

**Pseudo-Hermitian Hamiltonians generating waveguide mode evolution**Penghua Chen<sup>1</sup> and Y. D. Chong<sup>1,2,\*</sup><sup>1</sup>*Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore 637371, Singapore*<sup>2</sup>*Centre for Disruptive Photonic Technologies, Nanyang Technological University, Singapore 637371, Singapore*  
(Received 31 March 2017; published 19 June 2017)

We study the properties of Hamiltonians defined as the generators of transfer matrices in quasi-one-dimensional waveguides. For single- or multimode waveguides obeying flux conservation and time-reversal invariance, the Hamiltonians defined in this way are non-Hermitian, but satisfy symmetry properties that have previously been identified in the literature as “pseudo-Hermiticity” and “anti- $\mathcal{PT}$  symmetry”. We show how simple one-channel and two-channel models exhibit transitions between real, imaginary, and complex eigenvalue pairs.

DOI: [10.1103/PhysRevA.95.062113](https://doi.org/10.1103/PhysRevA.95.062113)**I. INTRODUCTION**

In 1998, Bender and co-workers [1–3] pointed out that Hamiltonians which are symmetric under a combination of parity and time reversal ( $\mathcal{PT}$ ) possess an interesting feature: despite being non-Hermitian, they can have eigenvalues that are strictly real. Moreover, tuning the Hamiltonian parameters can induce a non-Hermitian symmetry-breaking transition, between  $\mathcal{PT}$ -unbroken eigenstates with real eigenvalues and  $\mathcal{PT}$ -broken eigenstates with complex and conjugate-paired eigenvalues. The original intention of Bender *et al.* was to use  $\mathcal{PT}$  symmetry to extend fundamental quantum mechanics, but in 2008 Christodoulides and co-workers showed that  $\mathcal{PT}$  symmetry could be realized in optical structures with balanced gain and loss [4–7]. Since then, research into  $\mathcal{PT}$  symmetric optics has progressed rapidly, and the idea of “gain and loss engineering” in photonics, based on  $\mathcal{PT}$  symmetry, has led to devices with highly promising applications, such as low-power optical isolation [8,9] and laser mode selection [10,11].

In this paper, we look at a class of physically motivated non-Hermitian Hamiltonians that are *not*  $\mathcal{PT}$  symmetric in the original sense of Bender *et al.* [1–3], but nonetheless exhibit symmetry-breaking transitions between real and complex eigenvalues. These Hamiltonians are the generators of transfer matrices in single- or multichannel waveguides *without* gain or loss, at a fixed frequency (or energy). They were first studied in a 1997 paper by Mathur [12], prior to the development of  $\mathcal{PT}$  symmetry; one of our goals is to reevaluate them in light of subsequent developments in the theory of non-Hermitian Hamiltonians. We show that they form a subset of the “pseudo-Hermitian” matrices, a class of non-Hermitian matrices identified by Mostafazadeh and co-workers as a generalization of the  $\mathcal{PT}$  symmetry concept [13–19]. This subset is restricted further by a generalized anti- $\mathcal{PT}$  symmetry [20–23], where the  $\mathcal{P}$  operation interchanges forward-going and backward-going waveguide modes. A similar anti- $\mathcal{PT}$  symmetry was previously identified by Sukhorukov *et al.* in the context of beam evolution in parametric amplifiers [21]. Mostafazadeh and co-workers have also studied the Hamiltonians that generate transfer matrices in waveguides containing gain and/or loss, i.e., without flux conservation and time-reversal invariance

[17–19]. When those symmetries *are* present, however, we show that the resulting pseudo-Hermiticity and anti- $\mathcal{PT}$  symmetries give rise to non-Hermitian transitions between purely imaginary, purely real, and complex values. These non-Hermitian transitions are reminiscent of  $\mathcal{PT}$  symmetry-breaking transitions, and we show that they have physical consequences for the transmission properties of single- and multimode waveguides under parameter change.

For an  $N$ -channel waveguide (either an optical waveguide or a quantum electronic waveguide [12]) that obeys flux conservation as well as time-reversal invariance, it is known [24] that the group of transfer matrices, at a given operating frequency or energy, has a one-to-one mapping to the symplectic group  $\text{Sp}(2N, \mathbb{R})$ . The transfer matrices are generated by  $2N \times 2N$  matrices that are typically non-Hermitian; we can regard each such generator,  $H$ , as a Hamiltonian. The  $H$  matrices map onto the group of real matrices of the “Hamiltonian” type,  $\text{sp}(2N, \mathbb{R})$ , which are the generators of  $\text{Sp}(2N, \mathbb{R})$ .

The eigenvalues of  $H$  are not energies or frequencies, but rather the modal wave numbers of a translationally invariant waveguide. Real eigenvalues correspond to propagating modes, and complex eigenvalues correspond to evanescent (in-gap) modes. As shown below,  $H$  supports real eigenvalues despite being non-Hermitian because it satisfies a certain pair of symmetries: pseudo-Hermiticity [13–16] and anti- $\mathcal{PT}$  symmetry [20–23]. These symmetries are tied to the physical conditions of flux conservation and time-reversal invariance in the underlying waveguide.

