2)}^2 & (|x| \geq L'). \end{cases} \quad (53)$$

and thus the values of $\theta_1$ and $\theta_2$ change at two points $x = \pm L'$. We call the region $|x| < L'$ (|x| $\geq L'$) the inner (outer) region. We fix $L' = 50$ and $\theta_{1(2)}^1, \theta_{1(2)}^2 = (\frac{\pi}{4}, \frac{3\pi}{4})$ [the black circle in Fig. 3(b)] in the rest of this section, thus the topological number in the inner region $\nu^i$ is 0. Then, we consider several sets of $\theta_{1(2)}^i$ and $\theta_{1(2)}^o$ in order to change the topological number in the outer region, $\nu^o$. $\nu^o$ represents the difference of topological numbers in the inner and outer regions due to $\nu^i = 0$.

In Fig. 3 we plot eigenvalue distributions of the time-evolution operator $U_3$ in Eq. 13 with inhomogeneous coin parameters. These eigenvalues are calculated by numerical diagonalization for a finite system size ($|x| \leq 100$) with periodic boundary conditions. Except $\nu^o = 0$ [Fig. 4(a)], isolated eigenvalues appear on the real axis. The corresponding eigenstates are edge states of the three-step quantum walk, whose real part of quasi-energy $\varepsilon$ is 0 or $\pi$. First we consider unitary time evolution [Fig. 4(e)]. In this case six eigenstates with eigenvalues $\pm 1$ are degenerate. Since there are two boundaries where the topological number changes, the bulk-edge correspondence tells us that the number of edge states is twice as large as the difference of the topological numbers. In this case, edge states with eigenvalues $\pm 1$ appear and the number of edge states is twice as large as $\nu^o$, which corresponds with the result of bulk-edge correspondence.

Next we consider the case of non-unitary time evolution [Fig. 4(a)-(d)]. The eigenvalues of the edge states $\lambda$ satisfy $|\lambda| \neq 1$ [or equivalently $\text{Im}(\varepsilon) \neq 0$] and this means that the edge states break $\mathcal{PT}$ symmetry. Figure 4(f) shows the probability distribution of an edge state. This state apparently breaks $\mathcal{PT}$ symmetry because the probability distribution shows a peak only near the boundary $x = L'$ and thus is not symmetric in position space. As shown in Fig. 4(a)-(d), the number of edge states with $\text{Re}(\varepsilon) = 0, \pi$ are twice as large as $\nu^o$. Therefore, the bulk-edge correspondence holds even in the non-unitary
quantum walk with the large topological number in these parameters.

Finally, we verify the bulk-edge correspondence in the whole parameter region of $\theta_1^*$ and $\theta_2^*$ for the fixed parameters $(\theta_1^*, \theta_2^*) = (\frac{7}{5} \pi, \frac{1}{10} \pi)$. Figure 5 shows the number of edge states with Re(\varepsilon) = 0 as a function of $\theta_1^*$ and $\theta_2^*$. Compared with Fig. 3(b), the number of edge states is twice as large as the topological number of outer regions $\nu^*$. Hence the bulk-edge correspondence holds for the non-unitary three-step quantum walk belonging to the BDI class with the large topological number. We also confirmed the same result for edge states with Re(\varepsilon) = \pi.

FIG. 5. $\theta_1^*$ and $\theta_2^*$ dependences of the number of edge states with Re(\varepsilon) = 0. There are no edge states because bulk states close the band gap when $(\theta_1^*, \theta_2^*)$ are located in regions filled white (unfilled regions) without numbers.

IV. COUNTING NUMBER OF EDGE STATES BY SYMMETRY BREAKING PERTURBATION

We have confirmed that the bulk-edge correspondence holds for the non-unitary three-step quantum walk by counting the number of eigenstates satisfying Re(\varepsilon) = 0 or Re(\varepsilon) = \pi in the previous section. However, in the standard experiments of the quantum walk, only the probability distribution of walkers can be observed. Figure 6(a) and (b) show probability distributions in cases $\nu^* = 2$ and $\nu^* = 3$, respectively. Apparently, we cannot determine the number of edge states from these probability distributions. In this section we show that we can determine the number of edge states from time-step dependences of probability distributions by introducing a symmetry breaking perturbation.
A. Perturbation on degenerate edge states

In this section we put $\gamma = 0$ to realize unitary dynamics since the value of topological number does not depend on $\gamma$ as long as the band gaps are open. By modifying $U_0$, we introduce a perturbed time-evolution operator $U_\delta$

$$U_\delta := SC(\theta_2)SC(\theta_2 + \delta)SC(\theta_1),$$

(54)

where $\delta$ denotes strength of the perturbation. The time-evolution operator $U_\delta$ only has particle-hole symmetry instead of time-reversal symmetry and chiral symmetry. Thereby, the system belongs to class D whose topological number is 0 or 1 [49]. For these two topological numbers the relation $\nu_0 = \nu_\pi$ still holds because $U_\delta$ still takes sublattice structures. We naively expect that if the topological number for the unperturbed system is odd (even), the topological number for the perturbed system is changed to one (zero). We also note that particle-hole symmetry also ensures that the time-evolution operator $U_\delta$ has complex conjugate pairs of eigenvalues.

