Topology and geometry of singularities

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May 22, 2024

Motivation

Physical background

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

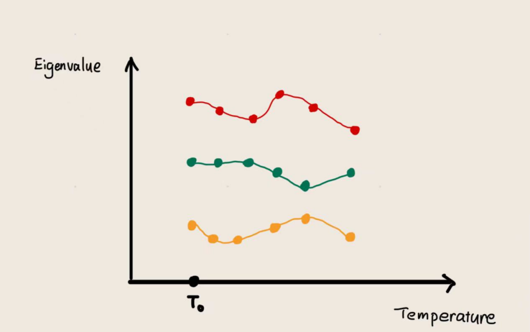


Figure 1: Energy bands

n-band: n is the number of eigenvalues

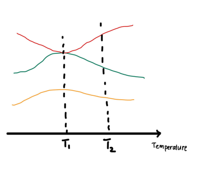


Figure 2: Gapless or Gapped

T_1: singular points (points where eigenvalues degenerate)

$H(T_1)$: gapless Hamiltonian

$H(T_2)$: gapped Hamiltonian

Exotic phenomina 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:

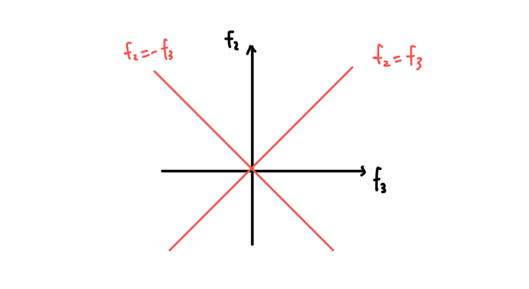
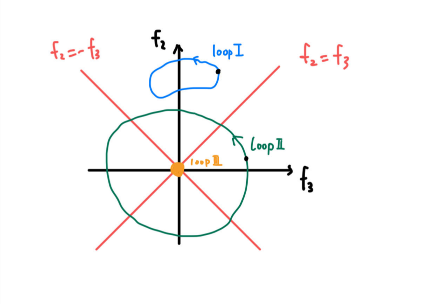


Figure 3: Degeneracy line



The following numbers means the number of eigenvalues

- Type I: 2
- Type II: $2 \to 1 \to 2 \to 1 \to 2 \to 1 \to 2 \to 1 \to 2$
- 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,$\cdots$

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

Physical picture for this bundle

- A 3-band gapped Hermitian Hamiltonian can be written as $H = \sum_{j=1}^{3} j \left|u^j\right\rangle \left\langle u^j\right|$
- H can be determined by a set of "right hand" orthonormal vectors ($\left|u^1\right\rangle$, $\left|u^2\right\rangle$, $\left|u^3\right\rangle$ form an element in $SO(3)$)
  H is unchanged for two of eigenvectors flip:$\left|u^j\right\rangle \mapsto -\left|u^j\right\rangle$(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 $\phi : X \to Gr_1(\mathbb{R}^\infty) \times Gr_1(\mathbb{R}^\infty)$, such that $\pi : SO(3) \to X$ appears in the pullback of ϕ and $f \times f$:

$$\begin{tikzcd} SO(3) \arrow[r] \arrow[d, "\pi"] & V_1(\mathbb{R}^\infty) \times V_1(\mathbb{R}^\infty) = ED_2 \arrow[d, "f \times f"] \\ X \arrow[r, "\phi"'] & Gr_1(\mathbb{R}^\infty) \times Gr_1(\mathbb{R}^\infty) = BD_2 \end{tikzcd}$$

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

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

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

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

$$\operatorname{span} \left(\begin{bmatrix} a & 0 & 0 & \cdots \end{bmatrix} \right) = \operatorname{span} \left(v_1 \right), \operatorname{span} \left(\begin{bmatrix} b & 0 & 0 & \cdots \end{bmatrix} \right) = \operatorname{span} \left(v_2 \right) \}$$