To motivate the interpretation of transfer matrix generators as “Hamiltonians” [12,17–19], consider a segment of an  $N$ -channel waveguide with negligible back-reflection. The position along the waveguide axis,  $z$ , can be thought of as playing the role of “time.” At a given energy  $E$ , the transfer matrix is a  $2N \times 2N$  block-diagonal matrix of the form

$$M = \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix}, \quad (1)$$

where  $U_1$  and  $U_2$  describe the mode mixing of the forward- and backward-going modes, respectively. In the absence of gain or loss,  $U_1$  and  $U_2$  are unitary, and  $M$  is generated by a

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$2N \times 2N$  Hermitian matrix  $H$  such that

$$M = \exp(iHz) = \begin{pmatrix} e^{iH_1z} & 0 \\ 0 & e^{iH_2z} \end{pmatrix}, \quad (2)$$

where  $H_1$  and  $H_2$  are Hermitian submatrices of  $H$ . The eigenvalues of  $H_{1,2}$  are the wave numbers of the forward- and backward-going modes. For such a reflection-free waveguide, we could focus on the Hermitian submatrix  $H_1$  as the Hamiltonian of the  $N$  forward modes; this leads to the well-known mapping between beam propagation and the Schrödinger wave equation [25].

When backreflection is non-negligible, due to inhomogeneities in the waveguide (e.g., a fiber Bragg grating [26–28]),  $M$  is no longer block diagonal; its generator  $H$  is neither block diagonal nor Hermitian [12]. However, the eigenvalues of  $H$  can still be regarded as modal wave numbers, which now consist of a mix of forward-going and backward-going components. Band extrema correspond to exceptional points of  $H$ , where its eigenvectors coalesce and the matrix becomes defective. At these points, the modal wave numbers exhibit “symmetry-breaking” transitions between real pairs (propagating modes), and either purely imaginary pairs (purely evanescent gap modes) or complex pairs (quasievanescent gap modes). This is reminiscent of  $\mathcal{PT}$  symmetry breaking [1,2], but, as we shall see, it is not  $\mathcal{PT}$  symmetry that is responsible for these eigenvalue transitions.

## II. HAMILTONIAN SYMMETRIES

We begin with a brief summary of the definitions of  $\mathcal{PT}$  symmetry and some of its variants and generalizations [29–31]. First, a Hamiltonian  $H$  is “ $\mathcal{PT}$  symmetric” if it is invariant under a combination of a unitary parity operator  $\mathcal{P}$  and an antiunitary time-reversal operator  $\mathcal{T}$  (which we take to be the complex conjugation operator), as follows [1–3]:

$$H = (\mathcal{PT})H(\mathcal{PT})^{-1}. \quad (3)$$

Conventionally, a parity operator must be involutory ( $\mathcal{P}^2 = I$ ), but we can generalize the  $\mathcal{PT}$  symmetry concept by dropping this assumption, and requiring only the combined antiunitary operator  $\mathcal{PT}$  to be involutory [3,29–31]. Equation (3) then implies that eigenvalues of  $H$  are either purely real, or form complex conjugate pairs. Next, “pseudo-Hermiticity” is a slightly different concept from  $\mathcal{PT}$  symmetry [13–16]: given a linear invertible Hermitian operator  $\eta$ , a Hamiltonian  $H$  is said to be pseudo-Hermitian under  $\eta$  if

$$H^\dagger = \eta H \eta^{-1}. \quad (4)$$

The  $\eta$  operator then serves as the metric operator for a possibly indefinite inner product. If  $H$  is a  $\mathcal{PT}$  symmetric matrix whose eigenvalues are all real, then  $H$  is necessarily pseudo-Hermitian under some operator  $\eta$ , but not vice versa [13–16]. Finally, we say that Hamiltonian is “anti- $\mathcal{PT}$  symmetric” if

$$-H = \mathcal{PT}H(\mathcal{PT})^{-1}. \quad (5)$$

In this case, the eigenvalues are either purely imaginary, or occur in negative-conjugate pairs [20–23]. A physical example of such a symmetry can be found in parametric amplifiers, where the  $\mathcal{P}$  operator interchanges signal and idler waveguide channels [21].

We now consider a waveguide that supports  $N$  channels (waveguide modes), operating at a single fixed frequency or energy. At each position  $z$  along the waveguide axis, the wave function can be expressed by  $2N$  complex wave amplitudes:

$$|\Psi(z)\rangle \equiv \begin{pmatrix} \Psi^+(z) \\ \Psi^-(z) \end{pmatrix}, \quad \text{where} \quad \Psi^\pm(z) \equiv \begin{pmatrix} \psi_1^\pm(z) \\ \vdots \\ \psi_N^\pm(z) \end{pmatrix}. \quad (6)$$

Here,  $\pm$  denotes wave components moving in the  $\pm\hat{z}$  direction, and the wave components are normalized so that  $|\psi_n^\pm|^2$  is an energy flux. The wave functions at any two points,  $z_1$  and  $z_2$ , are related by a transfer matrix:

$$M(z_1, z_2) |\Psi(z_2)\rangle = |\Psi(z_1)\rangle. \quad (7)$$

Let us assume that the waveguide is flux-conserving and time-reversal invariant [24]. This imposes two symmetry constraints on  $M$ . First, flux conservation states that the incoming flux into the segment between  $z_1$  and  $z_2$  must equal the outgoing flux, which implies that

$$\Sigma_z = M^\dagger \Sigma_z M, \quad \text{where} \quad \Sigma_z \equiv \begin{pmatrix} \mathcal{I} & \mathbf{0} \\ \mathbf{0} & -\mathcal{I} \end{pmatrix}. \quad (8)$$

