The topological vacuum in exceptional Brillouin zone

Ye Xiong

Department of Physics and Institute of Theoretical Physics, Nanjing Normal University, Nanjing 210023, P. R. China

The vacuum of a band system, with respect to particles or holes, can become topologically nontrivial when the exceptional points of the non-hermitian Hamiltonian spread over the whole Brillouin zone. The coalescence of the eigenstates eliminates the geometric multiplicity of the Hamiltonian and puts the remaining bands on a topological background. We find several distinct phenomena in these systems: a single band topological model, a two-band Chern insulator in which the topological number of the low band does not compensate to that of the up band, a topologically protected boundary state that is less damping when stronger dissipative forces are subjected and topologically protected in-gap extended states. Our results are presented by the vibrational spectrum on a classical lattice. The active constrains are the key ingredient to collapse the demanding Hilbert subspace.

Introduction.—In condensed matter physics, a band must be topologically trivial when its project operator, \( \hat{P}_n = \sum_k |n(k)\rangle\langle n(k)| \), commutes with the translation operator in the reciprocal space, \( e^{i\delta k} \), where \( |n(k)\rangle \) is the eigenstate of the \( n \)th band, \( \delta k \) is an infinitesimal displacement along the Wilson loops in the Brillouin zone (BZ) \([1,11]\). If there is only one band or counting all bands as a whole (which is the case when the Fermi energy is below or above all the bands), the project operator retrogresses to identity matrix or to zero matrix and the topological number must take trivial value, i.e., the total Zak phase of two bands in 1-dimensional (1D) Su-Schrieffer-Heeger (SSH) model is \( 2n\pi \) (\( n \) is an integer) \([12,16]\) and the Chern number of the entire bands on a 2-dimensional (2D) lattice must be 0 \([15]\). In this article, the above statement can be violated when the non-hermitian Hamiltonian is intrinsically defective in the BZ. The eigenstates will only cover a subspace of the Hilbert space \([15]\), which is referred as the vacuum of band in this article.

Our models are classical vibration lattices made up by mass points (MPs) connected by the springs. The key ingredient is the active constrains (ACs) subjected on each MPs. Compared with the passive constrains, the ACs need extra steps such as measurement and analysis. For instance, in Fig. 1(a), we show the ACs with many measurement instruments. Each MP is rigidly bonded with the pointer of speedometer on the next MP. In the first model, we find a chain with only one band. But its Zak phase is \( \pi \). As there is only one band contributes, only one boundary state is topologically protected. It will stay at either right or left end of the chain. In the absence of the chiral symmetry, the vibration frequency of this boundary state is not 0. But when the frictional forces dominated, an effective chiral symmetry restores. So an interesting phenomenon emerges: as subtracting stronger frictional forces, the damping rate of the boundary state is less. In the second model, we study a 2D lattice with two bands. Each band contributes the Chern number 1 so that the Chern number of the whole bands is 2 instead of 0. The boundary states will not always connect different bands continuously. But in order to compensate the pumped bulk states due to the nonzero Chern number, the boundary state must have a moment to spread to the bulk. So another abnormal behavior appears: the in-gap states are topologically protected to extend to the bulk.

1D lattice model.—The 1D classical lattice is made up by identical MPs with masses \( m = 1 \). Only the movements in the direction along the chain are considered. When ACs are applied, one band will be frozen and only one band persists. After a Fourier transformation, the constrains become \( x_k - e^{i\lambda_k} \dot{x}_k = 0 \). So the states on the vibration band must be

\[
|\psi_k\rangle \equiv \begin{pmatrix} x_k \\ \dot{x}_k \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ e^{-i\lambda_k} \end{pmatrix}.
\]

One should be careful in applying the Lagrange multiplier \( \lambda \). The variational term \( \lambda \) does not appear in the equation of motion. This is because when representing \( \lambda_i \) as the stress force induced by the \( i \)th bond, the reaction force in the bond does not act back to the \((i + 1)\)th MP but to the pointer of the speedometer. After appending the Fourier transformation of \( \lambda_i \) to the MP’s kinetic state \( |\psi_k\rangle \), the equation of motion for \( |\psi'_k\rangle \equiv (x_k, \dot{x}_k, \lambda_k)^T \) is

\[
\begin{pmatrix} 1 & 0 & 0 \\ 0 & m & 0 \\ 0 & 0 & 0 \end{pmatrix} |\psi'_k\rangle = \begin{pmatrix} 0 & 1 & 0 \\ -4K \sin^2(k/2) & -\Gamma & 1 \\ 1 & -e^{i\lambda_k} & 0 \end{pmatrix} |\psi'_k\rangle.
\]