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

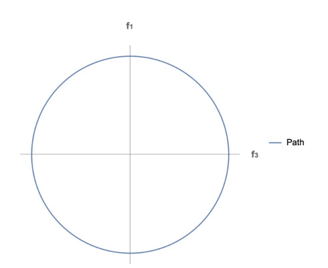
2-band Hermitian systems

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

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

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

Hermitian system

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

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

Hopf bundle

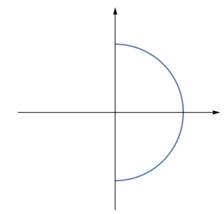
$$v_+' = \frac{1}{\sqrt{2(f_1^2+f_3^2) - 2f_3\sqrt{f_1^2+f_3^2}}} \begin{bmatrix} f_1 \\ -f_3 + \sqrt{f_1^2+f_3^2} \end{bmatrix},$$

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 $\pi : \mathbf{R}_{>0} \times E \to \mathbf{R}_{>0} \times S^1$, 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 $S^0 \hookrightarrow S^1 \to S^1$.

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:

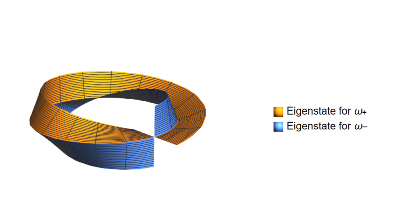
$$v_+^{'} = \begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{bmatrix}, \quad v_-^{'} = \begin{bmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{bmatrix}.$$

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:



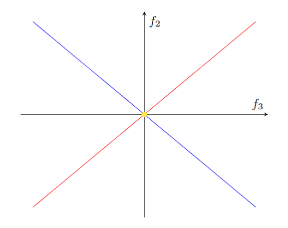
2-band non-Hermitian systems

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 $W_1 = \mathbf{R}^2 - \{(f_3, 0), f_3 \leq 0\}, \quad W_2 = \mathbf{R}^2 - \{(f_3, 0), f_3 \geq 0\}$, 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,

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

Non Hermitian system

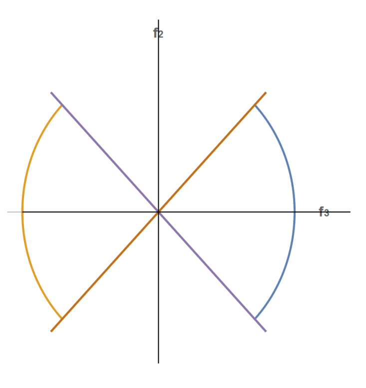
And the transition map of v_+ from W_1 to W_2 can be written by

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

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 $\{f_3^2 + f_2^2 = 1\}$.



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

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

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

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

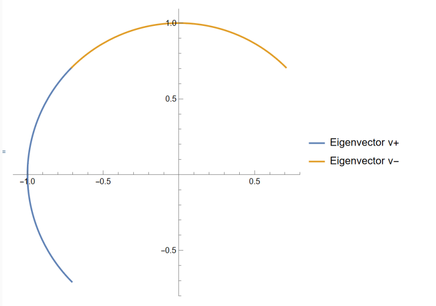
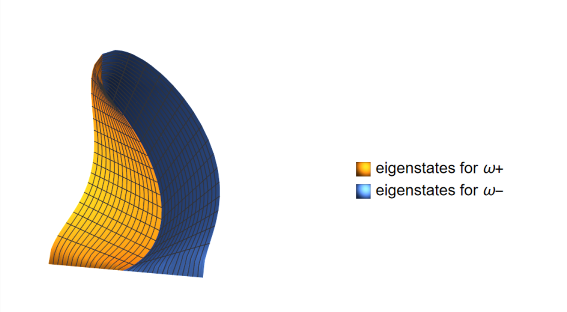


Figure 4: When $\theta = -\frac{\pi}{4}$, $v_+ = -v_-$,then v_+ travels clockwise while v_- travels counterclockwise, When $\theta = 0$, $v_+ \perp v_-$, and $v_+ = v_-$ when $\theta = \frac{\pi}{4}$.