Secondly, time-reversal invariance states that for each solution, there is also a solution obtained by taking the complex conjugate of the wave functions. Hence

$$M^* = \Sigma_x M \Sigma_x, \quad \text{where} \quad \Sigma_x \equiv \begin{pmatrix} \mathbf{0} & \mathcal{I} \\ \mathcal{I} & \mathbf{0} \end{pmatrix}, \quad (9)$$

with  $\mathcal{I}$  denoting the  $N \times N$  identity matrix. Both of these symmetry relations are preserved under composition of transfer matrices.

The combination of Eqs. (8) and (9) implies that waveguide propagation is reciprocal. Note that Eq. (8) can be rewritten as  $M \Sigma_z M^\dagger = \Sigma_z$ . We can combine this with Eq. (9) to obtain

$$M^T J M = J, \quad (10)$$

where

$$J \equiv \Sigma_z \Sigma_x = \begin{pmatrix} \mathbf{0} & \mathcal{I} \\ -\mathcal{I} & \mathbf{0} \end{pmatrix}. \quad (11)$$

This implies that the waveguide is reciprocal [32]; to see this, consider two arbitrary independent sets of wave amplitudes  $\psi_A^\pm$  and  $\psi_B^\pm$ , such that

$$M \begin{pmatrix} \Psi_A^+ \\ \Psi_A^- \end{pmatrix} = \begin{pmatrix} \Phi_A^+ \\ \Phi_A^- \end{pmatrix}, \quad M \begin{pmatrix} \Psi_B^+ \\ \Psi_B^- \end{pmatrix} = \begin{pmatrix} \Phi_B^+ \\ \Phi_B^- \end{pmatrix}. \quad (12)$$

We can also define the scattering matrix  $S$ , which relates incoming to outgoing waves:

$$S \begin{pmatrix} \Psi^+ \\ \Phi^- \end{pmatrix} = \begin{pmatrix} \Psi^- \\ \Phi^+ \end{pmatrix}, \quad (13)$$

for both  $A$  and  $B$  subscripts. By applying Eqs. (10)–(12) to Eq. (13), we can show that

$$\begin{pmatrix} \Psi_A^+ \\ \Phi_A^- \end{pmatrix}^T (S - S^T) \begin{pmatrix} \Psi_B^+ \\ \Phi_B^- \end{pmatrix} = 0. \quad (14)$$

Since this holds for independent sets of wave amplitudes, we conclude that  $S$  must be symmetric [32]. It is important to

note, however, that Eqs. (8) and (9) together form a set of constraints that is stronger than just the reciprocity condition (10). For instance, in optical waveguides with gain and/or loss, Eqs. (8) and (9) are violated, but Eq. (10) still holds.

We can now define a ‘‘Hamiltonian’’  $H$  that is the infinitesimal generator of the transfer matrix, via the Schrödinger-like equation

$$\begin{aligned} -i \frac{\partial}{\partial z} M(z, z_0) &= H(z) M(z, z_0) \\ \Leftrightarrow -i \frac{\partial}{\partial z} \left| \Psi(z) \right\rangle &= H(z) \left| \Psi(z) \right\rangle. \end{aligned} \quad (15)$$

The goal of this paper is to understand and interpret the symmetry properties of  $H$ . This matrix is Hermitian if and only if  $M$  is unitary, which corresponds to the case of the reflection-free waveguide discussed in Sec. I.

In the more general case where  $M$  is nonunitary,  $H$  is non-Hermitian. To determine the symmetry constraints on  $H$ , we use the well-known fact that the exponential map commutes with the adjoint action:

$$e^{J^{-1}(iH\Delta x)J} = J^{-1} e^{iH\Delta x} J, \quad (16)$$

where  $J$  is defined in Eq. (11). Applying this to Eqs. (8) and (9) gives the following pair of symmetry relations for  $H$ :

$$\Sigma_z H \Sigma_z = H^\dagger, \quad (17)$$

$$\Sigma_x H \Sigma_x = -H^*. \quad (18)$$

Based on the definitions introduced at the beginning of this section,  $H$  is pseudo-Hermitian under the operator  $\Sigma_z$  [18] and anti- $\mathcal{PT}$  symmetric under the operator  $\Sigma_x$ .

