

Topology and geometry in topological singularities

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Motivation

Hamiltonian is a matrix corresponding to the system we considered.

$$\text{Hamiltonian } H = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} \begin{cases} \text{eigenvalue: energy} \\ \text{eigenvector: state} \end{cases}$$

If Hamiltonian is parametrized, such as parametrized by temperature T :

$$H(T) = \begin{bmatrix} a_{11}(T) & a_{12}(T) & a_{13}(T) \\ a_{21}(T) & a_{22}(T) & a_{23}(T) \\ a_{31}(T) & a_{32}(T) & a_{33}(T) \end{bmatrix}$$

We can draw the energy band

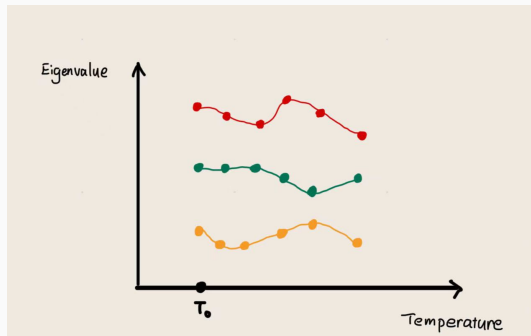


Figure 1: Energy bands

n -band: n is the number of eigenvalues

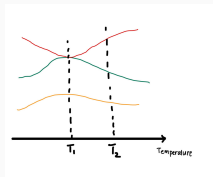


Figure 2: Gapless or Gapped

T_1 : singular points (points where eigenvalues degenerate)

$H(T_1)$: gapless Hamiltonian

$H(T_2)$: gapped Hamiltonian

Exotic phenomena emerge at singular points, so whether a loop in parameter space touches singular points is considerable.

Consider the matrix

$$H = \begin{bmatrix} f_3 & f_2 \\ -f_2 & -f_3 \end{bmatrix}$$

$$f_3, f_2 \in \mathbb{R}$$

Draw the degeneracy line:

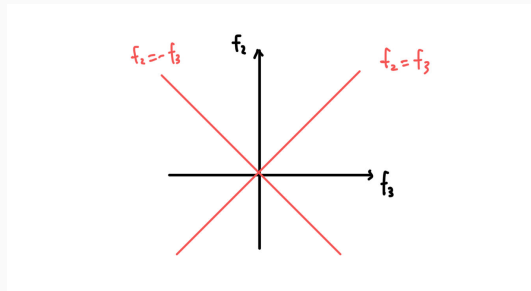
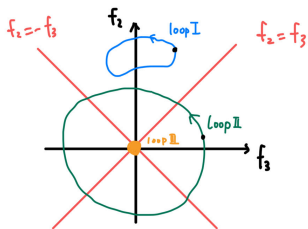


Figure 3: Degeneracy line



The following numbers means the number of eigenvalues

- Type I: 2
- Type II: $2 \rightarrow 1 \rightarrow 2 \rightarrow 1 \rightarrow 2 \rightarrow 1 \rightarrow 2 \rightarrow 1 \rightarrow 2$
- Type III: 1

Goal: Algebraic topology (computable invariants) for those loops to classify the evolution of eigenvalues and eigenstates.

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There are many cases: Hermitian/non-Hermitian, 2-band/3-band/ n -band, whether loop can intersect singular points, \dots

D_2 -bundle over $SO(3)/D_2$

Physical picture for this bundle

- A 3-band gapped Hermitian Hamiltonian can be written as $H = \sum_{j=1}^3 j |u^j\rangle \langle u^j|$
- H can be determined by a set of “right hand” orthonormal vectors $(|u^1\rangle, |u^2\rangle, |u^3\rangle)$ form an element in $SO(3)$
H is unchanged for two of eigenvectors flip: $|u^j\rangle \mapsto -|u^j\rangle$ (modulo D_2).
- H can be describe by $SO(3)/D_2$

Consider the bundle

$$D_2 \hookrightarrow SO(3) \xrightarrow{\pi} SO(3)/D_2 =: X, \quad \pi(x) = \bar{x}$$

Goal: The isomorphism classes of principal D_2 -bundles over X are denoted by $Prin_{D_2}(X)$ and $Prin_{D_2}(X) \simeq [X, BD_2]$ where BD_2 is the classifying space of D_2 . The following will show which $\phi \in [X, BD_2]$ corresponds to the principal D_2 -bundle we considered.