We refer to a state which changes from an edge state with $\varepsilon = 0$ or $\pi$ to the state with $\varepsilon \neq 0$ and $\pi$ by the perturbation as a defective edge state. In this section we define the coin parameters as

$$\theta_{1(2)}(x) = \begin{cases} \theta^{L}_{1(2)} & (x < 0) \\ \theta^{R}_{1(2)} & (x \geq 0) \end{cases}.\hspace{1cm} (55)$$

Here, we devide the system into two regions at $x = 0$ since parity is not essential for unitary time evolution with $\gamma = 0$. We define a quantity $\Delta \nu$ as the difference of two (left and right) topological numbers before adding the perturbation. The quasi-energies of the defective edge states are shifted by $\pm \omega_\delta$ because $U_\delta$ has complex conjugate pairs of eigenvalues. Note that $\omega_\delta$ becomes zero if $\delta = 0$. We also expect that a pair of defective edge states emerge for finite $\delta$ when $\Delta \nu = 2$ or 3. Here, we focus on the probability of detecting the walker at $x = 0$, $p_0(t)$. If a single edge state emerges, $p_0(t)$ takes a large value since the edge state strongly localizes near $x = 0$. Similarly if a pair of defective edge states emerges, the value of $p_0(t)$ oscillates since defective edge states also localize at $x = 0$ and must give rise to interference between two defective edge states. Detailed calculations of $p_0(t)$ are provided in Appendix. [A] Summarizing the above discussions, $p_0(t)$ takes a large value and oscillates if $\Delta \nu = 3$, takes a small value and oscillates if $\Delta \nu = 2$, and takes a large value if $\Delta \nu = 1$.

B. Numerical results

To verify the previous discussion, we numerically calculate the probability $p_0(t)$ by simulating the time evolution at $\delta \neq 0$. In this section the initial state and the coin parameters in $x < 0$ are given as $|\psi(0) = 0\rangle \otimes \frac{1}{\sqrt{2}}(|L\rangle + i|R\rangle)$ and $(\theta^L_1, \theta^L_2) = (\frac{\pi}{8}, \frac{1}{10}\pi)$, respectively. The value of the topological number in $x < 0$ is $\nu_{L} = 0$. First, we fix coin parameters for $x \geq 0$ as $\theta^R_1 = -\frac{1}{2}\pi, \theta^R_2 = -\frac{1}{12}\pi$ (the topological number in $x \geq 0$ is $\nu_{R} = 3$). The time evolution of the probability $p_0(t)$ is illustrated in the left column of Fig. 7. Figure 7 shows that oscillations with relatively long period appear in the case of $\delta \neq 0$. To clarify the oscillating nature we perform the discrete Fourier transform as

$$c(\omega) = \sum_{t=0}^{T} p_0(t)e^{-i\omega t}, \hspace{1cm} \omega = \frac{2\pi}{T+1}n, \hspace{0.5cm} n = 0, 1, \cdots, T+1,$$

(56)

where $c(\omega)$ represents the complex amplitude of the mode $\omega$ and $T$ denotes the total number of time-steps. In this section we set $T = 10000$. The value of $p_0(t)$ must be zero if $t$ is odd because the time-evolution operator $U_\delta$ contains three shift operators, and thus we have a mode with $\omega = \pi$ in all cases. In the right column of Fig. 7 we clearly see extra oscillating modes near $\omega = 0$ and $\pi$. These results agree well with the calculation in Appendix. [A] Then we conclude that these modes originate from the defective edge states and has the frequency $\omega_\delta$ and $\pi - \omega_\delta$.

Figure 8 shows that how the frequency $\omega_\delta$ and its amplitude $|c(\omega_\delta)|$ depend on the perturbation strength $\delta$. As shown in Fig. 8 we observe that $\omega_\delta$ is proportional to $\delta$ and $|c(\omega_\delta)|$ tends to decrease as $\delta$ increases.
FIG. 8. Dependence of (a) the frequency $\omega_\delta$ and (b) its Fourier coefficient $|c(\omega_\delta)|$ on the perturbation strength $\delta$.

FIG. 9. (left column) Time evoluion of the probability $p_0(t)$ in the case of $\delta = 0.05$. (right column) Absolute values of the Fourier coefficient $|c(\omega)|$ calculated from $p_0(t)$. (a) $\theta_1^R = -\frac{\pi}{10}, \theta_1^R = 2\pi (\Delta \nu = 2)$. (b) $\theta_1^R = -\frac{1}{10} \pi, \theta_1^R = 2\pi (\Delta \nu = 1)$.

As shown in Fig. 10 we observe that the value of $p_0(t)$ is still large after several time-steps if $\Delta \nu$ is odd. On the other hand $p_0(t)$ quickly decays if $\Delta \nu$ is even. Thus we can determine whether the number of edge states is odd or even for several time-steps. In practice, we can identify the two edge states (due to $\Delta \nu = 2$) by the following procedure. First, we prepare the three-step quantum walk with $\gamma \neq 0$ and $\delta = 0$, and observe a probability distribution in which a peak appears near the boundary as shown in Fig. 6 (a). Next, by changing $\gamma = 0$ and $\delta \neq 0$, but keeping the coin parameters unchanged, we observe the probability near the boundary. If the peak of the probability distribution near the boundary decays quickly, we can see that the number of edge states appearing at the boundary is two.

V. REALIZATION OF THE THREE-STEP QUANTUM WALK ON IBM Q

In the previous section, we show that the number of edge states can be determined by the long time dynamics of the probability distribution by introducing the perturbation into the time-evolution operator $U_3$. While quantum walks implemented by classical optical systems can realize the long time dynamics, the time step of quantum walks in quantum systems (such as a quantum optics with entangled photons) is still less than one hundred. To make possible alternatives, in this section, we consider to realize the three-step quantum walk by using a quantum computer IBM Q, motivated by Ref. [48]. We show that this approach enables us to well simulate the long time quantum dynamics, though it is limited to the unitary dynamics in a small system at the moment.

In this section, we set $\gamma = 0$ and impose periodic

the present experiments and show the results in Fig. 10.

$\delta$ implies that the period of oscillation becomes shorter but the amplitude of oscillation becomes weaker with increasing $\delta$.

Next, we consider cases of $\Delta \nu = 1$ and 2. We calculate $p_0(t)$ and $c(\omega)$ in a similar way and show the results in Fig. 9. Figure 9 (a) shows that in the case of $\Delta \nu = 2$, $p_0(t)$ oscillates and takes relatively smaller values compared with that of the case of $\Delta \nu = 3$. Figure 9 (b) shows that in the case of $\Delta \nu = 1$, $p_0(t)$ does not oscillate at all, except $\omega = \pi$ mode, but takes a large value. These results agree well with the predictions provided in the previous subsection. Taking these results into account, we can determine the number of edge states from time dependence of the probability detecting the walker at $x = 0$.