Figure

Moreover, the eigenbundle can be then visualized as below.



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

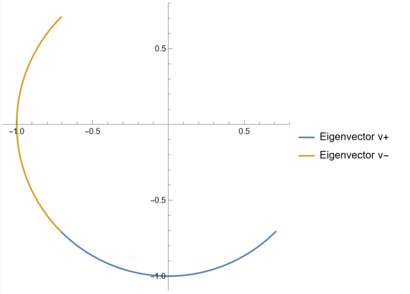
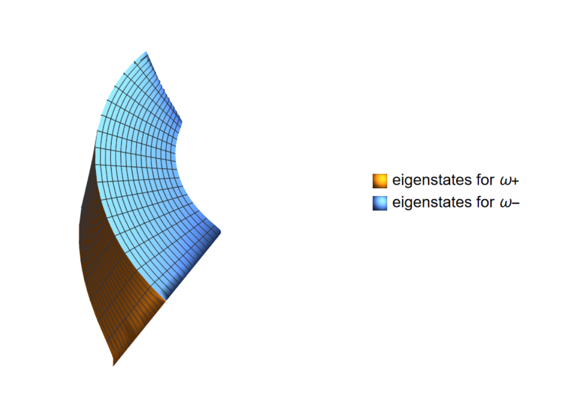


Figure 5: When $\theta = \frac{3\pi}{4}$, $v_+ = v_-$,then v_+ travels counterclockwise while v_- travels clockwise, When $\theta = \pi$, $v_+ \perp v_-$, and $v_+ = -v_-$ when $\theta = \frac{5\pi}{4}$.

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:

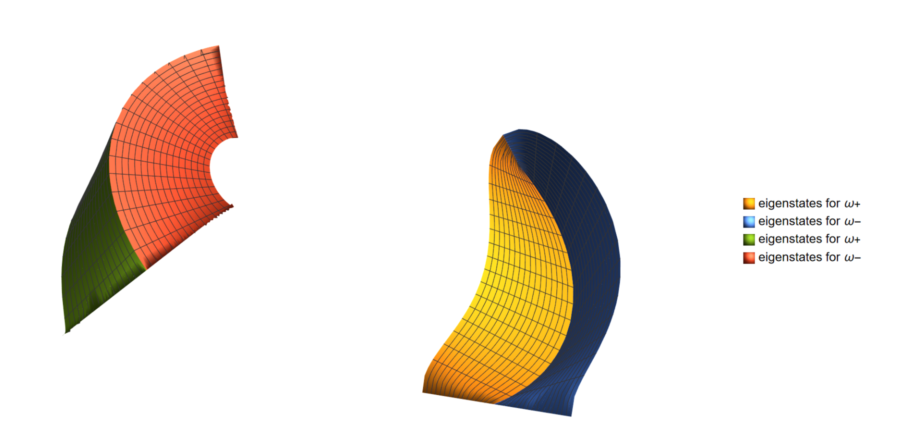


Figure 6: The right one corresponds to $\theta \in [-\frac{\pi}{4}, \frac{\pi}{4}]$, and the left one corresponds to $\theta \in [\frac{3\pi}{4}, \frac{5\pi}{4}]$.

Complex eigenvalues

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 $\vec{a} = (a_1, a_2, \cdots, a_n), \vec{b} = (b_1, b_2, \cdots, b_n)$, where $a_i, b_j \in \mathbf{C}$.
$\vec{A} = (A_1, A_2, \cdots, A_{2n}), \vec{B} = (B_1, B_2, \cdots, B_{2n})$, where $A_{2i-1} = Re(a_i), A_{2i} = Im(a_i)$, $B_{2i-1} = Re(b_i), B_{2i} = Im(b_i)$.

