Topological and geometric perspectives on non-Hermitian Hamiltonians

Non-Hermitian physics has become an emerging area of research in condensed matter physics, with far-reaching applications to materials science. Resulting from symmetry beyond classical Hermiticity, complexity of the topological structure in such quantum mechanical systems poses challenges to mathematical modeling while affording unconventional physical phenomena. In this talk, I'll report on joint work with physicists Hongwei Jia, Jing Hu, C. T. Chan et al., in which we investigate stratified singularity in the moduli spaces of such systems using intersection homology for homotopical classifications. I'll then explain joint work in progress with Zhou Fang, Chenlu Huang, Qingrui Qu, Wenhui Yang, and Zhiwang Yu towards an understanding of hyperbolic geometry therein, through Higgs bundles modeling eigenbundles, and Minkowski light-cones modeling exceptional surfaces, with examples.

Topological and geometric perspectives on non-Hermitian Hamiltonians

Joint with H. Jia, J. Hu, C. T. Chan (physically),
Z. Fang, C. Huang, Q. Qu, W. Yang, Z. Yu (mathematically), et al.

Yifei Zhu

Southern University of Science and Technology

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Motivations: Quantum materials and their math modeling

As an umbrella term in condensed matter physics, **quantum materials** refer to solids with *exotic/exceptional/not found in nature* ... physical properties at the *macroscopic* level that arise from the interactions of their electrons at the *microscopic* level, beginning at atomic and subatomic scales where the extraordinary effects of quantum mechanics cause unique and unexpected behaviors.

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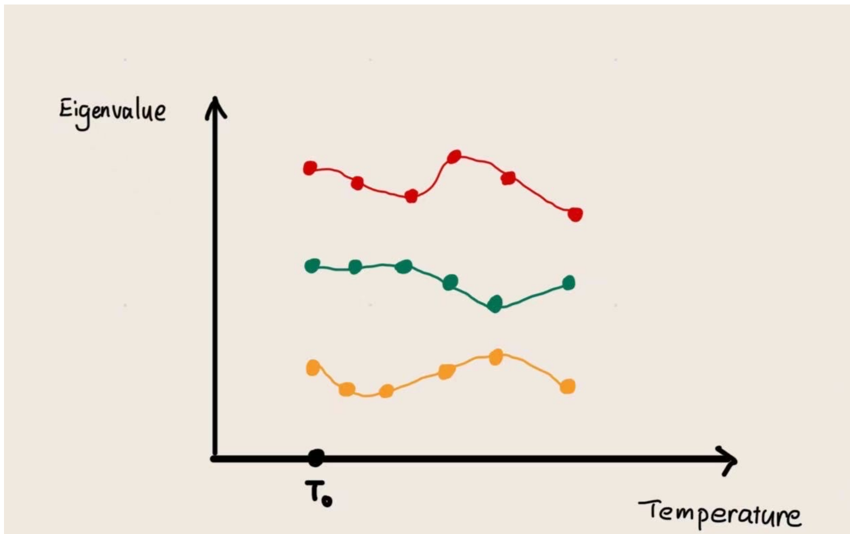
- U.S. Department of Energy, Office of Science issued a brochure *Basic research needs for quantum materials: Research to discover, harness, and exploit exotic electronic properties* in 2016.

- Zhong Fang et al. of the Chinese Academy of Sciences won the 2023 National Natural Science Award First Prize for *Computational prediction of topological electronic materials*.

- Ashvin Vishwanath of Harvard University delivered the Buckley prize talk *The unreasonable effectiveness of topology in the science of quantum materials* at the 2024 APS March Meeting in Minneapolis.

Motivations: Quantum materials and their math modeling

Mathematical modeling of electronic energy *band structures* therein



energy ⟷ *eigenvalue*

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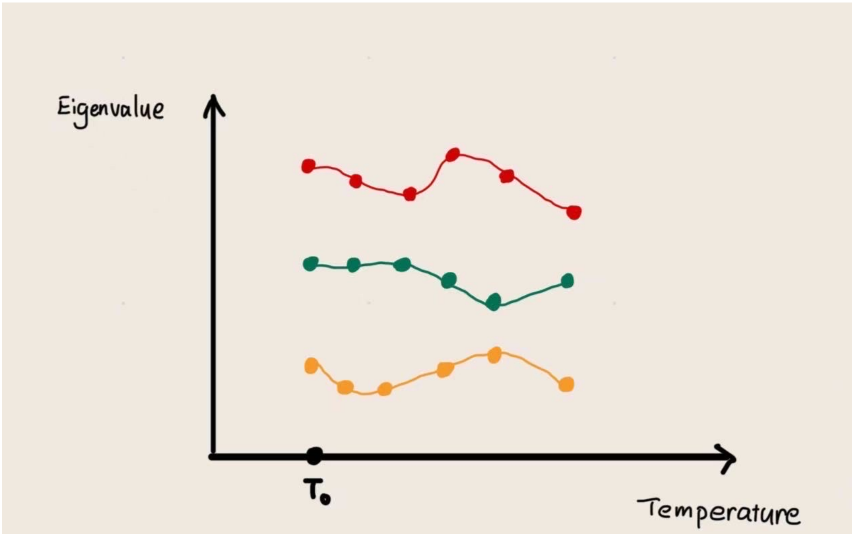