These results tell us that we need, at least, several hundreds steps to observe the oscillation of $p_0(t)$. Unfortunately, implementing such long time-step is not easy in the present experiments. Instead, we focus on the value of $p_0(t)$ at small time step $t$ which can be accessible by

$\delta$ in the case of $\Delta \nu = 1$, $p_0(t)$ does not oscillate at all, except $\omega = \pi$ mode, but takes a large value.

These results agree well with the predictions provided in the previous subsection. Taking these results into account, we can determine the number of edge states from time dependence of the probability detecting the walker at $x = 0$.

These results tell us that we need, at least, several hundreds steps to observe the oscillation of $p_0(t)$. Unfortunately, implementing such long time-step is not easy in the present experiments. Instead, we focus on the value of $p_0(t)$ at small time step $t$ which can be accessible by

$\delta$ in the case of $\Delta \nu = 1$, $p_0(t)$ does not oscillate at all, except $\omega = \pi$ mode, but takes a large value.

These results agree well with the predictions provided in the previous subsection. Taking these results into account, we can determine the number of edge states from time dependence of the probability detecting the walker at $x = 0$.

These results tell us that we need, at least, several hundreds steps to observe the oscillation of $p_0(t)$. Unfortunately, implementing such long time-step is not easy in the present experiments. Instead, we focus on the value of $p_0(t)$ at small time step $t$ which can be accessible by

$\delta$ in the case of $\Delta \nu = 1$, $p_0(t)$ does not oscillate at all, except $\omega = \pi$ mode, but takes a large value.

These results agree well with the predictions provided in the previous subsection. Taking these results into account, we can determine the number of edge states from time dependence of the probability detecting the walker at $x = 0$.

These results tell us that we need, at least, several hundreds steps to observe the oscillation of $p_0(t)$. Unfortunately, implementing such long time-step is not easy in the present experiments. Instead, we focus on the value of $p_0(t)$ at small time step $t$ which can be accessible by

$\delta$ in the case of $\Delta \nu = 1$, $p_0(t)$ does not oscillate at all, except $\omega = \pi$ mode, but takes a large value.

These results agree well with the predictions provided in the previous subsection. Taking these results into account, we can determine the number of edge states from time dependence of the probability detecting the walker at $x = 0$.

These results tell us that we need, at least, several hundreds steps to observe the oscillation of $p_0(t)$. Unfortunately, implementing such long time-step is not easy in the present experiments. Instead, we focus on the value of $p_0(t)$ at small time step $t$ which can be accessible by

$\delta$ in the case of $\Delta \nu = 1$, $p_0(t)$ does not oscillate at all, except $\omega = \pi$ mode, but takes a large value.

These results agree well with the predictions provided in the previous subsection. Taking these results into account, we can determine the number of edge states from time dependence of the probability detecting the walker at $x = 0$.

These results tell us that we need, at least, several hundreds steps to observe the oscillation of $p_0(t)$. Unfortunately, implementing such long time-step is not easy in the present experiments. Instead, we focus on the value of $p_0(t)$ at small time step $t$ which can be accessible by

$\delta$ in the case of $\Delta \nu = 1$, $p_0(t)$ does not oscillate at all, except $\omega = \pi$ mode, but takes a large value.

These results agree well with the predictions provided in the previous subsection. Taking these results into account, we can determine the number of edge states from time dependence of the probability detecting the walker at $x = 0$. 
boundary conditions on the position space so that the
time-evolution operator $U_3$ in Eq. (13) retains unitarity
in a finite system size. We denote the number of sites as
$N$, and for convenience we rewrite the shift operator $S$
as $S = L_- \otimes |L\rangle \langle L| + L_+ \otimes |R\rangle \langle R|$, where $L_\pm$ are unitary
operators and satisfy $L_\pm = \sum_x |x\pm 1\rangle \langle x|$. We
note that $L_N^\pm = I_N$ and $L_1^\pm = L_\mp$, where $I_N$ is an identity
operator in $N$ dimensions. Following the convention
of quantum information, we denote the Pauli matrices as
$X, Y, Z$ instead of $\sigma_1, \sigma_2, \sigma_3$ in this section.

### A. homogeneous case

In order to realize long time dynamics of the three-
step quantum walk on IBM Q, we apply the method in
Ref. [48] for a split step quantum walk. First we consider
a homogeneous system with coin parameters $\theta_1 = \frac{\pi}{2} + \epsilon$, $\theta_2 = \epsilon$. Here we set $\epsilon$ sufficiently small. In this case, the
coin operators are written as

$$C(\theta_1) = I_N \otimes \begin{pmatrix} -\epsilon & -1 \\ 1 & -\epsilon \end{pmatrix}, \quad \text{(57)}$$

$$C(\theta_2) = I_N \otimes \begin{pmatrix} 1 & -\epsilon \\ \epsilon & 1 \end{pmatrix}, \quad \text{(58)}$$

up to the first order of $\epsilon$. Then we expand the time-
evolution operator $U_3$ in Eq. (13) with $\gamma = 0$ in $\epsilon$ as

$$U_3 = A - \epsilon B + O(\epsilon^2), \quad \text{(59)}$$

$$A = L_3^\pm \otimes |R\rangle \langle L| - L_3^\mp \otimes |L\rangle \langle R|, \quad \text{(60)}$$

$$B = (L_3^+ + L_-) \otimes |L\rangle \langle L| + (L_- + L_+) \otimes |R\rangle \langle R|. \quad \text{(61)}$$