We need to find $\phi : X \rightarrow Gr_1(\mathbb{R}^\infty) \times Gr_1(\mathbb{R}^\infty)$, such that $\pi : SO(3) \rightarrow X$ appears in the pullback of ϕ and $f \times f$:

$$\begin{array}{ccc}
 SO(3) & \longrightarrow & V_1(\mathbb{R}^\infty) \times V_1(\mathbb{R}^\infty) = ED_2 \\
 \downarrow \pi & & \downarrow f \times f \\
 X & \xrightarrow{\phi} & Gr_1(\mathbb{R}^\infty) \times Gr_1(\mathbb{R}^\infty) = BD_2
 \end{array}$$

Claim: $\phi : SO(3)/D_2 \rightarrow Gr_1(\mathbb{R}^\infty) \times Gr_1(\mathbb{R}^\infty)$ is

$$\phi \left(\overline{\begin{bmatrix} a \\ b \\ c \end{bmatrix}} \right) = (span \left(\begin{bmatrix} a & 0 & 0 & \cdots \end{bmatrix} \right), span \left(\begin{bmatrix} b & 0 & 0 & \cdots \end{bmatrix} \right))$$

The pullback of ϕ and $f \times f$ is constructed as:

$$S = X \times_{BD_2} ED_2 = \left\{ \left(\overline{\begin{bmatrix} a \\ b \\ c \end{bmatrix}}, (v_1, v_2) \right) \mid \overline{\begin{bmatrix} a \\ b \\ c \end{bmatrix}} \in X, (v_1, v_2) \in V_1(\mathbb{R}^\infty) \times V_1(\mathbb{R}^\infty), \right. \\ \left. \text{span} \left(\begin{bmatrix} a & 0 & 0 & \cdots \end{bmatrix} \right) = \text{span}(v_1), \text{span} \left(\begin{bmatrix} b & 0 & 0 & \cdots \end{bmatrix} \right) = \text{span}(v_2) \right\}$$

Since v_1, v_2 are orthonormal, we have $v_1 = [\pm a, 0, 0, \dots]$, $v_2 = [\pm b, 0, 0, \dots]$.

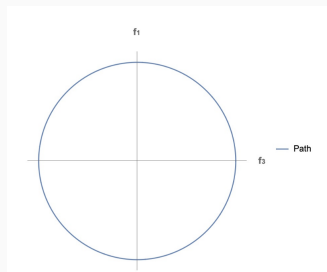
2-band Hermitian systems

Set-up for Hermitian systems

For a Hermitian system, denote the matrix and the eigenvalues by

$$H'_2 = H'_2(f_1, f_3) = \begin{bmatrix} f_3 & f_1 \\ f_1 & -f_3 \end{bmatrix}, \omega'_\pm = \pm \sqrt{f_1^2 + f_3^2}.$$

It has two distinct eigenvalues when $(f_3, f_1) \neq (0, 0)$. So a parameter space for this Hamiltonian H'_2 is $\mathbf{R}^2 - \{(0, 0)\}$:



Hermitian system

For a Hermitian system, $H'_2 = H'_2(f_1, f_3) = \begin{bmatrix} f_3 & f_1 \\ f_1 & -f_3 \end{bmatrix}$, the eigenvalues

$$\omega'_\pm = \pm \sqrt{f_1^2 + f_3^2}.$$

Let $U_1 = \{\mathbf{R}^2 - \{(f_3, 0), f_3 \leq 0\}\}$, $U_2 = \{\mathbf{R}^2 - \{(f_3, 0), f_3 \geq 0\}\}$, then we know that $U_1 \cup U_2 = \mathbf{R}^2 - \{(0, 0)\}$.

In U_1 , the corresponding eigenvectors are

$$v'_+ = \frac{1}{\sqrt{2(f_1^2 + f_3^2) + 2f_3\sqrt{f_1^2 + f_3^2}}} \begin{bmatrix} f_3 + \sqrt{f_1^2 + f_3^2} \\ f_1 \end{bmatrix},$$

$$v'_- = \frac{1}{\sqrt{2(f_1^2 + f_3^2) + 2f_3\sqrt{f_1^2 + f_3^2}}} \begin{bmatrix} -f_1 \\ f_3 + \sqrt{f_1^2 + f_3^2} \end{bmatrix}.$$

In U_2 ,

$$v'_+ = \frac{1}{\sqrt{2(f_1^2 + f_3^2) - 2f_3\sqrt{f_1^2 + f_3^2}}} \begin{bmatrix} f_1 \\ -f_3 + \sqrt{f_1^2 + f_3^2} \end{bmatrix},$$

$$v'_- = \frac{1}{\sqrt{2(f_1^2 + f_3^2) - 2f_3\sqrt{f_1^2 + f_3^2}}} \begin{bmatrix} f_3 - \sqrt{f_1^2 + f_3^2} \\ f_1 \end{bmatrix}.$$

The transition map of v'_+, v'_- is

$$t_{\pm} = \begin{cases} 1, & f_1 > 0 \\ -1, & f_1 < 0 \end{cases}, \quad (1)$$

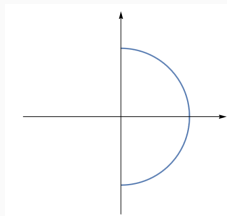
$$v'_+ = \frac{1}{\sqrt{2(f_1^2 + f_3^2) - 2f_3\sqrt{f_1^2 + f_3^2}}} \begin{bmatrix} f_1 \\ -f_3 + \sqrt{f_1^2 + f_3^2} \end{bmatrix},$$

Notice that v'_+, v'_- are invariant under scaling $(f_3, f_1) \mapsto (\lambda f_3, \lambda f_1)$ for $\lambda \in \mathbf{R}_{>0}$, so the normalized eigenbundle is of the form $\pi : \mathbf{R}_{>0} \times E \rightarrow \mathbf{R}_{>0} \times S^1$, where E is a principal S^0 -bundle over S^1 .

