Valley band structure in chiral-time symmetric non-Hermitian system

S. Lin and Z. Song
School of Physics, Nankai University, Tianjin 300071, China

We establish a connection between an arbitrary Hermitian tight-binding model with chiral ($\mathcal{C}$) symmetry and its non-Hermitian counterpart with chiral-time ($\mathcal{CT}$) symmetry. We show that such a kind of non-Hermitian Hamiltonian is pseudo-Hermitian. The eigenvalues and eigenvectors of the non-Hermitian Hamiltonian can be easily obtained from those of its parent Hermitian Hamiltonian. It provides a way to generate a class of non-Hermitian models with a tunable full real band structure by means of additional imaginary potentials. We also present an illustrative example that could achieve a valley structure from the energy band of a two-layer Hermitian square lattice model.

I. INTRODUCTION

Extra imaginary potentials induce many unusual features even in certain simple or trivial systems, which include quantum phase transition occurred in a finite system [1, 20], unidirectional propagation and anomalous transport [4, 21, 28], invisible defects [29, 31], coherent absorption [32] and self sustained emission [33, 35], loss-induced revival of lasing [38], as well as laser-mode selection [39, 40]. Most of these phenomena are related to the critical behaviours near exceptional or spectral singularity points. It opens a way for exploring novel quantum states. The basis of such approaches is to seek various non-Hermitian systems with exact solutions.

Recently, valleytronics based on graphene-like materials has attracted much attention. It refers to the technology of control over the valley degree of freedom of certain semiconductors [41, 42] that present multiple valleys inside the first Brillouin zone. It is expected that valley degree of freedom can be an analogue of the internal degree of freedom of spin to perform tasks involving both the storage and manipulation of quantum information [43–46]. Most of theoretical proposals and experiments were performed in natural systems, such as graphene [47], some Transition metal dichalcogenide monolayers [48], diamond [49], Bismuth [50], Silicon [44, 51, 52], Carbon nanotubes [46], Aluminium arsenide [53], and silicon [54]. Meanwhile, a natural question would emerge that whether one can find some artificial materials which have a valley band structure.

In this paper, we consider a method of constructing a variety of non-Hermitian systems which have full real spectra. We focus on the connection between an arbitrary Hermitian tight-binding model with chiral ($\mathcal{C}$) symmetry and its non-Hermitian counterpart with chiral-time ($\mathcal{CT}$) symmetry. We show that such a kind of non-Hermitian Hamiltonian is pseudo-Hermitian. The obtained result indicates that the eigenvalues and eigenvectors of the non-Hermitian Hamiltonian can be easily obtained from those of its parent Hermitian Hamiltonian and the reality of the spectrum is robust to the disorder. It also provides a way to generate a class of non-Hermitian models with a tunable full real band structure by means of additional imaginary potentials. We present an illustrative example, which is a two-layer square lattice model. By adding imaginary potentials, exact result shows that a valley band structure can be achieved.

The remainder of this paper is organized as follows. In Sec. III, we present a general formalism for the solution of an arbitrary non-Hermitian $\mathcal{CT}$ symmetric system. Sec. III is devoted to present an illustrative example of a two-layer square lattice model. Finally, we present a summary and discussion in Sec. IV.

II. MODEL AND FORMALISM

The main interest of this work is focused on the relation between an arbitrary Hermitian tight-binding model with $\mathcal{C}$ symmetry and a non-Hermitian model which is constructed based on the former by adding additional imaginary potentials. The latter is a non-Hermitian counterpart of the former in the context of this work.

Consider the Hamiltonian of a non-Hermitian tight-binding model

$$H = H_0 + H_\gamma, \quad (1)$$

with

$$H_0 = \sum_{i,j} J_{ij} \langle i | A | j \rangle_B + H.c., \quad (2)$$

$$H_\gamma = i\gamma \sum_j (| j \rangle_A \langle j | A - | j \rangle_B \langle j | B), \quad (3)$$

on a bipartite lattice $\Lambda = 2N$ which can be decomposed into two sublattices $\Lambda_A$ and $\Lambda_B$. Here we only consider the case with identical sublattice numbers $\Lambda_A = \Lambda_B = N$ for simplicity. A schematic illustration of the model is presented in Fig. 1(a).