Because of $A^2 = -I_N \otimes I_2$, $U_3^4$ satisfies

$$U_3^4 = I_N \otimes I_2 + -i\epsilon \{2i\{A, B\}) + O(\epsilon^2), \quad \text{(62)}$$

where $\{\cdot, \cdot\}$ denotes an anti-commutator. Then the equation

$$U_3^{4s} = [I_N \otimes I_2 - i\epsilon \{2i\{A, B\})]^s + O(\epsilon^2) \quad \text{(63)}$$

holds. We introduce a new continuous parameter $\tau$ such that

$$\epsilon \tau = \tau, \quad \text{(64)}$$

where $s \in \mathbb{N}$ denotes the number of time steps of $U_3^4$. We
take the limit as $\epsilon \to 0$ and $s \to \infty$ while $\tau = s\epsilon$ remains
finite. Then higher order terms of $\epsilon$ vanishes and $U_3^{4s}$ is expressed as

$$U_3^{4s} = e^{-iH\tau}, \quad H = 2i\{A, B\}. \quad \text{(65)}$$

As shown in Eq. (65), the time evolution $U_3^{4s}$ is
considered as the time evolution generated by the “effective
Hamiltonian” $H$, and the time is determined by $\tau$. Using

this effective Hamiltonian, we can simulate the time evolu-
tion of a three-step quantum walk with $4s = \frac{4\pi}{\epsilon}$ time
steps.

We obtain an explicit form of the effective Hamiltonian
by using Eqs. (60) and (61):

$$H = 2i(I_N + 2L_3^+ + L_3^\mp) \otimes |R\rangle \langle L| - 2i(I_N + 2L_3^+ + L_3^\mp + L_3^\pm) \otimes |L\rangle \langle R|. \quad \text{(66)}$$

To simulate the above Hamiltonian on IBM Q, we fix
the number of the sites to $N = 4$ hereafter, then we
represent the operator $L_\pm$ as matrices for the position
basis $(|0\rangle, |1\rangle, |2\rangle, |3\rangle)^T$,

$$L_+ = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}, \quad L_\mp = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad \text{(67)}$$

Using the relations $L_4^1 = I_4$, $L_2^2 = L_2^\pm$, we obtain the effective Hamiltonian for $N = 4$ as

$$H_4 = 6(I_0I_1Y_c + X_0I_1Y_c). \quad \text{(68)}$$

Here $Y_c$ and $X_0$ are one of the Pauli matrices acting on
qubit labelled by $c$ and 0, respectively, and $I_j$ is an identity
matrix acting on qubit $j$. The corresponding time-
evolution operator is written as

$$e^{-ih_4\tau} = e^{-6iI_0I_1Y_c}e^{-6iX_0I_1Y_c\tau}, \quad \text{(69)}$$

where we can rigorously decompose $e^{-ih_4\tau}$ as the right part of
Eq. (69) because two terms of $H_4$ commute.

We have to decompose the time-evolution operator in
Eq. (69) into single qubit operations and CNOT gates
to implement $e^{-ih_4\tau}$ on IBM Q. We perform such decom-
position by using the following relation:

$$C_{ct}Y_cI_cC_{ct}^\dagger = Y_cX_t, \quad \text{(70)}$$

where $C_{ct}$ represents the CNOT gate between control
qubit $c$ and target qubit $t$. Figure [11] shows a quantum
circuit implementing the time-evolution operator (69).
Figure [12] shows probability distributions obtained by
the following methods; (i) experiment of the quantum circuit
in Fig. [11] implemented by IBM Q, (ii) numerical simu-
lation of the quantum circuit, and (iii) direct numerical
calculation of the time-evolution operator in Eq. (13).
We also emphasize that long time steps [128 steps in Fig. 12(a) and 196 in Fig. 12(b)] is set even in the experiment on IBM Q. We note that the equivalent coin parameters and time steps are implemented for these three methods. As shown in Fig. 12, the results of simulation agree well with those of numerical calculation. In order to evaluate the accuracy of implementation on IBM Q, we introduce a squared statistical overlap (SSO) between two probability distributions \(p(x)\) and \(q(x)\) \((x = 0, 1, \ldots, N - 1)\) \cite{50}, defined by

\[
\text{SSO}(p(x), q(x)) := \left( \sum_{x=0}^{N-1} \sqrt{p(x)q(x)} \right)^2.
\]

For any probability distribution, the SSO satisfies \(0 \leq \text{SSO} \leq 1\) and the value of SSO becomes large as two probability distributions are similar to each other. In both cases in Figs. 12(a) and (b), the values of SSO between the numerical calculation and the simulation are larger than 0.999. Furthermore, the values of SSO between the experiments and the numerical calculations are 0.962 in Fig. 12(a) and 0.918 in Fig. 12(b). Thereby, the quantum circuit shown in Fig. 11 can experimentally simulate the dynamics of the homogeneous three-step quantum walk even in long time-steps. In Appendix B we provide the results of \(N = 8\) homogeneous case.

**B. inhomogeneous case**

In this subsection we consider inhomogeneous three-step quantum walks by introducing position dependent coin parameters as

\[
(\theta_1, \theta_2) = \begin{cases} 
(\theta_1^+, \theta_2^+) = \left(-\frac{\pi}{2} - \epsilon, \epsilon\right), & 0 \leq x \leq \frac{N}{2} - 1, \\
(\theta_1^-, \theta_2^-) = \left(\frac{\pi}{2} + \epsilon, \epsilon\right), & \frac{N}{2} \leq x \leq N - 1.
\end{cases}
\]

\[
(72)
\]

FIG. 12. Probability distributions of the homogeneous three-step quantum walk obtained by the numerical simulation of the quantum circuit (red densely filled bars), experiment by IBM Q (green diagonal square crossed bars), and direct numerical calculation of the time-evolution operator (blue sparsely filled bars). (a) \(\epsilon = \frac{\pi}{4}, \tau = 4\). The corresponding time-step is 128. The initial state is \(|\psi(0)\rangle = |2\rangle \otimes \frac{1}{\sqrt{2}}(|L\rangle + |R\rangle)\). (b) \(\epsilon = \frac{\pi}{16}, \tau = 3\). The corresponding time-step is 196. The initial state is \(|\psi(0)\rangle = |1\rangle \otimes \frac{1}{\sqrt{2}}(|L\rangle + \frac{1+i}{\sqrt{2}} |R\rangle)\).