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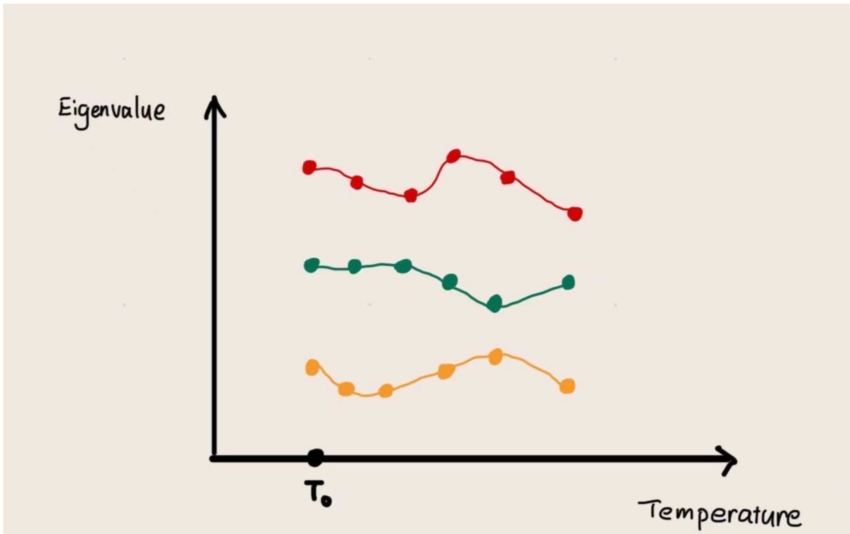

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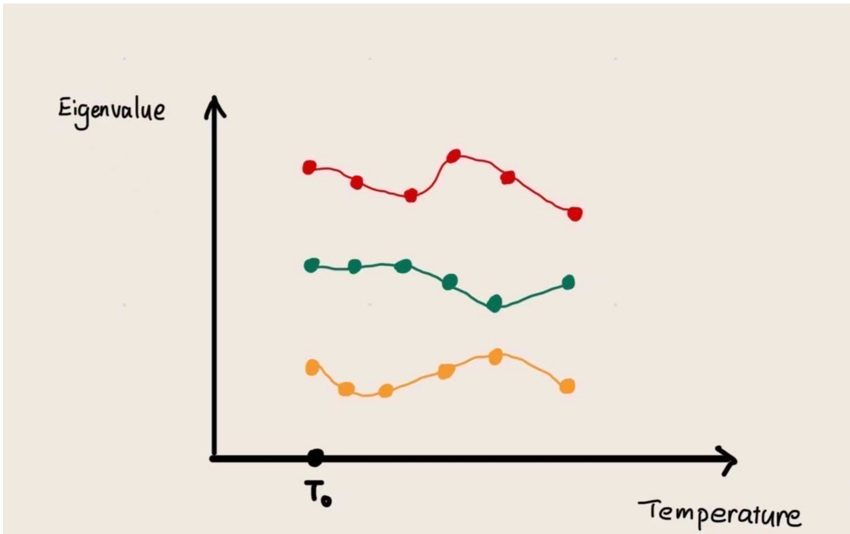

Hermitian

real eigenvalues (observable energies)

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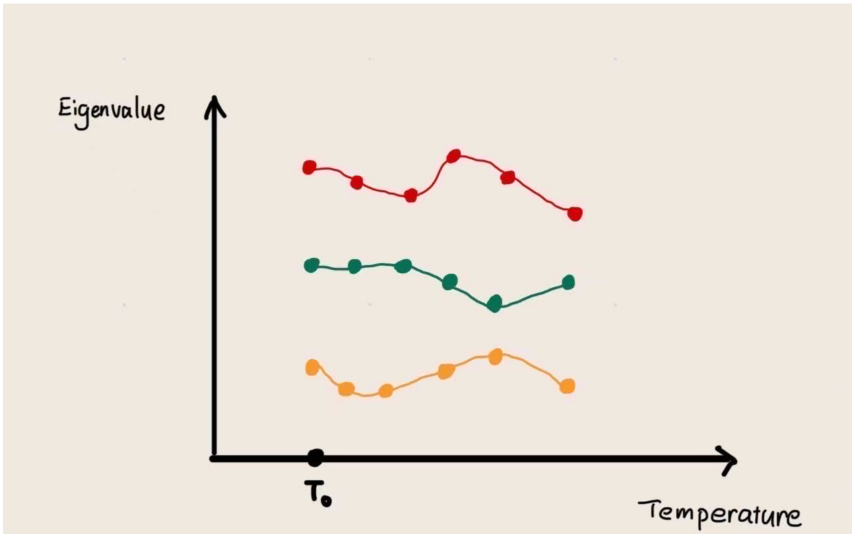