The Hamiltonian $H_0$ has both $\mathcal{C}$ and time-reversal ($\mathcal{T}$) symmetries, i.e.,

$$\mathcal{C}H_0\mathcal{C}^{-1} = -H_0, \quad \mathcal{T}H_0\mathcal{T}^{-1} = H_0. \quad (4)$$
Hermitian Hamiltonian and there is a simple relation between the spin representation. We will show that under the mapping \( \mathcal{C} \) symmetry is broken. However, if \( \varepsilon \) is an imaginary number, we always have \( \mathcal{C}T |\psi\rangle = |\psi\rangle \), i.e., \( |\psi\rangle \) has \( \mathcal{C}T \) symmetry. It is not a surprising result that one can treat the \( \mathcal{C}T \) symmetry in the context of \( \mathcal{PT} \) symmetry under the mapping \( H \rightarrow iH \), which obeys \( [\mathcal{C}T, iH] = 0 \).

Now we investigate the Hamiltonian \( H \) in a pseudo spin representation. We will show that \( H \) is a pseudo-Hermitian Hamiltonian and there is a simple relation between the spectra of \( H \) and \( H_0 \). Due to the \( \mathcal{C} \) symmetry, the Hamiltonian \( H_0 \) can be diagonalized as the form

\[
H_0 = \sum_{n=1}^{N} \varepsilon_0(n) \left( |\varphi_n^+\rangle \langle \varphi_n^+ | - |\varphi_n^-\rangle \langle \varphi_n^- | \right),
\]

where \( \varepsilon_0(n) > 0 \) is the positive energy spectrum with \( n \in [1, N] \), and

\[
|\varphi_n^\pm\rangle = \frac{1}{\sqrt{2}}(|\phi_n\rangle_A \pm |\phi_n\rangle_B),
\]

are eigenstates with eigenenergies \( \pm \varepsilon_0(n) \). Here states \( |\phi_n\rangle_A \) and \( |\phi_n\rangle_B \) are single-particle states with particle probability only distributed on sublattices A and B, respectively. Due to the \( \mathcal{C} \) symmetry of \( H_0 \), it is easy to check that \( |\varphi_n^+\rangle = \mathcal{C} |\varphi_n^-\rangle \). One can express the Hamiltonian in the representation of pseudo spins

\[
H_0 = \sum_{n=1}^{N} \varepsilon_0(n) \sigma_n^x,
\]

where

\[
\sigma_n^x = |\phi_n\rangle_B \langle \phi_n|_A + |\phi_n\rangle_A \langle \phi_n|_B
\]

is the \( x \)-component of the Pauli matrix. Accordingly, we could rewrite the Hamiltonian \( H \) as the form

\[
H = \sum_{n=1}^{N} \vec{B}(n) \cdot \vec{\sigma}_n,
\]

which describes an ensemble of non-interacting half spins in a complex external magnetic field. Here the field and the Pauli matrices are

\[
\vec{B}(n) = [\varepsilon_0(n), 0, i\gamma],
\]

\[
\sigma_n^x = |\phi_n\rangle_A \langle \phi_n|_A - |\phi_n\rangle_B \langle \phi_n|_B,
\]

\[
\sigma_n^y = i |\phi_n\rangle_B \langle \phi_n|_A - i |\phi_n\rangle_A \langle \phi_n|_B.
\]

Based on this analysis, the eigenstates and eigenenergies of Hamiltonian \( H \) are

\[
|\psi_n^{\pm}\rangle = \frac{1}{\sqrt{\Omega_{\pm}}} (|\phi_n\rangle_A \pm e^{\pi i \theta} |\phi_n\rangle_B),
\]

\[
\varepsilon(n) = \pm \sqrt{\varepsilon_0(n)^2 - \gamma^2},
\]

where \( \theta = \text{arccos} \sqrt{1 - |\gamma/\varepsilon_0(n)|^2} \) and the Dirac normalized coefficients are \( \Omega_{\pm} = 1 + \exp(\pm 2i \pi \theta) \).