Topological numbers of left \((x \in \left[0, \frac{N}{2} - 1\right]\) and right \((x \in \left[\frac{N}{2}, N - 1\right]\) region are \(\nu_L = 3\) and \(\nu_R = 0\), respectively, as shown in Fig. 3(a). Thereby, edge states would appear at the interface of two regions. For convenience we define projection operators:

\[
P := \sum_{x=0}^{\frac{N}{2}-1} |x\rangle \langle x|, \quad Q := \sum_{x=\frac{N}{2}}^{N-1} |x\rangle \langle x|, \quad \Pi := P - Q. \tag{73}
\]

Using these operators, we can rewrite the coin operators as \(C(\theta_{1(2)}) = P \otimes \tilde{C}(\theta_{1(2)}) + Q \otimes \tilde{C}(\theta_{1(2)})\), where

\[
\tilde{C}(\theta) := \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}.
\]

We expand the time-evolution operator for sufficiently small \(\epsilon\) as follows:

\[
U_3 = A + \epsilon B + \epsilon^2 C + O(\epsilon^3)
\]

\[
A = L_3^2 \Pi \otimes |L\rangle \langle R| - L_3^2 \Pi \otimes |R\rangle \langle L|
\]

\[
B = (L_+ + L_-) \Pi \otimes \mathbb{1}_2 - L_3^2 \otimes |L\rangle \langle L|
\]

\[
\quad - L_3^2 \otimes |R\rangle \langle R|
\]

\[
C = \left(\frac{3}{2} L_+ \Pi - L_- \Pi + L_+ - L_-\right) \otimes |L\rangle \langle R|
\]

\[
\quad + \left(\frac{3}{2} L_- \Pi - L_+ \Pi - L_+ - L_-\right) \otimes |R\rangle \langle L|.
\]

Because \(A^4 = I_N \otimes \mathbb{1}_2\) is satisfied for any \(N\), we can derive the effective Hamiltonian in a way similar to the previous subsection as

\[
H = i \{A^2, \{A, B\}\}. \tag{79}
\]

In order to proceed further, we fix \(N = 4\). Then we find that \(H = 0\), and thus \(U_3^4\) is written as

\[
U_3^4 = I_N \otimes \mathbb{1}_2 + D\epsilon^2 + O(\epsilon^3)
\]

\[
D = \{A^2, \{A, C\} + B^2\} + \{A, B\}^2
\]

\[
= 4i(Y_0L_1L_z + Y_0Z_1Z_z).
\]

Since Eq. (81) shows that \(D\) is the anti-Hermitian operator, \(D\) is written in term of a Hermitian operator \(H'\) as \(D = -iH'\). Then the equation

\[
U_3^{4s} = (I_N \otimes \mathbb{1}_2 - i\epsilon^2 H')^s + O(\epsilon^3)
\]

holds. We define \(\tau\) instead of Eq. (64) as:

\[
s\epsilon^2 = \tau. \tag{82}
\]

Taking the limit as \(\epsilon \to 0\) and \(s \to \infty\) while \(\tau = s\epsilon^2\) is kept finite, we obtain

\[
U_3^{4s} = e^{-iH'\tau} \tag{83}
\]

Then we can simulate time evolution of the three-step quantum walk with \(4s = \frac{4\pi}{\epsilon^2}\) time-steps using this time-evolution operator in Eq. (84).
Figure 13 shows the quantum circuit simulating the time evolution governed by the Hamiltonian $H'$. Figure 14 shows probability distributions obtained by using the circuit in Fig. 13 and direct numerical calculations. Since we can write the effective Hamiltonian $H'$ as

$$H' = 8i(|0\rangle \otimes |L\rangle \langle L| + |1\rangle \otimes |R\rangle \langle R|) + \text{h.c.}, \tag{85}$$

the states $|x = \text{odd}\rangle \otimes |L\rangle$ and $|x = \text{even}\rangle \otimes |R\rangle$ are unaffected by the time-evolution operator $e^{-iH't}$. Figure 14 (a) reflects this property, since the state remains at the initial position when the initial state is $|\psi(0)\rangle = |1\rangle \otimes |L\rangle$. In this case, the value of SSO between the simulation of the circuit and the numerical calculation is larger than 0.999, the value of SSO between the experiment and the numerical calculation is 0.840. On the other hand, for the initial state including the term $|2\rangle \otimes |L\rangle$, the probability distribution of the numerical calculation and the simulation show shifts to the other positions, as shown in Fig. 14. In this case, the value of SSO between the simulation and the numerical calculation is 0.946 and that between the experiment and numerical calculation is 0.915. Hence the quantum circuit in Fig. 13 can simulate the dynamics of the inhomogeneous three-step quantum walk. We note that the performance of the quantum circuit to simulate the inhomogeneous three-step quantum walk is a bit reduced, though we can still observe the high probability at $x = 2$, originating from the edge states in Fig. 14. The less performance would result from contributions of ignored higher order terms in $\tau$ of the time-evolution operator. In the inhomogeneous case, the order of the leading correction term is $O(\tau^2)$ due to Eq. (85), while that in the homogeneous case $O(\tau^2)$ due to Eq. (63).

VI. SUMMARY

We have investigated the bulk-edge correspondence of $\mathcal{PT}$ symmetric open quantum systems with large topological numbers. To this end, we define the non-unitary three-step quantum walk with $\mathcal{PT}$ symmetry and other symmetries required for the BDI class in Ref. [34]. We have numerically confirmed the validity of the bulk-edge correspondence for this model since the number of eigenvalues corresponding to multiple edge states agree well with the difference of topological numbers. However, detecting the number of edge states is not easy in experiments. Thereby, we have developed a procedure to distinguish the number of edge states from time dependences of the probability distribution which is available in the standard experiments of quantum walks. In addition, we have also demonstrated that long time dynamics of the three-step quantum walk can be well simulated on the quantum computer IBM Q. Our study contributes to the future experimental verification of the bulk-edge correspondence in non-Hermitian systems.