Hermitian vs. non-Hermitian

real eigenvalues (observable energies) vs. eigenvalues with imaginary part (counts for energy exchange with surrounding environment or other systems)

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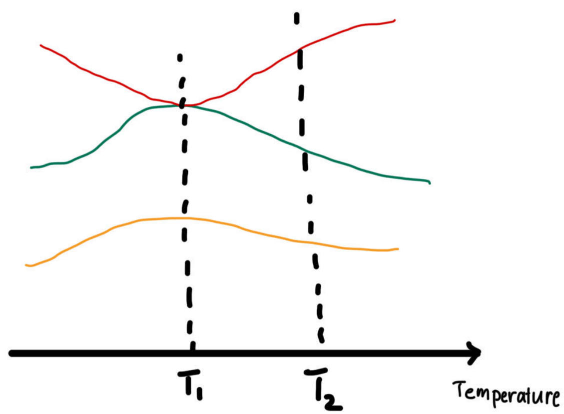

phases of matter
H_2O*: solid, liquid, gas*

T_1 : singular points (points where eigenvalues degenerate)
$H(T_1)$: gapless Hamiltonian
$H(T_2)$: gapped Hamiltonian

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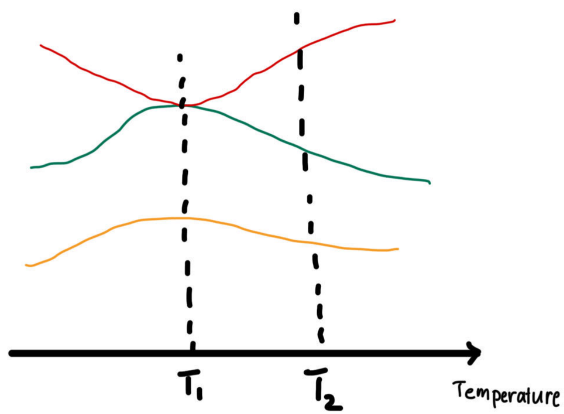
Development of sensing and absorbing devices



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*Guzman et al., Model-free characterization of topological edge and corner states in mechanical networks, **PNAS** 2024.*

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Thanks to Hopf bundles and Higgs bundles as *eigenbundles*, we now have a conceptually more systematic, visibly more intuitive understanding of the topic. The structure of Higgs bundles also hints at certain deeper aspects of mathematics as well as physics.

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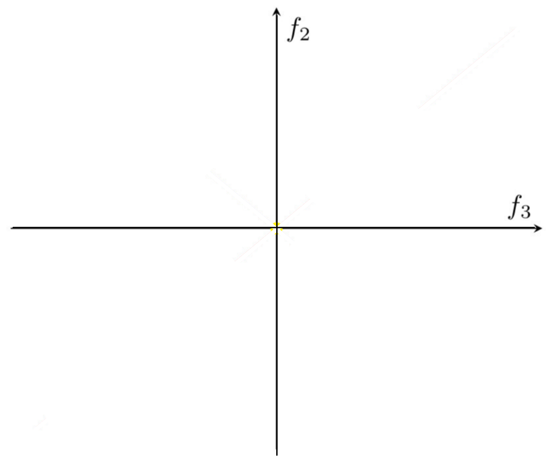

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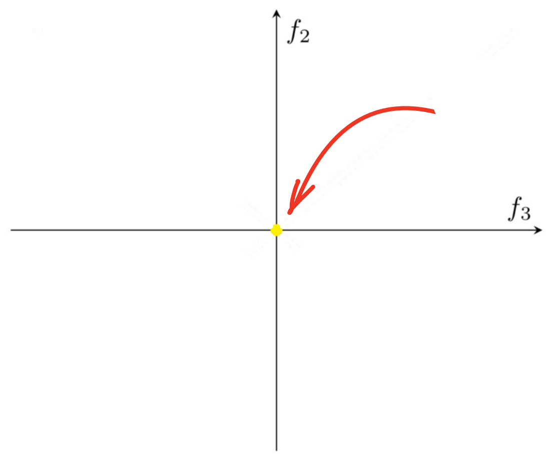

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0. Over {(0, 0)}, H has a double eigenvalue, whose eigenspace is 2-dimensional.