A  $2N \times 2N$  matrix  $H$  satisfies these two symmetries, (17) and (18), if and only if it has the form

$$H = \begin{pmatrix} \mathcal{H} & \mathcal{A} \\ -\mathcal{A}^* & -\mathcal{H}^* \end{pmatrix}, \quad (19)$$

where  $\mathcal{H}$  and  $\mathcal{A}$  are  $N \times N$  matrices satisfying

$$\mathcal{H} = \mathcal{H}^\dagger, \quad \mathcal{A} = \mathcal{A}^T. \quad (20)$$

These  $H$  matrices are closely connected to the symplectic structure of the transfer matrices. It is known that the transfer matrices can be mapped to the real symplectic group  $\text{Sp}(2N, \mathbb{R})$  [24]. In a similar way, we can show that the  $H$  matrices are isomorphic (in the vector space sense) to the real-valued Hamiltonian matrices,  $\text{sp}(2N, \mathbb{R})$ , which are the Lie algebra generators of  $\text{Sp}(2N, \mathbb{R})$ . To prove this, we first note, via Eqs. (8) and (9), that the transfer matrices take the form

$$M = \begin{pmatrix} \mathcal{C} & \mathcal{B} \\ \mathcal{B}^* & \mathcal{C}^* \end{pmatrix}, \quad (21)$$

where  $\mathcal{B}$  and  $\mathcal{C}$  are complex  $N \times N$  matrices satisfying

$$\mathcal{C}\mathcal{C}^\dagger - \mathcal{B}\mathcal{B}^\dagger = 1, \quad \mathcal{C}\mathcal{B}^T = \mathcal{B}^T\mathcal{C}. \quad (22)$$

Define  $\mathcal{C} = \mathcal{X} + i\mathcal{Y}$  and  $\mathcal{B} = \mathcal{F} + i\mathcal{G}$ , where  $\{\mathcal{X}, \mathcal{Y}, \mathcal{F}, \mathcal{G}\}$  are real  $N \times N$  matrices. Then  $M$  maps to a real  $2N \times 2N$  matrix as follows [24]:

$$f(M) = W = \begin{pmatrix} \mathcal{X} - \mathcal{G} & \mathcal{F} - \mathcal{Y} \\ \mathcal{F} + \mathcal{Y} & \mathcal{X} + \mathcal{G} \end{pmatrix}. \quad (23)$$

The  $f$  map is one-to-one and onto, and one can show that  $W$  is symplectic (i.e.,  $W J W^T = J$ ) if and only if  $M$  satisfies Eqs. (21) and (22). Note, however, that the group operation of  $\text{Sp}(2N, \mathbb{R})$ —i.e., multiplication of the  $W$  matrices—does not correspond to the composition operation (matrix multiplication) of the transfer matrices.

The map  $f$  defined in Eq. (23) can also be applied to the  $H$  matrices, which are the generators of  $M$  satisfying Eqs. (19) and (20). We can then show that

$$if(H) = \begin{pmatrix} -\text{Im}(\mathcal{H}) - \text{Re}(\mathcal{A}) & -\text{Re}(\mathcal{H}) - \text{Im}(\mathcal{A}) \\ \text{Re}(\mathcal{H}) - \text{Im}(\mathcal{A}) & -\text{Im}(\mathcal{H}) + \text{Re}(\mathcal{A}) \end{pmatrix}, \quad (24)$$

which is a real  $2N \times 2N$  matrix of the Hamiltonian form. This means that

$$[Jf(H)]^T = Jf(H), \quad (25)$$

where  $J$  is the skew-symmetric matrix defined in Eq. (11). [The Hamiltonian matrices are so-called because they occur naturally in systems of equations formed by Hamilton’s equations of classical mechanics [33]; the terminology is unrelated to our interpretation of the  $H$  matrices as Hamiltonians, which is based on the Schrödinger-like Eq. (15).] Equation (24) is one-to-one, and thus constitutes an isomorphism to the group of Hamiltonian matrices, where the group operations are addition operations on the  $H$  matrices as well as the Hamiltonian matrices. In turn, the group of Hamiltonian matrices is the Lie algebra  $\text{sp}(2N, \mathbb{R})$  that generates the Lie group  $\text{Sp}(2N, \mathbb{R})$ .

### III. EIGENVALUE PROPERTIES

The  $H$  matrices defined in the previous section are pseudo-Hermitian under  $\Sigma_z$ , due to the flux conservation condition (17), and anti- $\mathcal{PT}$  symmetric under  $\Sigma_x$ , due to the time-reversal invariance condition (18). These symmetries offer the prospect of non-Hermitian transitions in the eigenvectors and eigenvalues of  $H$ , analogous to the  $\mathcal{PT}$ -breaking transition.

First, however, let us discuss the physical meaning of the eigenvectors and eigenvalues of  $H$ . If a waveguide is invariant under translation by some  $L$ , each waveguide mode is describable by a state vector  $|\Psi\rangle$  satisfying [34]

$$M(z + L, z) |\Psi\rangle = \exp(i\kappa L) |\Psi\rangle, \quad (26)$$

for some wave number  $\kappa$ . Then  $|\Psi\rangle$  and  $\kappa$  are an eigenvector and eigenvalue of  $H$ , the generator of  $M$ . The components of the state vector  $|\Psi\rangle$  describe the waveguide mode’s decomposition into forward-going and backward-going modes of an ‘‘empty’’ (reflection-free) waveguide. These forward and backward modes are coupled via inhomogeneities in the waveguide, such as a Bragg grating where  $L$  is a multiple of the grating period [26–28].