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

Angles in complex vectors

- Kähler angle

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

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

Computations

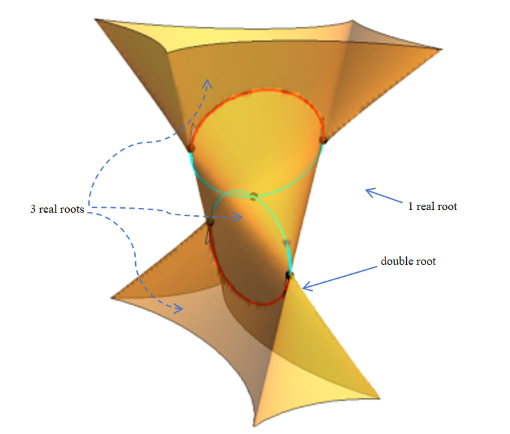
The Hermitian product of v_+ and v_-

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

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

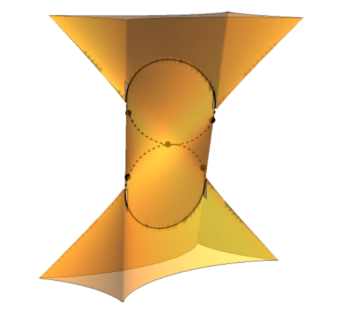
3-band non-Hermitian systems

3-band non-Hermitian systems



$$H[f_1, f_2, f_3] = \begin{bmatrix} 1 & f1 & f2 \\ -f1 & -1 & f3 \\ -f2 & f3 & -1 \end{bmatrix}$$

3-band non-Hermitian systems



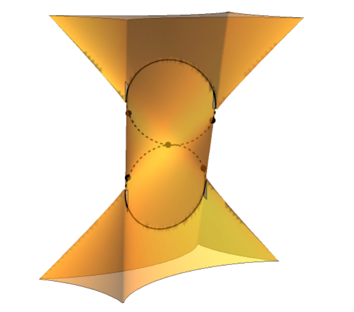
- 4 NLs and 2 NILs

They are two circles:

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

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

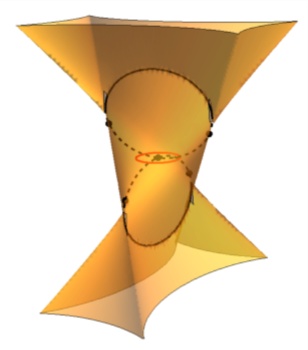
3-band non-Hermitian systems



- 5 MPs

$$(0, 0, 0)$$
$$(\frac{2\sqrt{2}}{3}, -\frac{2\sqrt{2}}{3}, \frac{2}{3})$$
$$(-\frac{2\sqrt{2}}{3}, \frac{2\sqrt{2}}{3}, \frac{2}{3})$$
$$(\frac{2\sqrt{2}}{3}, \frac{2\sqrt{2}}{3}, -\frac{2}{3})$$
$$(-\frac{2\sqrt{2}}{3}, -\frac{2\sqrt{2}}{3}, -\frac{2}{3})$$