There are only two principal S^0 -bundles over S^1 (up to isomorphism). The total space is a connected space, so the bundle is isomorphic to a Hopf bundle $S^0 \hookrightarrow S^1 \rightarrow S^1$.

Hermitian system

If we let $(f_3, f_1) \in U_1$ varies along the path $\{f_3^2 + f_1^2 = 1\}$, we may assume $(f_3, f_1) = (\cos \theta, \sin \theta)$, where $\theta \in [-\frac{\pi}{2}, \frac{\pi}{2}]$.



Then $\omega'_+ = 1, \omega'_- = -1$, and the eigenvectors can be written as:

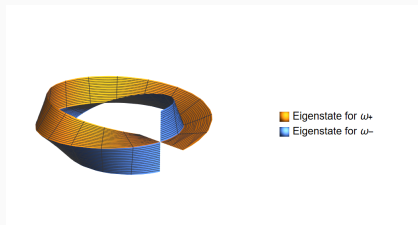
$$v'_+ = \begin{bmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{bmatrix}, \quad v'_- = \begin{bmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{bmatrix}.$$

Hermitian system

Similarly, let $(f_3, f_1) \in U_2$ varies along the path $\{f_3^2 + f_1^2 = 1\}$, assume $(f_3, f_1) = (\cos \theta, \sin \theta)$, where $\theta \in [\frac{\pi}{2}, \frac{3\pi}{2}]$. We can know that

$$v'_+ = \begin{bmatrix} \cos \frac{\theta}{2} \\ \sin \frac{\theta}{2} \end{bmatrix}, \quad v'_- = \begin{bmatrix} -\sin \frac{\theta}{2} \\ \cos \frac{\theta}{2} \end{bmatrix}.$$

Hence, we can see that the eigenstates of a Hermitian system can be visualized as:



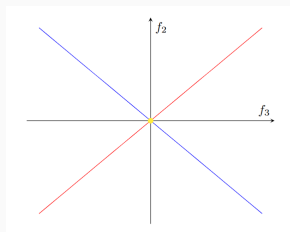
2-band non-Hermitian systems

Set-up for Non-Hermitian systems

For a non-Hermitian system, denote the matrix and the eigenvalues by

$$H_2 = H_2(f_2, f_3) = \begin{bmatrix} f_3 & f_2 \\ -f_2 & -f_3 \end{bmatrix}, \omega_{\pm} = \pm \sqrt{f_3^2 - f_2^2}.$$

It has a double root if and only if $f_2 = \pm f_3$. As a parameter space for this Hamiltonian H_2 , the $f_2 f_3$ -plane becomes a stratified space:



Non Hermitian system

For a non-Hermitian system, $H_2 = H_2(f_2, f_3) = \begin{bmatrix} f_3 & f_2 \\ -f_2 & -f_3 \end{bmatrix}$, $\omega_{\pm} = \pm \sqrt{f_3^2 - f_2^2}$.

Let $W_1 = \mathbf{R}^2 - \{(f_3, 0), f_3 \leq 0\}$, $W_2 = \mathbf{R}^2 - \{(f_3, 0), f_3 \geq 0\}$, then we know that $W_1 \cup W_2 = \mathbf{R}^2 - \{(0, 0)\}$.

In W_1 ,

$$v_+ = \frac{1}{\|*\|} \begin{bmatrix} -f_3 - \sqrt{f_3^2 - f_2^2} \\ f_2 \end{bmatrix}, v_- = \frac{1}{\|*\|} \begin{bmatrix} -f_2 \\ f_3 + \sqrt{f_3^2 - f_2^2} \end{bmatrix}.$$

In W_2 ,

$$v_+ = \frac{1}{\|*\|} \begin{bmatrix} -f_2 \\ f_3 - \sqrt{f_3^2 - f_2^2} \end{bmatrix}, v_- = \frac{1}{\|*\|} \begin{bmatrix} f_3 - \sqrt{f_3^2 - f_2^2} \\ -f_2 \end{bmatrix}.$$

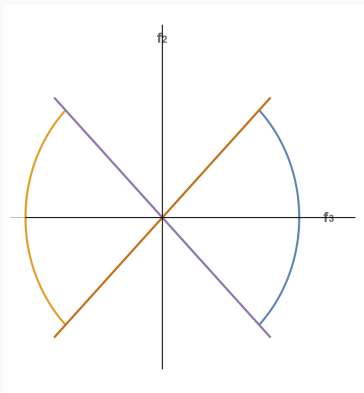
And the transition map of v_+ from W_1 to W_2 can be written by

$$t_+ = \begin{cases} 1, & f_2 > 0 \\ -1, & f_2 < 0 \end{cases} \quad (2)$$

Meanwhile, the transition map t_- of v_- from W_1 to W_2 has the same formula as v_+ .