This result has many implications. (i) Non-Hermitian Hamiltonian \( H \) is pseudo-Hermitian, since it has either a real spectrum or else its complex eigenvalues always occur in complex conjugate pairs. In contrast, there is no such proof for a \( \mathcal{PT} \)-symmetric system. (ii) It explicitly connects the complete set \( \{\varepsilon(n), |\psi_n^{\pm}\rangle\} \) to \( \{\pm \varepsilon_0(n), |\varphi_n^\pm\rangle\} \). Only an extra phase is added in \( |\psi_n^z\rangle \) from \( |\varphi_n^z\rangle \), which indicates that the two states have the same Dirac probability distribution when \( \varepsilon(n) \) is real. (iii) The exceptional points occur at \( \gamma = \gamma_n = \pm \varepsilon_0(n) \), which correspond to the \( \mathcal{C}T \) symmetry breaking of states \( |\varphi_n^\pm\rangle \).
It allows a variety of non-Hermitian models with a wide range of disorder parameters to have a full real spectrum and the modulation of band structure is due to the non-Hermiticity. In the next section, we will show its application in an example.

To demonstrate these features, we consider an example model, a generalized non-Hermitian Rice-Mele model, which has been investigated in Ref. [56, 57]. The corresponding Hermitian Hamiltonian has the form

$$H_0 = \sum_{j=1}^{N} (J_{2j-1} |j\rangle_A \langle j|_B + J_{2j} |j\rangle_B \langle j+1|_A) + \text{H.c.}$$

with the periodic boundary condition $|2N+1\rangle_A = |1\rangle_A$. The hopping amplitude between two sublattices is $J_{j} = 1 + (-1)^j \delta$, where $\delta$ is the dimerization factor. The generalized non-Hermitian Rice-Mele Hamiltonian has been completely solved and the obtained result can be recovered by the present method. In this case, we have

$$\varepsilon(k) = \pm \sqrt{\varepsilon_0(k)^2 - \gamma^2},$$

$$\varepsilon_0(k) = 2 \sqrt{\delta^2 + (1 - \delta^2) \cos^2(k/2)},$$

with $k = 2\pi n/N$, $n \in [1, N]$. In the absence of $\gamma$, the energy gap is $4\delta$, which determines the exceptional point occurring at $\gamma = \gamma_c = \pm 2\delta$ for the non-Hermitian Rice-Mele Hamiltonian. In other words, the energy gap of $H_0$ protects the $CT$ symmetry of the eigenstates of $H$. This is still true in the presence of noise in $J_j$. In contrast to a $PT$ symmetric system, the reality of the spectrum for a $CT$ symmetric one is more robust to the disorder of coupling constants.

### III. VALLEY STRUCTURE

The connection between $H_0$ and $H$ can be employed to modulate the band structure of $H$, which has some intriguing properties induced by the non-Hermitian term $H_\gamma$. In traditional condensed matter theories, the energy band structure plays a crucial role in the theory of electron conductivity in the solid state and explains why materials can be classified as insulators, conductors, and semiconductors. Moreover, much attention has been paid to the honeycomb lattice [58], which is relevant to high electron mobility and topological phase, as exemplified by the graphene. On the other hand, a local maximum (minimum) on the valence (conduction) band has been proposed as a valley degree of freedom, stimulating a promising field, valleytronics which is in analogy to spintronics [59].

In the Hermitian realm, the band structures of most kinds of systems have been well studied. Nevertheless, non-Hermitian parameters may induce an unusual band structure which is difficult to achieve in a Hermitian system. As an example, Eq. (20) provides a way to accomplish this task that imaginary potentials can deform the shape of a given band structure without altering its topology except the situation when the system contains the exceptional points. In the following, we will present an example which realizes a valley structure on a square lattice.