The Hamiltonian  $H$  satisfies Eqs. (17) and (18), which implies that its eigenvalues come in pairs. If  $\kappa$  is an eigenvalue, then  $\kappa^*$  and  $-\kappa^*$  are also eigenvalues. To show this, suppose that

$$H \begin{pmatrix} v \\ w \end{pmatrix} = \kappa \begin{pmatrix} v \\ w \end{pmatrix} \quad (27)$$

for some  $v, w \in \mathbb{C}^N$  and  $\kappa \in \mathbb{C}$ . By the pseudo-Hermiticity relation (17),

$$H^\dagger \begin{pmatrix} v \\ -w \end{pmatrix} = \kappa \begin{pmatrix} v \\ -w \end{pmatrix}. \quad (28)$$

Since  $H$  and  $H^T$  share the same eigenvalues,  $\kappa^*$  is an eigenvalue of  $H$ . Furthermore, from the anti- $\mathcal{PT}$  symmetry relation (18), we obtain

$$H^* \begin{pmatrix} w \\ v \end{pmatrix} = -\kappa \begin{pmatrix} w \\ v \end{pmatrix}, \quad (29)$$

which implies that  $-\kappa^*$  is an eigenvalue of  $H$ . Based on these results, for each eigenvalue  $\kappa$ , either  $\kappa$  (i) is purely imaginary,  $\kappa$  (ii) is purely real, or (iii) there exist four eigenvalues  $\{\kappa, -\kappa, \kappa^*, -\kappa^*\}$  that are not purely real or imaginary. Note that case (iii) can only occur for  $N \geq 2$ .

We can induce transitions between these three cases by tuning various parameters in  $H$ . The transition from case (i) to case (ii) or (iii) corresponds to the breaking of the eigenvector's anti- $\mathcal{PT}$  symmetry; in case (i), the eigenvector has unbroken anti- $\mathcal{PT}$  symmetry and satisfies  $|v|^2 = |w|^2$  [see Eq. (29)], whereas in the other two cases, the eigenvector's anti- $\mathcal{PT}$  symmetry is broken. However, the transition from (ii) to (iii) does *not* seem to correspond to any obvious form of symmetry breaking (or “pseudo-Hermiticity breaking”) in the eigenvector, based on Eq. (28).

#### IV. IMPLICATIONS FOR WAVEGUIDE SCATTERING PARAMETERS

In  $\mathcal{PT}$  symmetric optics, the evolution of waveguide modes can be used to provide evidence for the  $\mathcal{PT}$  symmetry-breaking transition [4–7]. In the pioneering experimental demonstration of Ruter *et al.*, for instance, light is injected into one of a pair of  $\mathcal{PT}$  symmetric waveguides (which are assumed to have negligible backreflection) [7]. When the system is in the  $\mathcal{PT}$ -unbroken phase, the injected light beats, or oscillates, between the two waveguides with no net amplification or damping; but when the system is in the  $\mathcal{PT}$ -broken phase, the injected light experiences exponential amplification.

In a similar spirit, we will now show that the non-Hermitian transitions of  $H$  are tied to the modal evolution across a waveguide segment with *non-negligible* backreflection. This process is interpreted through the *backward*  $z$  evolution of the wave amplitudes. Unlike in Ref. [7], the different components of the state vector in our model consist of forward-going versus backward-going waves, rather than the excitations of gain versus loss waveguides. We can make use of the fact that, at the end of the waveguide, the transmitted wave is purely forward-going, with no backward component; this plays a role analogous to the initial state in the experiment of Ref. [7], in which light is injected into one of the two waveguides. Our non-Hermitian transitions correspond to the abrupt changes in reflection and transmission caused by passing through band extrema.

For a single-mode waveguide ( $N = 1$ ), the  $H$  matrix has the form

$$H = \begin{pmatrix} \mathcal{E} & a \\ -a^* & -\mathcal{E} \end{pmatrix}, \quad (30)$$

where  $\mathcal{E} \in \mathbb{R}$  and  $a \in \mathbb{C}$ . In the context of an optical waveguide,  $\mathcal{E}$  and  $a$  could parametrize the detuning and backreflection induced by a fiber Bragg grating [20–23]. Interestingly, a non-Hermitian Hamiltonian of this form has previously been investigated by Mathur [12], in the context of a quantum electronic waveguide formed by coupled chiral edge states in a quasi-one-dimensional quantum Hall gas. There, the chiral edge states satisfy the time-independent Schrödinger equation

$$\begin{pmatrix} -i\partial_z & -a(z) \\ -a(z)^* & i\partial_z \end{pmatrix} \begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} = \mathcal{E} \begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix}, \quad (31)$$

where  $\psi^\pm$  are the wave amplitudes for the chiral edge states on opposite edges,  $\mathcal{E}$  is the edge state energy, and  $a(z)$  is the coupling between the edge states. (If the sample is sufficiently narrow relative to the penetration depth of the edge states, such coupling can occur by evanescent tunneling; it spoils the topological protection that is normally enjoyed by the edge states [35,36]). Rearranging Eq. (31), and using the definition (15), yields Eq. (30).