Real eigenvalues

We first consider the situation when two eigenvalues are real, i.e, $f_3^2 - f_2^2 > 0$.
Again, let (f_3, f_2) varies along the path $\{f_3^2 + f_2^2 = 1\}$.



$$\text{In } W_1 \cap \{f_3^2 + f_2^2 = 1\} \cap \{f_3^2 - f_2^2 > 0\},$$

$$v_+ = \frac{1}{\sqrt{2f_3^2 + 2f_3\sqrt{f_3^2 - f_2^2}}} \begin{bmatrix} -f_3 - \sqrt{f_3^2 - f_2^2} \\ f_2 \end{bmatrix},$$

$$v_- = \frac{1}{\sqrt{2f_3^2 + 2f_3\sqrt{f_3^2 - f_2^2}}} \begin{bmatrix} -f_2 \\ f_3 + \sqrt{f_3^2 - f_2^2} \end{bmatrix}.$$

Figure

First if we look in a 2-dimensional plane, when θ ranges from $-\frac{\pi}{4}$ to $\frac{\pi}{4}$, we have

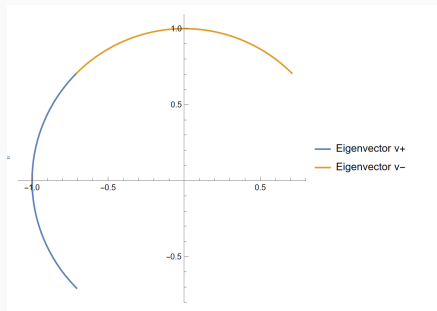
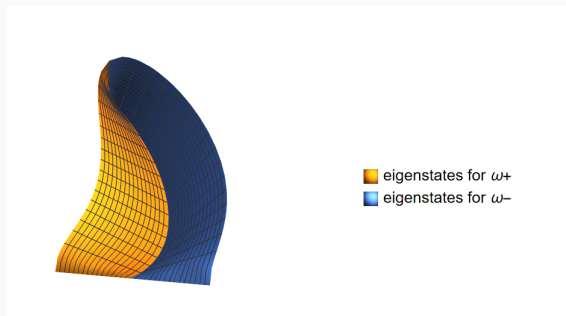


Figure 4: When $\theta = -\frac{\pi}{4}$, $v_+ = -v_-$, then v_+ travels clockwise while v_- travels counterclockwise, When $\theta = 0$, $v_+ \perp v_-$, and $v_+ = v_-$ when $\theta = \frac{\pi}{4}$.

Figure

Moreover, the eigenbundle can be then visualized as below.



Similarly, when θ ranges from $\frac{3\pi}{4}$ to $\frac{5\pi}{4}$,

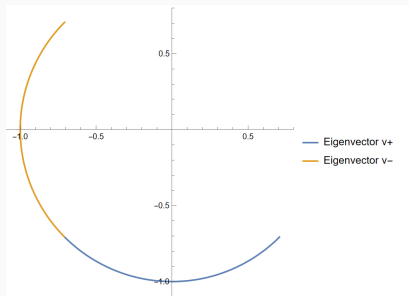
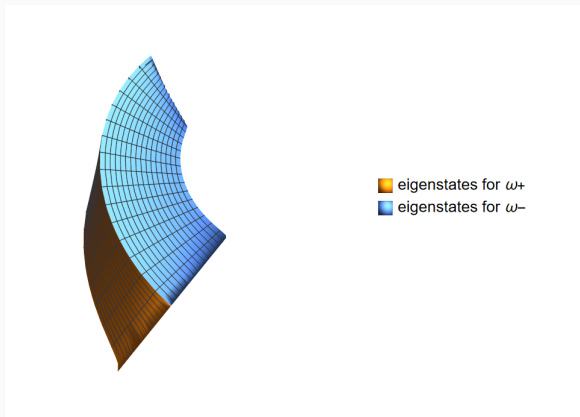


Figure 5: When $\theta = \frac{3\pi}{4}$, $v_+ = v_-$, then v_+ travels counterclockwise while v_- travels clockwise, When $\theta = \pi$, $v_+ \perp v_-$, and $v_+ = -v_-$ when $\theta = \frac{5\pi}{4}$.

For the part where θ ranges from $\frac{3\pi}{4}$ to $\frac{5\pi}{4}$, we can visualize it in a same manner.