After substituting \( |\psi'_k\rangle = e^{-i\omega t} |\psi'_k(\omega)\rangle \), the eigenfrequency \( \omega \) and the eigenstate \( |\psi'_k(\omega)\rangle \) are found by solving a general eigen-problem likes, \(-i\omega C |\psi'(\omega)\rangle = D |\psi'(\omega)\rangle\), where \( C \) is an irreversible matrix. As \( D \) is reversible, by multiplying \(-D^{-1} i\omega\) from the left, the above equation is equivalent to the eigen-problem of a non-hermitian matrix \(-D^{-1} C, -\frac{1}{\omega} |\psi'_k(\omega)\rangle = -D^{-1} C |\psi'_k(\omega)\rangle\).
FIG. 1. (a) MPs are connected with their nearest neighbors by springs whose spring constant $K = 1$. The ACs, $x_i - x_{i+1} = 0$, rigidly bond the displacement of the $i$th MP with the velocity of the next MP. Each MP feels the restoring force from a strong spring, $\lambda_i \sim -K'(x_i - x_{i+1})$, where $K' = 10^4$ in the calculations. (b) The spectrum when one spring is removed. There is no boundary state. (c) The spectrum when one constrain is removed. One boundary state emerges in this case. Its frequency is mixed with those of bulk states when $\Gamma = 0$. But when increasing $\Gamma$, it approaches to the original point. (d) When both spring and constrain are cut off, the spectrum is largely modified by the skin effect. The insert shows the spectrum near the center of complex plane. The topologically protected boundary state still survives.

The matrix must be right at exceptional point (EP) because, physically, constrains can only freeze vibration modes instead of introducing new ones. For the present 1D model, there are only two eigenvalues, $-1/\omega = e^{i\pi}$ and 0, where the first one is associated with the vibration band $|\psi_k^{(1)}(\omega)\rangle$ and the latter is two fold degenerated with only one corresponding eigenstate (in the frozen band), $|\psi_k^{(2)}(\omega)\rangle$. The part of the eigenstate that describes the motion of the MPs, $|\psi_k^{(1)}(\omega)\rangle$, is obtained by eliminating the stress variable $\lambda_k$ in $|\psi\rangle$. The operator $\sum_k |\psi_k^{(1)}(\omega)\rangle\langle \psi_k^{(1)}(\omega)\rangle$ cannot span the whole phase space and is not identical matrix. Evidently, such operator does not commute with $e^{L_i k}$ so that the single vibration band can have nontrivial topological phase. This problem is more clear when the AC bonds are replaced by strong springs. One immediately realize that the ACs are freezing a band and pushing their frequencies to $\infty$. The Zak phase of the frozen band is also $\pi$. So the problem can be read as: the visible band is left on the remnant of the frozen band.

Actually, the operator $\sum_k |\psi_k^{(1)}(\omega)\rangle\langle \psi_k^{(1)}(\omega)\rangle$ is no longer a project operator on the eigenstates. This leads to the debate on how to define the topological phase in non-hermitian systems. If one insists to define the topological phase from the project operator, the Zak phase should be $I \int_0^{2\pi} dk \langle \langle \psi_k^{(1)} (\omega)| \partial_k |\psi_k^{(1)}(\omega)\rangle\rangle$, where $\langle \langle \psi_k^{(1)}|\rangle\rangle$ are the left eigenstates of the matrix $D^{-1} C$. But this expression includes the contributions from the stress forces. The forces are extra variables which are introduced to complete the equation of motion. They have nothing to do with the phase space of the MPs. Furthermore, in principle, we can introduce similar auxiliary variables as many as possible, e.g., employing more variables like $\alpha_k = \beta_k = \lambda_k$ and appending all of them to $|\psi\rangle$. So there is no reason to count their contributions to the topological phase. Besides that, the above Zak phase is not real in general. If one would like to represent the topological phase back to the relative position of the Wannier function’s center in each unit cell, a complex position value is not acceptable. So in this article, we take the Zak phase as

$$I \int_0^{2\pi} dk \langle \langle \psi_k^{(1)} (\omega)| \partial_k |\psi_k^{(1)}(\omega)\rangle\rangle.$$  \hspace{1cm} (3)

In Fig. (b), (c) and (d), we show the vibration spectrum for a ring with different boundary conditions. A open boundary-like condition can be introduced by: (b) cutting off one spring , (c) cutting off one constrain and (d) cutting off both spring and constrain. In the calculations, we have used the trick by replacing all rigid constrains with the strong springs. The rigid constrains are restored when $K' \to \infty$.