When  $a$  is a nonzero constant,  $H$  has eigenvalues

$$\kappa = \pm \sqrt{\mathcal{E}^2 - |a|^2}. \quad (32)$$

The eigenvalues are either both imaginary (corresponding to unbroken anti- $\mathcal{PT}$  symmetry) or both real (corresponding to broken anti- $\mathcal{PT}$  symmetry). The transition between the two regimes occurs at  $\kappa = 0$ , and it corresponds to the familiar effects of crossing a band extremum, or of crossing the cutoff frequency of a waveguide. On one side of the transition, there is a pair of propagating modes (real  $\kappa$ ), and on the other side the modes are purely evanescent (imaginary  $\kappa$ ). Since there are only two eigenvalues, this anti- $\mathcal{PT}$ -breaking transition is the only type that occurs for  $N = 1$ .

In Fig. 1, we consider a waveguide segment between  $z = 0$  and  $z = Z$ . Within the segment, the parameter  $a$  varies smoothly from zero (at the end points) to a nonzero value  $a_0$ , as shown in Fig. 1(a), whereas outside the segment, we set  $a = 0$  corresponding to a reflection-free waveguide; we also set  $\mathcal{E} = 1$  everywhere. Suppose that there is an input wave with amplitude  $\psi^+(0) = 1$  at the start of the segment. This gives rise to a reflected wave with amplitude  $\psi^-(0) = r$ , and a transmitted wave with amplitude  $\psi^+(Z) = t$ . Since there is no backward-going wave at the end of the segment,  $\psi^-(Z) = 0$ . Due to linearity, we can rescale the wave amplitudes so that  $\psi^+(0) = 1/t, \psi^-(0) = r/t$  at the start of the segment, and  $\psi^+(Z) = 1, \psi^-(Z) = 0$  at the end.

This reflection-and-transmission scenario can be mathematically described by the *backward* evolution of the non-Hermitian Schrödinger-like equation (15), with the end conditions  $\psi^+(Z) = 1$  and  $\psi^-(Z) = 0$ . Upon integrating Eq. (15) backwards from  $z = Z$  to  $z = 0$ , we obtain  $\psi^+(0) = 1/t$  and  $\psi^-(0) = r/t$ . In Figs. 1(b) and 1(c), we plot  $|\psi^+(z)|^2$  and  $|\psi^-(z)|^2$  against  $z$ , obtained through the backward evolution calculation described above. When  $a_0 = 0.9$ , the entire waveguide segment is in the anti- $\mathcal{PT}$ -broken phase, where the eigenvalues of  $H$  are real; we observe beating between the forward-going and backward-going components, without exponential amplification or damping. When  $a_0 = 1.01$ , the waveguide segment passes into the anti- $\mathcal{PT}$ -unbroken phase,



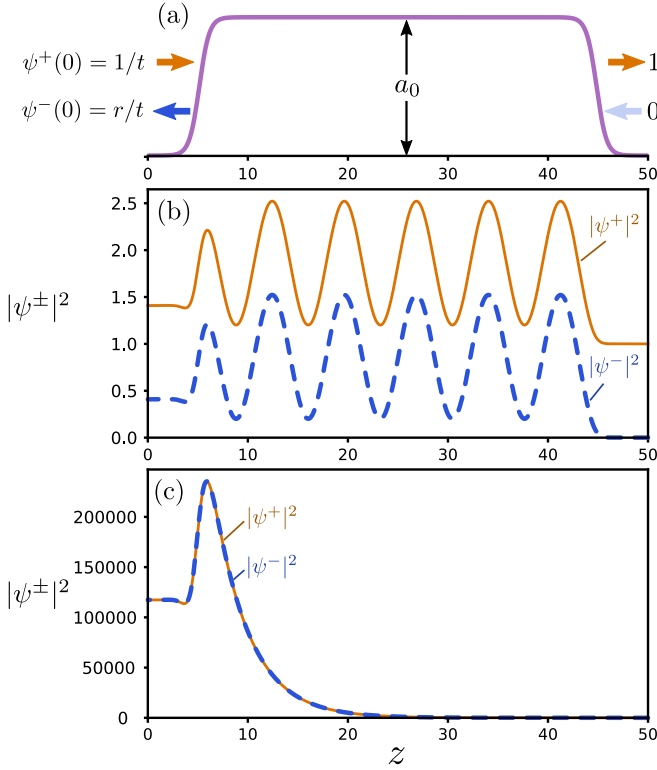


FIG. 1. Reflection and transmission for a waveguide segment. (a) Schematic of the scattering problem, showing input wave amplitude  $1/t$ , reflected amplitude  $r/t$ , and transmitted amplitude 1. The curve shows the profile of  $a(z)$ , which is taken to be  $a(z) = (a_0/2)[\tanh(z - z_1) - \tanh(z - z_2)]$ , where  $z_1 = 5$  and  $z_2 = 45$ . We set  $\mathcal{E} = 1$  everywhere, and  $a = 0$  outside the segment. (b),(c) Intensities of the forward and backward components,  $|\psi^\pm(z)|^2$ , vs  $z$ , for (b)  $a_0 = 0.9$  (anti- $\mathcal{PT}$ -broken) and (c)  $a_0 = 1.01$  (anti- $\mathcal{PT}$ -unbroken).

where the eigenvalues of  $H$  are imaginary; we observe that the state undergoes exponential “backward amplification” in going from  $z = Z$  to  $z = 0$ . Interpreted in terms of the forward-going wave injected at  $z = 0$ , the transmitted part is exponentially damped because, inside the segment, the waveguide passes through a band extremum (into a band gap, or under the waveguide cutoff). Most of the incident wave is hence reflected. The two distinct behaviors—oscillation and damping—correspond to the anti- $\mathcal{PT}$ -broken and anti- $\mathcal{PT}$ -unbroken phases of the non-Hermitian Hamiltonian  $H$ . This is in some sense the opposite of the  $\mathcal{PT}$  waveguide evolution experiment of Ruter *et al.*, where the symmetry-unbroken regime produces oscillations and the symmetry-broken regime produces amplification [7].