As we have demonstrated, the quantum walk enables us to define non-unitary time-evolution operators with various symmetries. Further, these non-unitary quantum walks can be experimentally realized in the quantum optical system [22]. Since symmetry classes increase up to 38 for topological phases in non-Hermitian systems, studying non-unitary quantum walks with different symmetries is important for further developments of topological phases in open quantum systems. We believe the quantum walk becomes an important arena to investigate fruitful novel phenomena in open quantum systems.

We have also demonstrated that the long time dynamics of the three-step quantum walk can be well simulated by IBM Q. Unfortunately, the current coherent time of IBM Q gives the strong constraint for the system size of the quantum walk. However, this problem should be solved in future since the long coherent time must be realized to make quantum computers (including IBM Q) useful. Furthermore, on IBM Q, the system size can exponentially increase with increasing the number of qubits. Therefore, this approach may solve the scalability problem of experiments for quantum walks.

ACKNOWLEDGMENTS

We thank Y. Asano, H. Hirori, R. Okamoto, and K. Yakubo for helpful discussions. This work was supported by KAKENHI (Grants No. JP18J20727, No. JP19H01838, No. JP18H01140, No. JP18K18733, and No. JP19K03646) and a Grant-in-Aid for Scientific Research on Innovative Areas (KAKENHI Grant No. JP15H05855 and No. JP18H04210) from the Japan Society for the Promotion of Science.
Appendix A: Detailed calculations of perturbed probabilities

In Appendix A, we derive the time dependences of the probability at the interface, where edge states dominate the dynamics, when the perturbed time-evolution operator $\hat{U}_\delta$ in Eq. (A4) is employed. We first consider the case of $\Delta \nu = 3$ where three edge states appear at the interface at the same quasi-energy when $\delta = 0$. The quasi-energies of defective edge states are $\pm \omega_3$ or $\pi \pm \omega_3$ because of particle-hole symmetry. We write the states whose eigenenergy is $\omega$ or $\omega \pm \omega_3$ as $|\psi_\omega\rangle$, $|\psi_{\omega \pm}\rangle$, where $\omega = 0, \pi$. We prepare an initial state $|\psi(t = 0)\rangle$ that localizes at $x = 0$, then we can expand $|\psi(t = 0)\rangle$ as a linear combination of the eigenstates of the time-evolution operator in Eq. (A4),

$$|\psi(t = 0)\rangle = a|\psi_0\rangle + be^{-i\omega_3 t}|\psi_{0+}\rangle + ce^{i\omega_3 t}|\psi_{0-}\rangle + p|\psi_\pi\rangle + q|\psi_{\pi+}\rangle + r|\psi_{\pi-}\rangle + \text{(linear combination of bulk states)},$$

(A1)

where $a, b, c, p, q, r$ denote wave function amplitudes. The state at time-step $t$ is written as

$$|\psi(t)\rangle = a|\psi_0\rangle + be^{-i\omega_3 t}|\psi_{0+}\rangle + ce^{i\omega_3 t}|\psi_{0-}\rangle + p(-1)^t|\psi_\pi\rangle + qe^{-i(\pi + \omega_3) t}|\psi_{\pi+}\rangle + re^{-i(\pi - \omega_3) t}|\psi_{\pi-}\rangle + \text{(linear combination of bulk states)},$$

(A2)

Then, the wavefunction at the interface $(x = 0)$ is given by:

$$\psi(t) = a|\psi_0\rangle + be^{-i\omega_3 t}|\psi_{0+}\rangle + ce^{i\omega_3 t}|\psi_{0-}\rangle + p(-1)^t|\psi_\pi\rangle + qe^{-i(\pi + \omega_3) t}|\psi_{\pi+}\rangle + re^{-i(\pi - \omega_3) t}|\psi_{\pi-}\rangle + \text{(linear combination of bulk wavefunctions)},$$

(A3)

We expand the initial state localized at $x = 0$ as the subsequent terms in Eq. (A4). Since the amplitudes of $\psi_\omega$ are much larger than those of $\psi_{\omega \pm}$, this is because that a defective edge state is not a edge state and thus the localization length of the defective edge state is much longer than that of the edge state. We observe that $p_0(t)$ takes a large value at long time-step $t$ because of the terms $|a|^2|\psi_0\rangle^2$ and $|p|^2|\psi_\pi\rangle^2$, and the value of $p_0(t)$ oscillates with frequency $\pi, \omega_3$ and $\pi - \omega_3$ because of the subsequent terms in Eq. (A4).

We further neglect the quadratic terms $\psi_{\omega \pm}^*\psi_{\omega \pm}$ in Eq. (A4) since the amplitudes of $\psi_\omega$ are much larger than those of $\psi_{\omega \pm}$. We expand the initial state localized at $x = 0$ as

$$|\psi(t = 0)\rangle = a'\ |\psi_0\rangle + b'\ |\psi_{0+}\rangle + b'\ |\psi_{0-}\rangle + q'|\psi_{\pi+}\rangle + q'|\psi_{\pi-}\rangle + \text{(linear combination of bulk states)},$$

(A5)

where $a', b', p', q'$ denote wavefunction amplitudes. We define the quasi-energies of the defective edge states $\pm \omega_3$ or $\pi \pm \omega_3$ again, then we obtain $p_0(t)$ as

$$p_0(t) \simeq |a'|^2|\psi_0\rangle^2 + |b'|^2|\psi_{0-}\rangle^2 + |p'|^2|\psi_{\pi+}\rangle^2 + |q'|^2|\psi_{\pi-}\rangle^2 + 2Re(a'^*b'e^{2i\omega_3 t}\psi_0^*\psi_{0-}) + 2Re(a'^*b'e^{-i(\pi + \omega_3) t}\psi_{\pi+}^*\psi_{\pi-}) + 2Re(b'^*p'e^{-i(\pi - \omega_3) t}\psi_0^*\psi_{\pi+}) + 2Re(b'^*p'e^{-2i\omega_3 t}\psi_{\pi-}^*\psi_{\pi-}),$$

(A6)

Since $p_0(t)$ in Eq. (A6) is governed by defective states and $|\psi_0\rangle$ and $|\psi_{\pi\pm}\rangle$ are smaller than $|\psi_0\rangle$ and $|\psi_{\pi}\rangle$, the
by substituting these representations we obtain the effective Hamiltonian (B5). We use the equation (B6) and neglect higher order terms of \( \tau \).