We consider a bilayer square lattice model which is shown in Fig. 2. The corresponding Hermitian Hamiltonian has the form

$$H_0 = H_1 + H_2 + H_{12},$$

$$H_\lambda = J \sum_{j,l=1}^{N} |\lambda, j, l\rangle \langle \lambda, j + 1, l| + \text{H.c.},$$

$$H_{12} = T \sum_{j,l=1}^{N} |1, j, l\rangle \langle 2, j, l| + \text{H.c.},$$

where $\lambda = 1$ or $2$ is the index that respectively labels the position in the top or bottom layers, and $(j, l)$ is the in-plane site index. Parameters $J$ and $T$ of this model are intra and interlayer hopping strengths. In this paper, we only consider the case of $T > 4J$. And the distribution of imaginary potentials is given as the form

$$H_\gamma = i\gamma \sum_{\lambda=1}^{2} \sum_{j,l=1}^{N} (-1)^{j+l} |\lambda, j, l\rangle \langle \lambda, j, l|. $$

The Hamiltonian $H_0$ can be easily diagonalized via Fourier transformation. Let us consider an individual rung, i.e. two sites with the same in-plane site index on the opposite layers. An occupied rung has two possible states that are bond and antibond states. The bond (antibond) state of a rung can only be transited to the
bond (antibond) state next to it. Therefore it can be decomposed into two independent single layer square lattices with on-site potentials $T$ and $-T$, respectively. The spectra and eigenvectors are

$$\varepsilon^{\pm}_0(k_x, k_y) = \pm \{2J[\cos(k_x) + \cos(k_y)] + T\}, \quad (28)$$

and

$$|\varphi^{\pm}(k_x, k_y)\rangle = \sum_{j,l=1}^{N} \frac{e^{i(k_x j + k_y l)}}{N^{1/2}} (|\lambda_A, j, l\rangle \pm |\lambda_B, j, l\rangle), \quad (29)$$

where $\pm$ denotes the two independent single layers, and $k_x = 2nx\pi/N, k_y = 2ny\pi/N$ with $n_x, n_y \in [1, N]$. States $|\lambda_A, j, l\rangle$ and $|\lambda_B, j, l\rangle$ are the position states of sublattices A and B with the layer labels $\lambda_A = \lfloor 3 - (-1)^{j+l}\rfloor / 2$ and $\lambda_B = \lfloor 3 - (-1)^{j+l}\rfloor / 2$. This band structure is trivial, but it would be a good parent to construct a valley structure by adding staggered imaginary potentials. Now we consider the corresponding non-Hermitian Hamiltonian $H = H_0 + H_\gamma$. According to the above result, the spectra and eigenvectors of $H$

$$\varepsilon^{\pm}(k_x, k_y) = \pm \sqrt{\varepsilon^{\pm}_0(k_x, k_y)^2 - \gamma^2}, \quad (30)$$

and

$$|\psi^{\pm}(k_x, k_y)\rangle = \sum_{j,l=1}^{N} \frac{e^{i(k_x j + k_y l)}}{N^{1/2}} i^{\pm i\gamma} (|\lambda_A, j, l\rangle \pm e^{\mp i\theta} |\lambda_B, j, l\rangle), \quad (31)$$

where

$$\theta = \arccos \sqrt{1 - (\gamma/\varepsilon^{\pm}_0)^2} \quad (32)$$

is real when the symmetry is not broken. In the exact $CT$-symmetric region, there are local maxima (minima) on the valence (conduction) band at points $(k_x^c, k_y^c) = (\sigma \pi, \sigma' \pi)$ ($\sigma, \sigma' = $ odd). The energy band gap is $2\sqrt{(T - 4J)^2 - \gamma^2}$ and the exceptional points occur at $\gamma = \gamma_c = \varepsilon_0(k_x^c, k_y^c) = T - 4J$. In the vicinity of $k_c$ and considering the case $0 < \gamma_c - \gamma \ll J$, we have an approximate relation