Put them together, we can get:

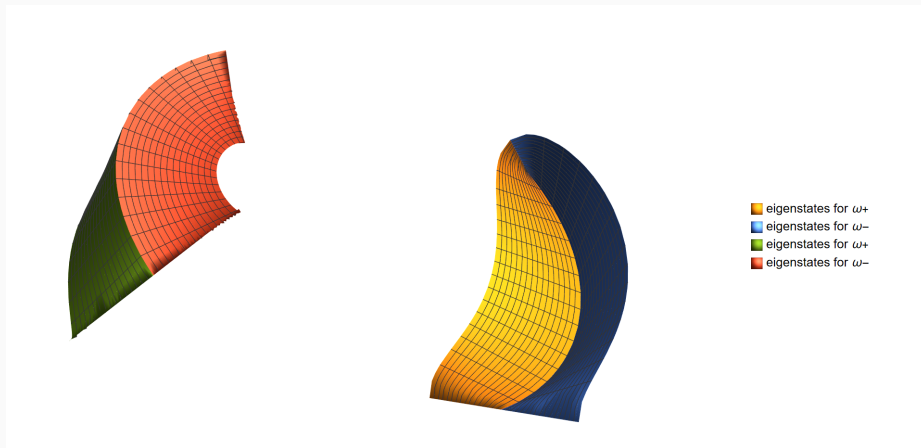


Figure 6: The right one corresponds to $\theta \in [-\frac{\pi}{4}, \frac{\pi}{4}]$, and the left one corresponds to $\theta \in [\frac{3\pi}{4}, \frac{5\pi}{4}]$.

If $f_2^2 - f_3^2 < 0$, two eigenvalues then become pure imaginary number, i.e.,

$$\omega_+ = i\sqrt{f_2^2 - f_3^2}, \quad \omega_- = -i\sqrt{f_2^2 - f_3^2}.$$

The two corresponding eigenvectors have the form of

$$v_+ = \frac{1}{\sqrt{2}|f_2|} \begin{bmatrix} -f_3 - i\sqrt{f_2^2 - f_3^2} \\ f_2 \end{bmatrix}, \quad v_- = \frac{1}{\sqrt{2}|f_2|} \begin{bmatrix} -f_3 + i\sqrt{f_2^2 - f_3^2} \\ f_2 \end{bmatrix}.$$

Angles in complex vectors

Let $\vec{a} = (a_1, a_2, \dots, a_n)$, $\vec{b} = (b_1, b_2, \dots, b_n)$, where $a_i, b_j \in \mathbf{C}$.

$\vec{A} = (A_1, A_2, \dots, A_{2n})$, $\vec{B} = (B_1, B_2, \dots, B_{2n})$, where $A_{2i-1} = \text{Re}(a_i)$, $A_{2i} = \text{Im}(a_i)$, $B_{2i-1} = \text{Re}(b_i)$, $B_{2i} = \text{Im}(b_i)$.

- Euclidean angle: $\cos(\vec{a}, \vec{b}) = \frac{(\vec{A}, \vec{B})}{|\vec{A}||\vec{B}|}$.

- Hermitian angle

Recall the Hermitian inner product of \vec{a}, \vec{b} is $(\vec{a}, \vec{b})_{\mathbf{C}} = \sum_{i=1}^n a_i \overline{b_i}$, it is a complex number, so we may assume $\frac{(\vec{a}, \vec{b})_{\mathbf{C}}}{|\vec{a}||\vec{b}|} = \rho e^{i\psi}$, where $0 < \rho \leq 1$ and $0 \leq \psi \leq 2\pi$.

Hence Hermitian angle: $\cos_H(\vec{a}, \vec{b}) = \rho$.

- Pseudo-angle is defined to be ψ .

- Kähler angle

Let $\vec{A}' = (-A_2, A_1, \dots, -A_{2n}, A_{2n-1})$, $\vec{B}' = (-B_2, B_1, \dots, -B_{2n}, B_{2n-1})$, where $A_{2i-1} = \operatorname{Re}(a_i)$, $A_{2i} = \operatorname{Im}(a_i)$, $B_{2i-1} = \operatorname{Re}(b_i)$, $B_{2i} = \operatorname{Im}(b_i)$.