Unfortunately, the current coherence time of IBM Q is insufficient to incorporate the Suzuki-Trotter expansion.

Figure (16) shows the quantum circuit realizing time evolution generated by the Hamiltonian in Eq. (B5) without the Suzuki-Trotter formula. We compare probability distributions obtained by numerical simulations and experiments on IBM Q using the circuit shown in Fig. 16.

In addition, we compare direct numerical calculations of the time-evolution operator and numerical simulation of the quantum circuit by applying Suzuki-Trotter formula (B7). These results are shown in Fig. 17 with different parameter sets.

First of all, we remark that the probability distributions of numerical calculations and simulations of the quantum circuit applying the Suzuki-Trotter expansions are similar to each other and the value of SSO between them becomes almost one. Therefore, we conclude that the effective Hamiltonian (B5) is able to describe dynamics of the three-step quantum walk with \( N = 8 \). However, the current coherent time of IBM Q is insufficient to apply the Suzuki-Trotter expansions. Then we compare results between simulation/experiments of the circuit in Fig. 16 below.

We first focus on the case of relatively short time-step \( \tau = 20 \) as shown in Fig. 17 (a). In this case, the value of SSO between the simulations and the numerical calculations is 0.891. Further, the value of SSO between the experiments and the numerical calculations (simulations) is 0.734 (0.686). Taking these values, we think that it is possible to simulate the proper short time dynamics of the three-step quantum walk with \( N = 8 \) by IBM Q.

Next, we focus on cases of longer time-steps as shown in Fig. 17 (b)-(d). The minimum value of SSO between the simulations of the circuit in Fig. 16 and the numerical
FIG. 17. Probability distributions of the homogeneous three-step quantum walk with $N = 8$ obtained by the numerical simulation of the quantum circuit (red densely filled bars), experiment by IBM Q (green diagonal square crossed bars), direct numerical calculation of the time-evolution operator (blue sparsely filled bars), and simulations of the quantum circuit with Suzuki-Trotter expansions (purple hashed bars). To approximate Suzuki-Trotter expansions, we truncate the expansion by setting $n = 1000$ for $e^{(A + B)\tau} \approx (e^{A\tau}e^{B\tau})^t$. (a) $\epsilon = \frac{1}{10}, \tau = 4$. The corresponding time step is 20. Initial state is $|\psi(0)\rangle = |0\rangle \otimes \frac{1}{\sqrt{2}} (|L\rangle + e^{i\frac{\pi}{4}} |R\rangle)$. (b) Parameters and initial state are the same as (a), except for $\tau$. In this case $\tau = \frac{\pi}{2}$ and the corresponding time-step is 160. (c) $\epsilon = \frac{1}{2}, \tau = 4$. The corresponding time-step is 128. Initial state is $|\psi(0)\rangle = |0\rangle \otimes |L\rangle$. (d) $\epsilon = \frac{1}{2}, \tau = \frac{\pi}{2}$. The corresponding time-step is 120. Initial state is $|\psi(0)\rangle = |1\rangle \otimes \frac{1}{\sqrt{2}} (|L\rangle + |R\rangle)$.

calculations is 0.616 in the case of Fig. 17(d). Because the value of SSO is small even for the simulation, it indicates that we cannot effectively simulate the probability distributions using the circuit constructed by Eq. (B6) due to non-commutativity of each terms and the short coherence time. Nevertheless, we show results comparing those of the simulations and experiments. The values of SSO between simulations and experiments are 0.564 (b), 0.559 (c), and 0.869 (d). [The higher SSO in (d) would be accidental.] The results of experiments using the circuit shown in Fig. 16 are in general different from the results of simulations due to the qubit’s coherence times and some errors. It also indicates that errors interrupt improving accuracy of an approximation, because the number of quantum gates becomes larger as accuracy of an approximation improves.