$$\frac{(k_x - k_x^c)^2}{a^2} + \frac{(k_y - k_y^c)^2}{b^2} - \frac{(\varepsilon^\pm)^2}{c^2} = -1, \quad (33)$$

with $c = \sqrt{\gamma_c^2 - \gamma^2}$ and $a = b = c/\sqrt{2J/\gamma_c}$, which indicates that the band structure is a hyperboloid of two sheets. For $\gamma = \gamma_c$, it reduces to a Dirac cone. The group velocity at the linear region is

$$v_g = J \sqrt{2(T/J - 4)}, \quad (34)$$

which indicates that $v_g$ strongly depends on the ratio of $J$ and $T$, while it only depends on the hopping strength in a honeycomb lattice. It seems that it has a similar band structure with that of graphene near the zero-energy plane. The difference between them is that the vertices of the cone of graphene are degenerate points, while the ones in the present model are exceptional points. For $\gamma < \gamma_c$, the energy gap and the group velocity are tunable by $\gamma$, $J$, and $T$. The valley band structures for different $\gamma$ are plotted in Fig. 3.

In addition, the density of states $D(\varepsilon)$ of energy bands for a square lattice can be expressed as follows

$$D(\varepsilon) = \frac{1}{4\pi^2} \int_B \delta [\varepsilon - \varepsilon^{\pm}(k_x, k_y)] \, dk_x dk_y, \quad (35)$$

which describes the number of states per unit energy per unit cell and therefore the function is properly normalized to $\int_B D(\varepsilon) \, d\varepsilon = 2$. Due to the symmetry of spectrum, we have $D(\varepsilon) = D(-\varepsilon)$. Here the densities of states for different $\gamma$ are plotted in Fig. 3. In the vicinity of $k_c$ and considering the case $0 \leq \gamma_c - \gamma \ll J$, Eq. 35 allows

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**FIG. 3.** (color online) 3D plots of band structures of bilayer square lattice with periodic boundary condition. Staggered imaginary potentials $\pm i\gamma$ are applied throughout the lattice and here we set $\lambda = \pm$. The parameters are (a) $T = 5J, \gamma = 0$, (b) $T = 5J, \gamma = 0.98J$, (c) $T = 5J, \gamma = J$. 

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us to derive an approximate expression for the density of states

\[ D(\varepsilon) = \begin{cases} \frac{1}{\pi \sqrt{\varepsilon - \gamma}} & |\varepsilon| \geq \sqrt{\frac{\gamma^2}{4} - \gamma^2} \\ 0 & |\varepsilon| < \sqrt{\frac{\gamma^2}{4} - \gamma^2} \end{cases} \]  

which is a linear function of energy. We plot this expression in Fig. 4 as comparison. It indicates that \( D(\varepsilon) \) shows a semimetallic behavior as that in graphene.

\[ \text{IV. SUMMARY} \]

In conclusion, we have studied the connection between an arbitrary Hermitian tight-binding model with \( C \) symmetry and its non-Hermitian counterpart with \( CT \) symmetry. It has been shown that such a kind of non-Hermitian Hamiltonian is pseudo-Hermitian, providing a way to generate a class of non-Hermitian models with a tunable full real band structure by adding additional imaginary potentials. Based on the exact results, it is found that the eigenvalues and eigenvectors of the non-Hermitian Hamiltonian can be easily obtained from those of its parent Hermitian Hamiltonian. The reality of the spectrum is robust to the disorder due to the protection of energy gap. Furthermore, as an illustrative example, we investigate the band structure of a two-layer square lattice model with staggered imaginary potentials. We find that a tunable valley band structure can be achieved. It should have wide applications in non-Hermitian synthetic graphene-like materials.

\[ \text{ACKNOWLEDGMENTS} \]

We acknowledge the support of the National Basic Research Program (973 Program) of China under Grant No. 2012CB921900 and CNSF (Grant No. 11374163).

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