Then

$$\cos_K(\vec{a}, \vec{b}) \sin(\vec{a}, \vec{b}) = \cos_K(\vec{A}, \vec{B}) \sin(\vec{A}, \vec{B}) = \cos(\vec{A}', \vec{B}').$$

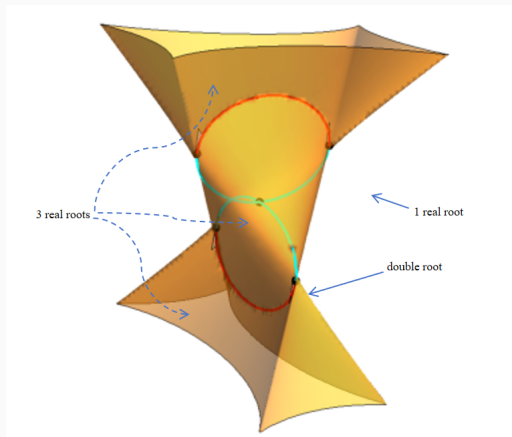
The Hermitian product of v_+ and v_-

$$\langle v_+, v_- \rangle = \frac{f_3}{f_2} \left(\frac{f_3}{f_2} + i \sqrt{1 - \left(\frac{f_3}{f_2} \right)^2} \right).$$

If we consider the Hermitian angle of v_+ and v_- , then we know $\cos_H \langle v_+, v_- \rangle = \left| \frac{f_3}{f_2} \right|$.
The Kähler angle of two real vectors is $\frac{\pi}{2}$.

3-band non-Hermitian systems

3-band non-Hermitian systems



$$H[f_1, f_2, f_3] = \begin{bmatrix} 1 & f_1 & f_2 \\ -f_1 & -1 & f_3 \\ -f_2 & f_3 & -1 \end{bmatrix}$$

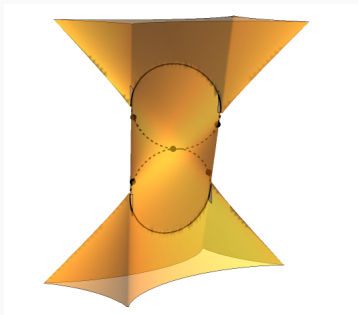
3-band non-Hermitian systems

- 4 NLs and 2 NILs

They are two circles:

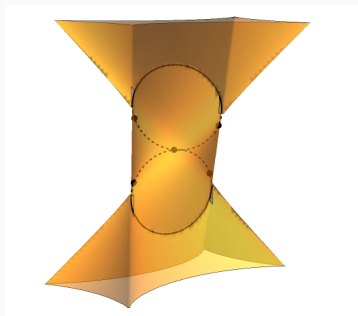
$$\begin{cases} f_1 = \cos t \\ f_2 = -\cos t \\ f_3 = 1 + \sin t \end{cases}, t \in [0, 2\pi)$$

$$\begin{cases} f_1 = \cos t \\ f_2 = \cos t \\ f_3 = -1 + \sin t \end{cases}, t \in [0, 2\pi)$$



3-band non-Hermitian systems

- 5 MPs



$$(0, 0, 0)$$

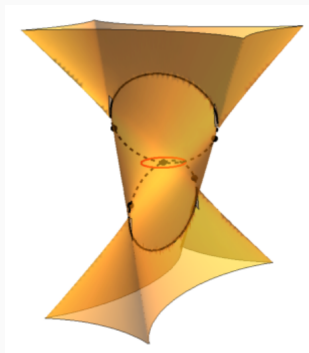
$$\left(\frac{2\sqrt{2}}{3}, -\frac{2\sqrt{2}}{3}, \frac{2}{3}\right)$$

$$\left(-\frac{2\sqrt{2}}{3}, \frac{2\sqrt{2}}{3}, \frac{2}{3}\right)$$

$$\left(\frac{2\sqrt{2}}{3}, \frac{2\sqrt{2}}{3}, -\frac{2}{3}\right)$$

$$\left(-\frac{2\sqrt{2}}{3}, -\frac{2\sqrt{2}}{3}, -\frac{2}{3}\right)$$

Loop1



$$\begin{cases} f_1 = \frac{1}{2} \cos t \\ f_2 = \frac{1}{2} \sin t \\ f_3 = 0 \end{cases}, t \in [0, 2\pi)$$

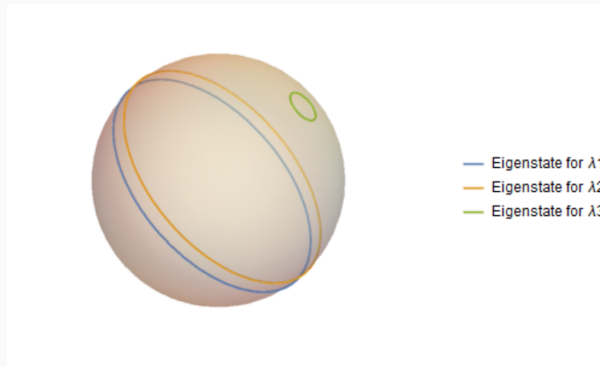
The eigenvalues are

$$\lambda_1 = -1, \lambda_2 = -\frac{\sqrt{3}}{2}, \lambda_3 = \frac{\sqrt{3}}{2},$$