In Fig. (b), with only one spring is cut off, the spectrum is same as that of the perfect ring. This is because the constrains keep restricting the possible vibration modes in the subspace that is identical to the perfect ring. The lost of spring cannot modify the spectrum.

In Fig. (c), when the constrain between the ends is removed, the bulk spectrum is similar to that of the perfect ring. But there is one boundary state at the right end of the chain. This single topologically protected boundary state can be understood by recalling the arguments in the electronic SSH model because their bulk band states
share the same equation. In the topological SSH model, there are two boundary states. Each one is contributed from the up and the low bands half by half. But in the present model, only one band contributes so that there is only half boundary state at each end. But as half states are unstable, they recombine to one state. We also find that its frequency is not zero when \( \Gamma \) is small and is on the imaginary axis. This is because there is no chiral symmetry in the non-hermitian Hamiltonian. But the equation of motion and the ACs are invariant under complex conjugation. So the frequency of the boundary state must stay at the imaginary axis because of \( \omega \to -\omega^* \) symmetry. When the frictional forces dominate, the equation of motion approaches to \( \ddot{x}_i = -\Gamma \dot{x}_i \). Under time reverse operation, this equation changes sign and the ACs become \( x_i + \dot{x}_{i+1} = 0 \). So after combining the time reversed model and the model itself, there are totally two bands and these two bands will mimic those in the SSH model. This means that an effective chiral symmetry restores in the combination and the frequency of the boundary state must be fixed at zero. This is why the damping rate of the boundary state decreases when \( \Gamma \) increases.

In Fig. 2(d), the spectrum is entirely different from that of the perfect ring. All bulk states are squeezed to the ends and their frequencies are largely modified as well. This is the skin effect in non-hermitian system [28–30]. We also found that this skin effect does not obey the Theorem I in Ref. 31 because the Hamiltonian is defective. Near the center of the complex plane, there are two states. One is originated from the topologically protected boundary state and the other is from the vibration mode released by the missing constrain. They hybrid together and can be separated by the frictional forces in bulk.

We know there are two equivalent ways to study topological physics in the hermitian systems: one is on the Hamiltonian, especially on the symmetry of the Hamiltonian and the other is on the Berry phase. One of our motivations is to find what will happen when this equivalence breaks down: there are topological-like eigenstates but the non-hermitian Hamiltonian does not have the corresponding symmetry. The above model shows that the bulk-boundary correspondence still holds. But the number of the boundary states and their frequencies are different from those of the hermitian case. Our next model is to find what will happen when this idea is applied to the 2D Hall system.

2D Hall model. — The 2D model is shown in Fig. 2(a). Here we only study the transverse-mode of the wave. Each unit cell has two MPs (denoted as A and B types of MPs) with the identical mass \( m = 1 \). The ACs are only acted on the B type of MPs by the restriction

\[
B_{\vec{k}} - G(\vec{k}, A_{\vec{k}}, B_{\vec{k}}) = 0,
\]

(4)

where

\[
G = -[\sin(k_x) + I \sin(k_y)]A_{\vec{k}} + [\cos(k_x) + \cos(k_y)]B_{\vec{k}} + \sqrt{(1 - \cos(k_x) - \cos(k_y))^2 + \sin^2(k_x) + \sin^2(k_y)}B_{\vec{k}}.
\]

(5)

Here \( \vec{k} \) is the wave vector and \( A_{\vec{k}}(B_{\vec{k}}) \) is the Fourier’s transformation of the displacements for the A(B) type MPs. Such constrains can be manipulated by the rigid connections between the B type MPs and the pointers of the machines whose outputs are \( G_{i,j} \), where \( G_{i,j} \) is the inverse Fourier’s transformation of \( G(\vec{k}, A_{\vec{k}}, B_{\vec{k}}) \),

\[
G_{i,j} = \frac{1}{2} \left[ I(A_{i+1,j} - A_{i-1,j}) + (A_{i,j-1} - A_{i,j+1}) + (B_{i+1,j} + B_{i-1,j} + B_{i,j+1} + B_{i,j-1}) + \sum_{i_1,j_1} V(i_1,j_1)B_{i-i_1,j-j_1} \right].
\]

(6)

Here \( A_{i,j}(B_{i,j}) \) is the displacement of the A (B) type MPs at the site \( (i,j) \), \( V(i,j) \) is the inverse Fourier’s transformation of \( V(i_1,j_1) \) and the summation is over all 2D lattices. As shown in Fig. 2 (b), \( V(i,j) \) decreases rapidly when \( i \) and \( j \) are away from the origin. The imaginary number \( I \) in Eq. 6 can be realized by a \( \pi/2 \) phase shift in the machines.