Loop1



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

Loop1

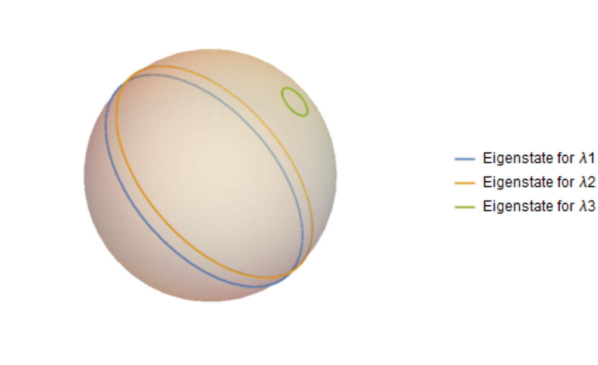
The eigenvalues are

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

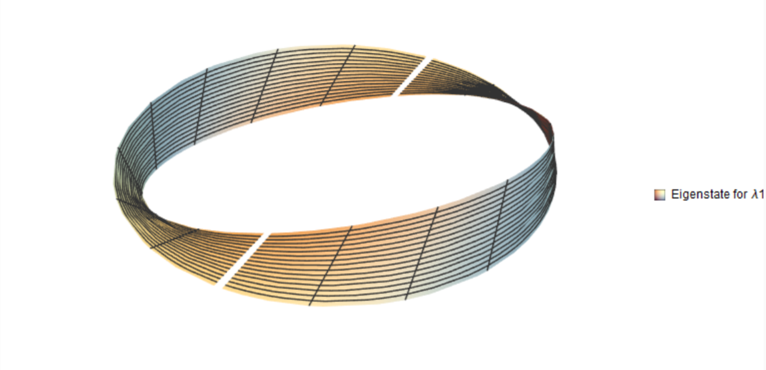
and the corresponding eigenvectors are

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

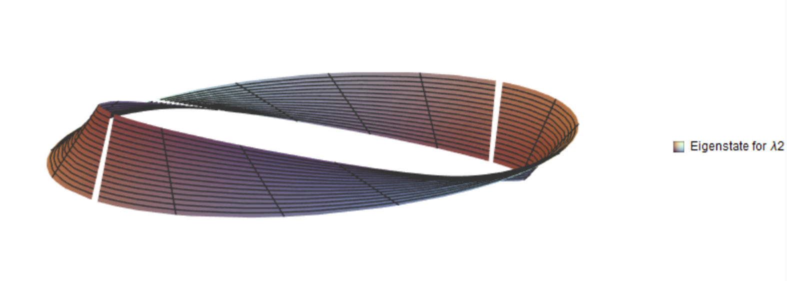
Traces of eigenstates



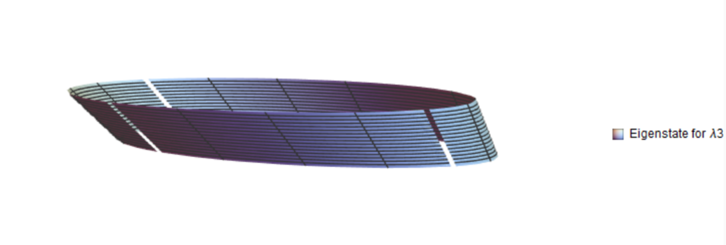
Vector bundles of Loop1

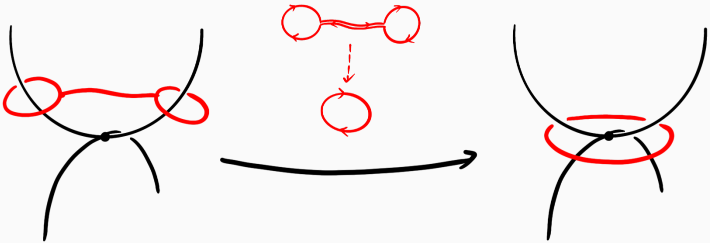


Vector bundles of Loop1

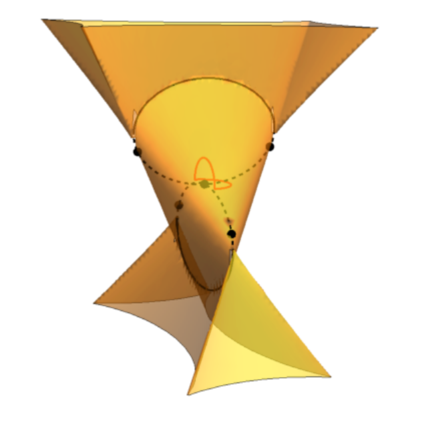


Vector bundles of Loop1





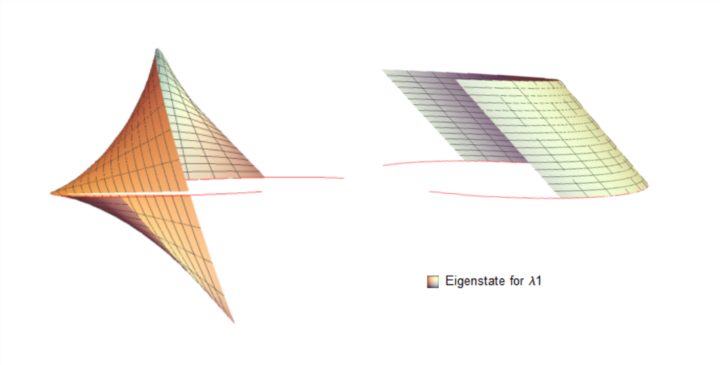
Loop2



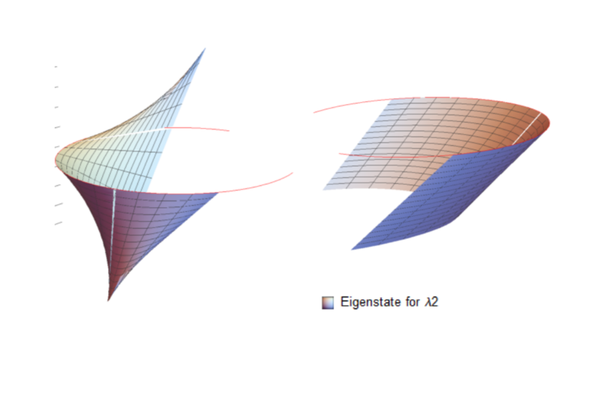