Next, we consider the  $N = 2$  case. The most general  $4 \times 4$  non-Hermitian Hamiltonian satisfying Eqs. (19) and (20) can be written as

$$H = \begin{pmatrix} \mathcal{E} & \eta & m_1 & a \\ \eta^* & \mathcal{E} & a & m_2 \\ -m_1^* & -a^* & -\mathcal{E} & -\eta^* \\ -a^* & -m_2^* & -\eta & -\mathcal{E} \end{pmatrix}, \quad (33)$$

where  $\mathcal{E} \in \mathbb{R}$  and  $\eta, a, m_1, m_2 \in \mathbb{C}$ . This could describe a dual-mode optical waveguide, in which inhomogeneities (e.g.,

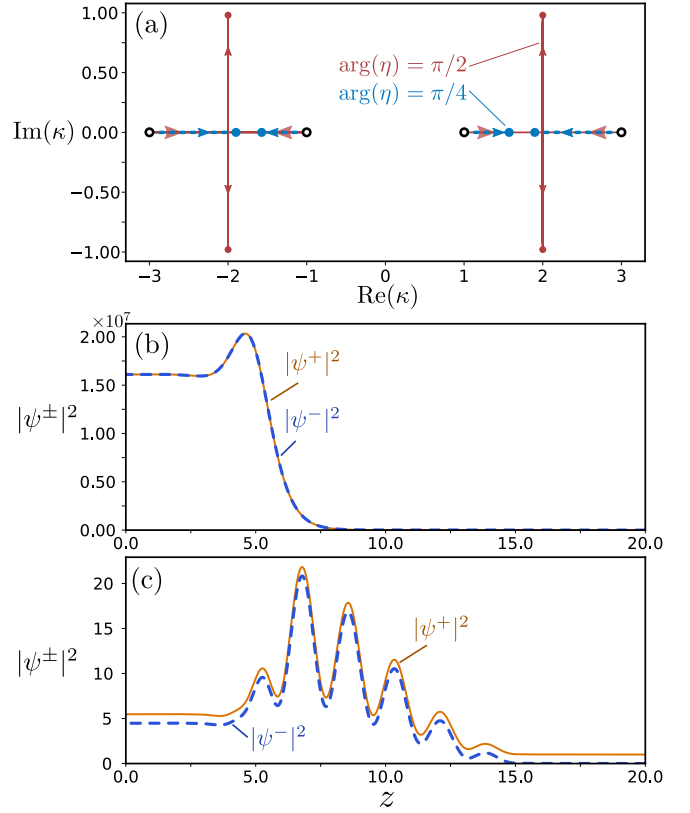


FIG. 2. Reflection and transmission behavior of an  $N = 2$  waveguide. (a) Complex plane trajectories of the eigenvalues  $\kappa$ , for the matrix given in Eq. (33) with  $\mathcal{E} = 1$ ,  $|\eta| = 2$ ,  $a = 0$ , and  $m_1 = m_2 = m$  varying from 0 to 1.4. The trajectory directions are indicated by arrows, the start points ( $m = 0$ ) are indicated by hollow circles, and the end points ( $m = 1.5$ ) are indicated by filled circles. The trajectories are dependent on  $\arg(\eta)$ , and two possible choices,  $\pi/4$  and  $\pi/2$ , are shown. (b),(c) Intensities of the forward and backward components,  $|\psi^\pm(z)|^2 = |\psi_\uparrow^\pm(z)|^2 + |\psi_\downarrow^\pm(z)|^2$ , vs  $z$ . We set  $\mathcal{E} = 1$ ,  $|\eta| = 2$ ,  $a = 0$ , and  $m = (1.4/2)[\tanh(z - z_1) - \tanh(z - z_2)]$ , where  $z_1 = 5$  and  $z_2 = 15$ . (b) For  $\arg(\eta) = \pi/4$ , the eigenvalues become complex within the waveguide segment, resulting in exponential wave damping. (c) For  $\arg(\eta) = \pi/2$ , the eigenvalues are real throughout, resulting in beating. The end-point condition is  $\psi_\uparrow^+(20) = 1$ ; varying the distribution of forward-going wave amplitudes at the end point does not significantly alter the results.