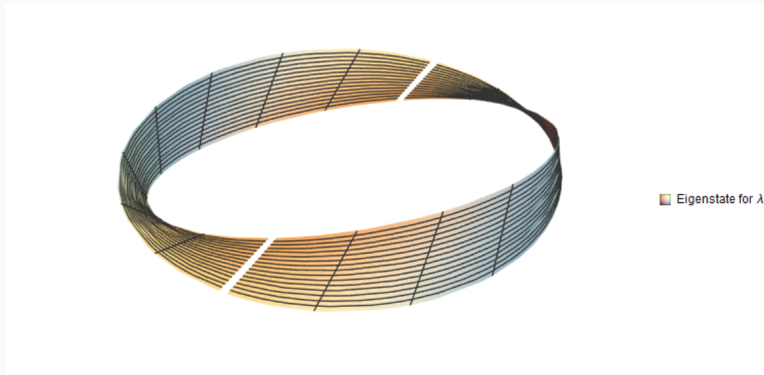
and the corresponding eigenvectors are

$$v_1 = \begin{pmatrix} 0 \\ -\tan t \\ 1 \end{pmatrix}, v_2 = \begin{pmatrix} (\sqrt{3} - 2) \csc t \\ \cot t \\ 1 \end{pmatrix}, v_3 = \begin{pmatrix} -(\sqrt{3} + 2) \csc t \\ \cot t \\ 1 \end{pmatrix}$$