$$\begin{cases} f_1 = \frac{1}{2}\cos(\frac{1}{4}\pi + t) \\ f_2 = \frac{1}{2}\sin(\frac{1}{4}\pi + t) \\ f_3 = 0 \end{cases}, t \in [0, \pi)$$

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

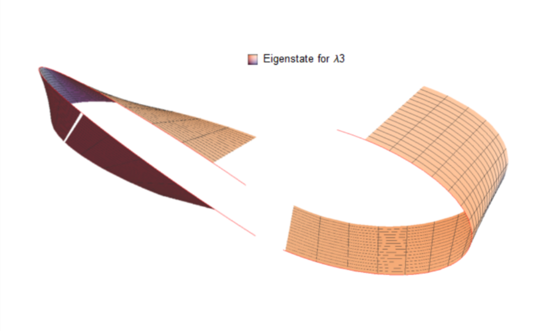
Vector bundles of Loop2



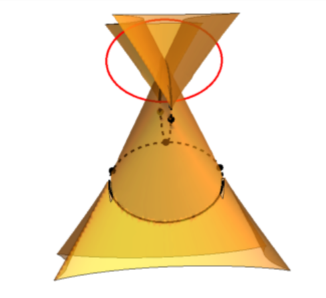
Vector bundles of Loop2



Vector bundles of Loop2



Loop3



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

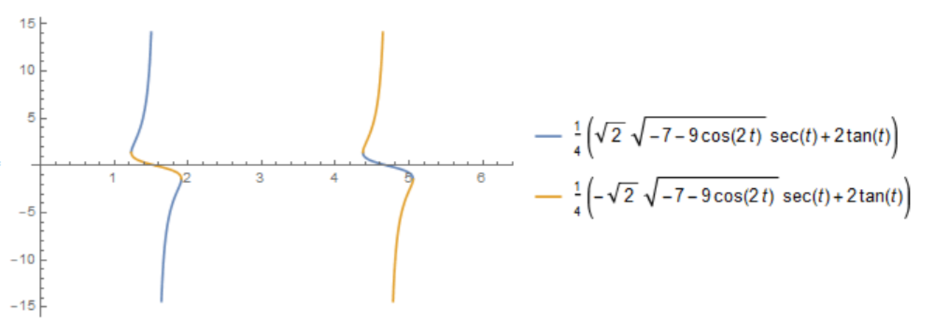
Loop3

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


15
10
5
−5
−10
−15
1
2
3
4
5
6
$\frac{1}{4}\left(\sqrt{2}\sqrt{-7-9\cos(2t)}\,\sec(t)+2\tan(t)\right)$
$\frac{1}{4}\left(-\sqrt{2}\sqrt{-7-9\cos(2t)}\,\sec(t)+2\tan(t)\right)$

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Thanks!