a Bragg grating) induce mixing between the two types of transverse modes, as well as between forward-going and backward-going modes. It could also be realized using a generalization of Mathur’s quantum Hall model [12] to the quantum spin Hall gas [37]. In a quasi-one-dimensional quantum spin Hall waveguide, shown schematically in Fig. 2(a), the coupled edge states can be described by the Schrödinger equation

$$\begin{pmatrix} -i\partial_z & -\eta & -m_1 & -a \\ -\eta^* & -i\partial_z & -a & -m_2 \\ -m_1^* & -a^* & i\partial_z & -\eta^* \\ -a^* & -m_2^* & -\eta & i\partial_z \end{pmatrix} \begin{pmatrix} \psi_\uparrow^+ \\ \psi_\uparrow^- \\ \psi_\downarrow^+ \\ \psi_\downarrow^- \end{pmatrix} = \mathcal{E} \begin{pmatrix} \psi_\uparrow^+ \\ \psi_\uparrow^- \\ \psi_\downarrow^+ \\ \psi_\downarrow^- \end{pmatrix}, \quad (34)$$

where  $\{\uparrow, \downarrow\}$  denote the spin polarizations of the various edge states,  $m_1$  and  $m_2$  represent the scattering amplitudes for spin-flip back-scattering along each edge,  $\eta$  represents

hopping between edges with spin flip, and  $a$  represents hopping between edges without spin flip. This Schrödinger equation is invariant under the time-reversal operation  $\psi_{\uparrow}^+ \leftrightarrow (\psi_{\downarrow}^-)^*$  and  $\psi_{\uparrow}^- \leftrightarrow (\psi_{\downarrow}^+)^*$ , which conjugates the wave amplitudes as well as reversing the spin and the direction of motion. Rearranging Eq. (34) yields the non-Hermitian matrix  $H$  given in Eq. (33) as the generator of the transfer matrix.

Returning to Eq. (33), let us examine the possible eigenvalues of  $H$ . There are two special cases: first, if  $m_1 = m_2 = 0$ , then the eigenvalues are

$$\kappa = \pm \sqrt{(\mathcal{E} \pm |\eta|)^2 - |a|^2}, \quad (35)$$

where the two  $\pm$  signs are independent. Secondly, if  $\eta = 0$  and  $m_1 = m_2 = m$ , then the eigenvalues are

$$\kappa = \pm \sqrt{E^2 - |a \pm m|^2}. \quad (36)$$

In both of these special cases, the eigenvalues are either real or purely imaginary, and the transitions occur at  $\kappa = 0$ . These are the transitions between cases (i) and (ii) discussed in Sec. III, and are essentially similar to the behavior seen in the  $N = 1$  waveguide. They correspond to passing through band extrema at  $k = 0$ .

When  $\eta \neq 0$  and  $m_1, m_2 \neq 0$ , there can also occur transitions between the cases (i) and (iii), or between (ii) and (iii), discussed in Sec. III. In other words, the eigenvalues go from purely real or purely imaginary numbers to a set of four distinct complex numbers. We can demonstrate such transitions by taking  $a = 0$  and  $m_1 = m_2 = m$ , and varying  $\eta$  and/or  $\mathcal{E}$ . It can be shown that bifurcations occur when

$$\mathcal{E} = \pm |m \sin[\arg(\eta)]|. \quad (37)$$

They occur along the real- $\kappa$  axis if  $|\eta| > |m \cos[\arg(\eta)]|$  and along the imaginary- $\kappa$  axis if  $|\eta| < |m \cos[\arg(\eta)]|$ . The former corresponds to passing through a pair of band extrema located at  $\pm \kappa$ . (Similar bifurcations occur if  $a \neq 0$ ; the expressions for the bifurcation points are simply more complicated.) As in the  $N = 1$  case, we can observe the eigenvalue transitions using a waveguide segment with varying

parameters. In Fig. 2, we study a waveguide segment in which  $m_1 = m_2$  varies from zero (no backreflection) to a nonzero value. Depending on the choice of  $\arg(\eta)$ ,  $\kappa$  may remain real, or undergo a real-to-complex bifurcation. Unlike the  $N = 1$  case, however, this bifurcation does not correspond to a breaking of an eigenstate symmetry. In the results obtained by backward integration of the non-Hermitian Schrödinger-like equation, we indeed observe exponential damping in the former case, and beating in the latter. For  $N > 2$ , we expect to see the same relationships between the reflection and transmission behavior of the waveguide and the underlying non-Hermitian transitions of  $H$ , based on the eigenvalue properties discussed in Sec. III.

## V. CONCLUSIONS

We have shown that the generator of the transfer matrix, when regarded as a non-Hermitian Hamiltonian, exhibits the features of pseudo-Hermiticity [13–16] and anti- $\mathcal{PT}$  symmetry [20–23]. In the literature on non-Hermitian systems, there has been a great deal of interest in such symmetries as generalizations of the  $\mathcal{PT}$  symmetry concept [1–3]. In previous works, realizing these symmetries has required the presence of phenomena such as negative-index materials [20] or parametric amplification [21]. In our case, they arise from the simple physical requirements of flux conservation and time-reversal symmetry. These Hamiltonians' non-Hermitian transitions, including the breaking of anti- $\mathcal{PT}$  symmetry, manifest physically as the effects of crossing a band extremum in a waveguide (e.g., the sharp decrease in transmission when entering a band gap).

## ACKNOWLEDGMENTS

We are grateful to M. V. Berry, J. Gong, D. Leykam, H. Wang, and Q. Wang for helpful comments. We acknowledge support from the Singapore MOE Academic Research Fund Tier 2 Grant No. MOE2015-T2-2-008 and the Singapore MOE Academic Research Fund Tier 3 Grant No. MOE2011-T3-1-005.

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