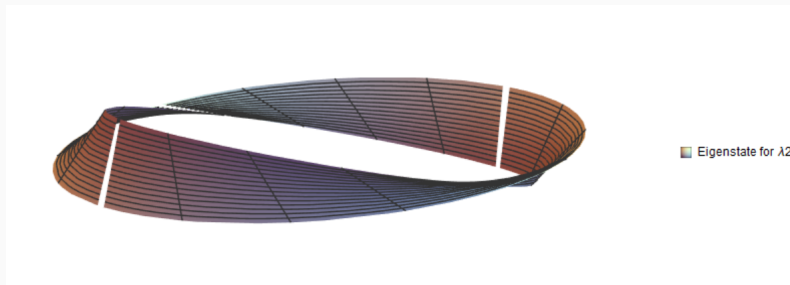
Traces of eigenstates



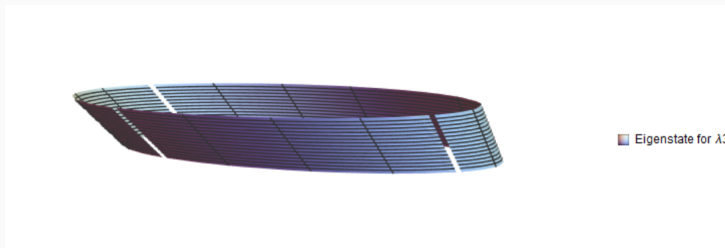
Vector bundles of Loop1

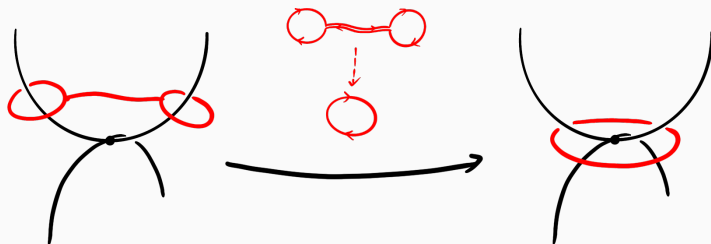


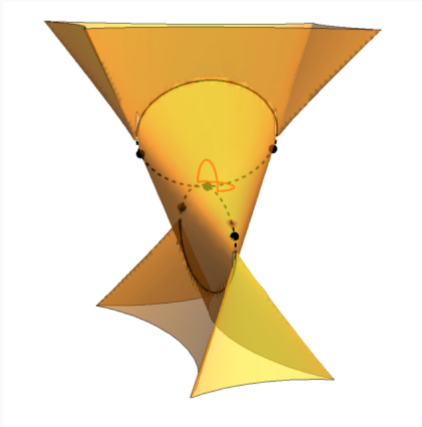
Vector bundles of Loop1



Vector bundles of Loop1



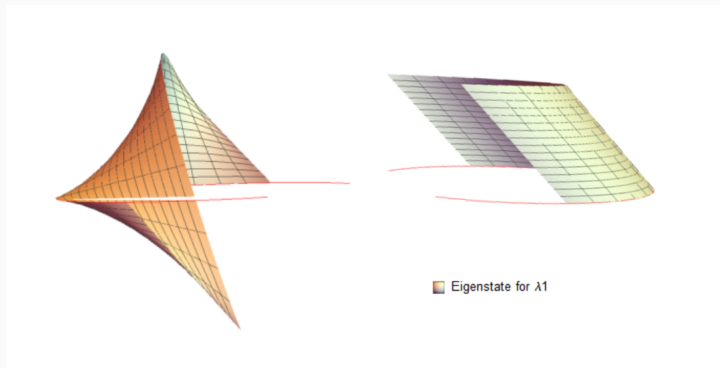




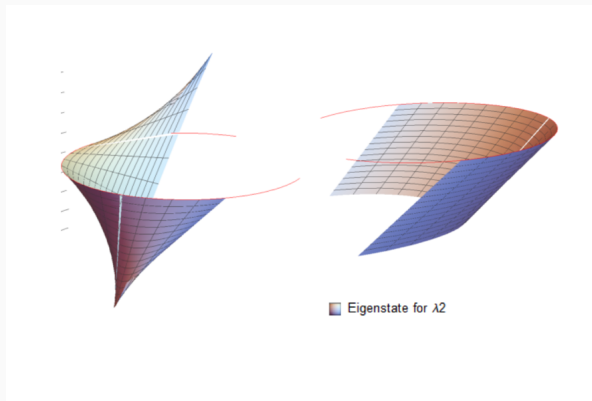
$$\begin{cases} f_1 = \frac{1}{2} \cos\left(\frac{1}{4}\pi + t\right) \\ f_2 = \frac{1}{2} \sin\left(\frac{1}{4}\pi + t\right) , t \in [0, \pi) \\ f_3 = 0 \end{cases}$$

$$\begin{cases} f_1 = \frac{1}{2\sqrt{2}} \cos t \\ f_2 = \frac{1}{2\sqrt{2}} \cos t , t \in [\pi, 2\pi) \\ f_3 = -\frac{1}{2} \sin t \end{cases}$$

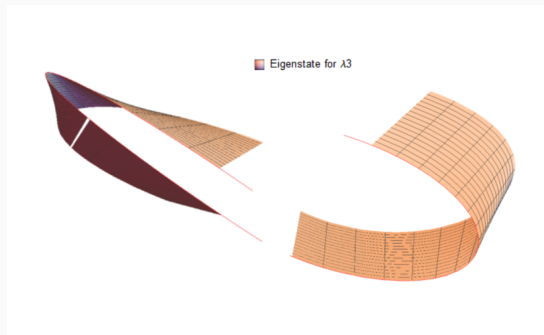
Vector bundles of Loop2

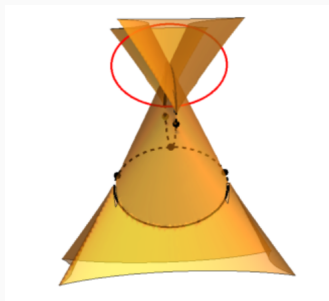


Vector bundles of Loop2



Vector bundles of Loop2





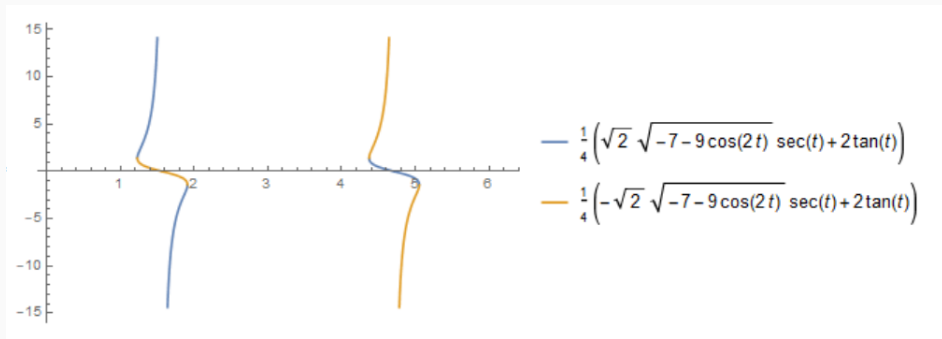
$$\begin{cases} f_1 = \cos t \\ f_2 = \cos t \\ f_3 = 2 + \sin t \end{cases}, t \in [0, 2\pi)$$

The corresponding eigenvectors are

$$v_1 = \begin{pmatrix} 0 \\ -1 \\ 1 \end{pmatrix}, v_2 = \begin{pmatrix} \frac{1}{4}(\sqrt{-14 - 18 \cos 2t} \sec t + 2 \tan t) \\ 1 \\ 1 \end{pmatrix}$$

$$v_3 = \begin{pmatrix} \frac{1}{4}(-\sqrt{-14 - 18 \cos 2t} \sec t + 2 \tan t) \\ 1 \\ 1 \end{pmatrix}$$

Loop3



1. Principal bundles, Hopf bundles and eigenbundles, Barbara Roos.
https://www.math.uni-tuebingen.de/de/forschung/maphy/personen/dr-barbara-roos/doc/theses/roos_semester_project.pdf
2. Non-Abelian band topology in noninteracting metals, Wu, QuanSheng and Soluyanov, Alexey A. and Bzdušek, Tomáš.
3. Angles in Complex Vector Spaces, Scharnhorst, K.

Thanks!