[1] C. M. Bender and S. Boettcher, Phys. Rev. Lett. 80, 5243 (1998).
[2] A. Mostafazadeh, J. Math. Phys. 43, 205 (2002).
[3] A. Mostafazadeh, J. Math. Phys. 43 2814 (2002).
[4] A. Mostafazadeh, J. Math. Phys. 43 3944 (2002).
[5] C. M. Bender, Rep. Prog. Phys. 70 947 (2007).
[6] A. Guo, G. J. Salamo, D. Duchesne, R. Morandotti, M. Volatier-Ravat, V. Aimez, G. A. Siviloglou, and D. N. Christodoulides, Phys. Rev. Lett. 103, 093902 (2009).
[7] C. E. Rüter, K. G. Makris, R. El-Ganainy, D. N. Christodoulides, M. Mordechai, and D. Kip, Nat. Phys. 6, 192 (2010).
[8] B. Peng, S. K. Özdemir, F. Lei, F. Monifi, M. Gianfreda, G. L. Long, S. Fan, F. Nori, C. M. Bender, and L. Yang, Nat. Phys. 10, 394 (2014).
[9] B. Peng, S. K. Özdemir, S. Rotter, H. Yilmaz, M. Liertzer, F. Monifi, C. M. Bender, F. Nori, and L. Yang, Science 346, 328 (2014).
[10] Z. Lin, H. Ramezani, T. Eichelkraut, T. Kottos, H. Cao, and D. N. Christodoulides, Phys. Rev. Lett. 106, 213901 (2011).
[11] A. Regensburger, C. Bersch, MA Miri, G. Onishchukov, D. N. Christodoulides, and U. Peschel, Nature 488, 167 (2012).
[12] A. Mostafazadeh, Phys. Rev. A 87, 012103 (2013).
[13] J. Wiersig, Phys. Rev. Lett. 112, 203901 (2014).
[14] J. Wiersig, Phys. Rev. A 93, 033809 (2016).
[15] Z. P. Liu, J. Zhang, S. K. Özdemir, B. Peng, H. Jing, X. Y. L’iu, C. W. Li, L. Yang, F. Nori, and Y. X. Liu, Phys. Rev. Lett. 117, 110802 (2016).
[16] W. Chen, S. K. Özdemir, G. Zhao, J. Wiersig, and L. Yang, Nature 548, 192 (2017).
[17] H. Hodaei, A. U. Hassan, S. Wittek, H. Garcia-Gracia, R. El-Ganainy, D. N. Christodoulides, and M. Khajavikhan, Nature 548, 187 (2017).
[18] L. Feng, R. El-Ganainy, and L. Ge, Nature Photonics 11, 752 (2017).
[19] R. El-Ganainy, K. G. Makris, M. Khajavikhan, Z. H. Musslimani, S. Rotter, and D. N. Christodoulides, Nat. Phys. 14, 11 (2018).
[20] T. Ozawa, H. M. Price, A. Amo, N. Goldman, M. Hafezi, L. Lu, M. C. Rechtsman, D. Schuster, J. Simon, O. Zilberberg, and I. Carusotto, Rev. Mod. Phys. 91, 015006 (2019).
[21] J. S. Tang, Y. T. Wang, S. Yu, D. Y. He, J. S. Xu, B. H. Liu, G. Chen, Y. N. Sun, K. Sun, Y. J. Han, C. F. Li,
and G. C. Guo, Nat. Photon. 10, 642 (2016).
[22] L. Xiao, X. Zhan, Z. H. Bian, K. K. Wang, X. Zhang, X. P. Wang, J. Li, K. Mochizuki, D. Kim, N. Kawakami, W. Yi, H. Obuse, B. C. Sanders, and P. Xue, Nat. Phys. 13, 1117 (2017).
[23] K. Mochizuki, D. Kim, and H. Obuse, Phys. Rev. A 93, 062116 (2016).
[24] D. Kim, K. Mochizuki, N. Kawakami, and H. Obuse, arXiv:1609.09650.
[25] X. Zhan, L. Xiao, Z. Bian, K. Wang, X. Qiu, B. C. Sanders, W. Yi, and P. Xue, Phys. Rev. Lett. 119, 130501 (2017).
[26] L. Xiao, X. Qiu, K. Wang, Z. Bian, X. Zhan, H. Obuse, B. C. Sanders, W. Yi, and P. Xue, Phys. Rev. A 98, 063847 (2018).
[27] K. Esaki, M. Sato, K. Hasebe, and M. Kohmoto, Phys. Rev. B 84, 205128 (2011).
[28] D. Leykam, K. Y. Bliokh, C. Huang, Y. D. Chong, and F. Nori, Phys. Rev. Lett. 118, 040401 (2017).
[29] L. Zhou and J. Gong, Phys. Rev. B 98, 205417 (2018).
[30] H. Shen, B. Zhen, and L. Fu, Phys. Rev. Lett. 120, 146402 (2018).
[31] F. K. Kunst, E. Edvardsson, J. C. Budich, and E. J. Bergholtz, Phys. Rev. Lett. 121, 026808 (2018).
[32] Z. Gong, Y. Ashida, K. Kawabata, K. Takasan, S. Higashikawa, and M. Ueda, Phys. Rev. X 8, 031079 (2018).
[33] K. Kawabata, K. Shiozaki, and M. Ueda, and M. Sato, arXiv:1812.09133.
[34] S. Yao and Z. Wang, Phys. Rev. Lett. 121, 086803 (2018).
[35] Y. Xiong, J. Phys. Commun. 2, 035043 (2018).
[36] A. Ghatak and T. Das, J. Phys.: Condens. Matter 31, 263001 (2019).
[37] M. Ezawa, Phys. Rev. B 99, 121411(R) (2019).
[38] D. S. Borgnia, A. J. Kruchkov, R.-J. Slager, arXiv:1902.07217.
[39] K. Kawabata, T. Bessho, and M. Sato, arXiv:1902.08479.
[40] K. Yokomizo and S. Murakami, arXiv:1902.10958.
[41] J. Kempe, Contemp. Phys. 44, 307 (2003).
[42] N. B. Lovett, S. Cooper, M. Everitt, M. Trevers, and V. Kendon, Phys. Rev. A 81, 042330 (2010).
[43] T. Kitagawa, M. A. Broome, A. Fedrizzi, M. S. Rudner, E. Berg, I. Kassal, A. Aspuru-Guzik, E.Demler, and A. G. White, Nat. Commun. 3, 882 (2012).
[44] J. K. Asbóth and H. Obuse, Phys. Rev. B 88, 121406(R) (2013).
[45] H. Obuse, J. K. Asbóth, Y. Nishimura, and N. Kawakami, Phys. Rev. B 92, 045424 (2015).
[46] A. Regensburger, C. Bersch, B. Hinrichs, G. Onishchukov, A. Schreiber, C. Silberhorn, and U. Peschel, Phys. Rev. Lett. 107, 233902 (2011).
[47] J. Boutari, A. Feizpour, S. Barz, C. Di. Franco, M. S. Kim, W. S. Kolthammer, and I. A. Walmsley, J. Opt. 18, 094007 (2016).
[48] R. Balu, D. Castillo, and G. Siopsis, Quantum Sci. Technol. 3, 035001 (2017).
[49] A. P. Schnyder, S. Ryu, A. Furusaki, and A. W. W. Ludwig, Phys. Rev. B 78, 195125 (2008).
[50] J. Chiaverini, J. Britton, D. Leibfried, E. Knill, M. D. Barrett, R. B. Blakestad, W. M. Itano, J. D. Jost, C. Langer, R. Ozeri, T. Schaetz, and D. J. Wineland, Science 308, 997 (2005).