We have calculated the vibration spectrum using the same trick introduced in the 1D case. The ACs freeze...
two bands and leave us with another two bands. They are also calculated the Chern number of each band by watching the Wannier function’s center as the function of \( k_x \), 
\[
\Phi(k_x) = \int dk_y \langle \psi_n(k_x, k_y) | i \frac{\partial}{\partial k_y} | \psi_n(k_x, k_y) \rangle,
\]
where \( |\psi_n\rangle \) is the kinetic state of the MPs for the \( n \)th band. As Fig. 2(d) shows, the Chern number of each band is 1. The figure also implies that the Chern numbers for the two frozen bands are 0. Interestingly, even after counting the contributions from the frozen bands, the total Chern number is 2 instead of 0. This is different from that in the 1D case.

![Figure 3](image)

**FIG. 3.** The spectrum for a 2D stripe. The width is \( W = 20 \). The data of the boundary states within the gap are closely spaced for the sake of clarity (the data are pasted from the calculation with higher density \( k_x \)). The spring constant and other parameters are the same as those in Fig. 2. The frictional coefficient is (a) \( \Gamma = 0 \), (b) 1.7 and (c) 2. The blue regions indicate that the states in them are extended in bulk.

Finally, the edge states are studied. Like that in the 2D quantum Hall effect, we consider an infinitely long stripe. It is placed along the \( x \) axis so that \( k_x \) is good number. All connections, including the springs and the components of the ACs, those across the edges are cut off. As Fig. 2 shows, unlike that in the quantum Hall effect, the boundary states do not link the two bands when \( \Gamma \) is small. Also the open boundary condition does not modify the bulk spectrum. So the nonzero Chern number of the bulk bands should topologically protect the existence of the boundary states. These two phenomena seem controversial when adopting the discussion from the quantum Hall effect: as \( k_x \) is varying by \( 2\pi \), one bulk state is pumped from one edge to the other and the energies of the edge states must cross over the gap to compensate this extra pumped state. Otherwise, the system is not periodic along \( k_x \) anymore. But our data clearly illustrate a different picture. It is more like a situation (not really exist) in quantum Hall effect that the neighboring bands disappear and spectrum of the edge states are connected by themselves. But in quantum Hall effect, they cannot be connected because the states are on the different edges. The above argument implies us to check the eigen-states of these boundary states. Interestingly, we find that they do become extended in the blue regions. So the situation changes to: as \( k_x \) is varying by \( 2\pi \), one bulk state is pumped to the edge while the boundary states dissipate the state back to the bulk. In doing so, the boundary states in the gap need to be extended in bulk at sometime. This is the topological reason behind the in-gap extended states.

**Discussions.**— Due to the skin effect in non-hermitian systems, it is known that the bulk-boundary correspondence cannot be applied directly because the topology of bulk states in the \( k \) space is different from that of skin states in the presence of open boundary.\[32–36\]. But in most cases of this article, the bulk spectrum does not change dramatically when the boundaries are introduced. So our discussions on the correspondence between boundary states and topology of the bulk states are still valid.

The models we presented here are different from the classical isostatic lattices proposed by Kane and coworkers\[37, 38\], where the passive constrains are subjected to the lattice and freeze all bulk vibration modes. Mostly, the topological index is winding number in any dimension and the topological boundary states are zero frequency modes. While in the above models, it is the ACs that split the Hilbert space into two twisted subspaces, the allowed and the forbidden subspaces. The bulk vibration states can still survive in the allowed subspace. The topological index is Zak phase, Chern number and others. The models are also different from the topological acoustic structures induced by strain\[39–42\], or Coriolis force\[43–45\].

The models imply that the topology of a band can be richer than those in the hermitian and the undefective non-hermitian systems. When the whole BZ becomes exceptional, the Hamiltonian and its symmetry cannot uniquely determine the topology and one needs to look back upon the truncated wave-functions. The aggregate of topological systems is greatly enlarged in this case.

**Acknowledgments.**— The work was supported by National Foundation of Natural Science in China Grant Nos. 10704040.