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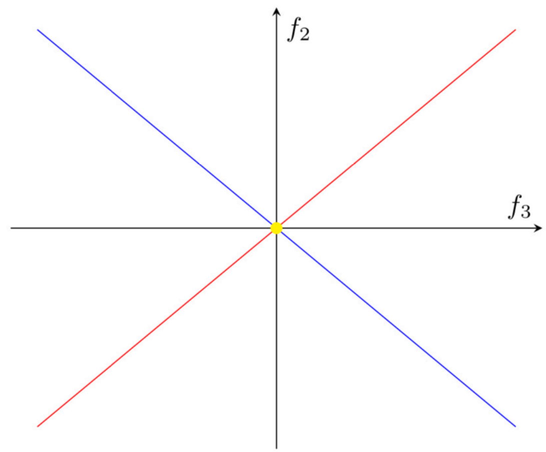

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1. Over $\{f_2 = \pm f_3\} - \{(0, 0)\}$, again H has a double eigenvalue, but its eigenspace is of dimension 1.

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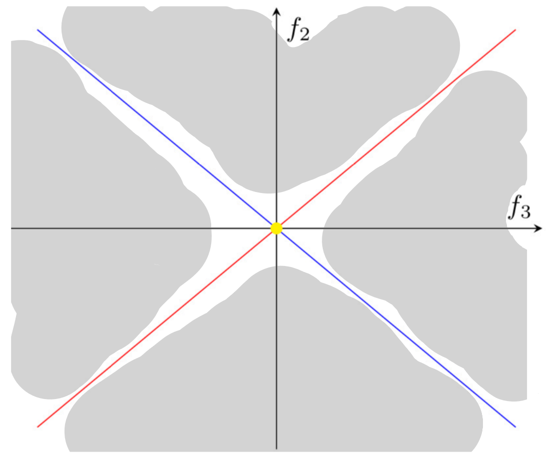

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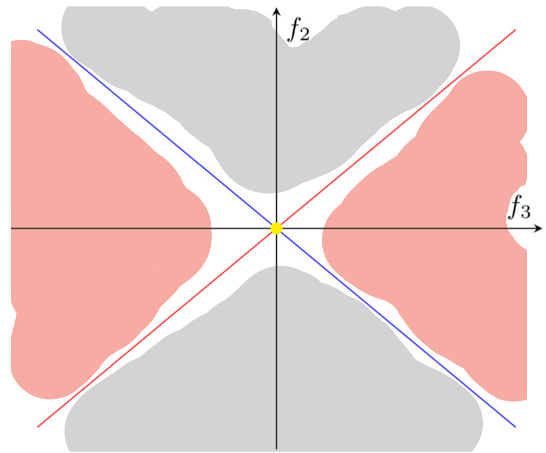

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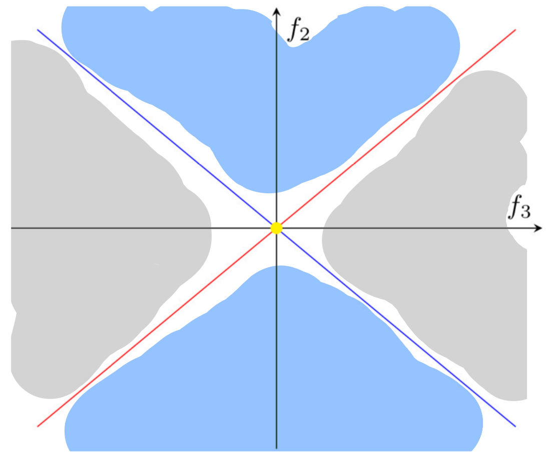

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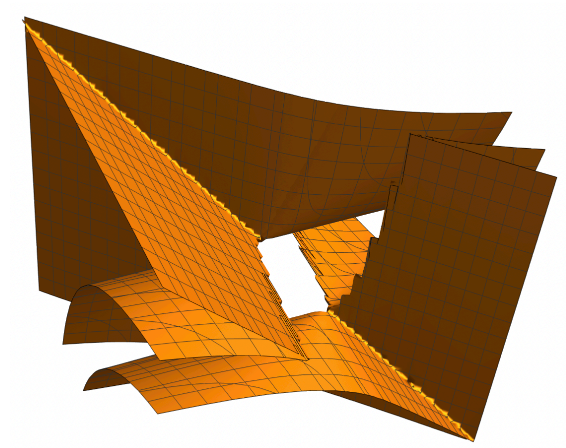
Another example of non-Hermitian "3-band systems" is also of particular interest to us. One such Hamiltonian takes the form

$$H_3 = \begin{bmatrix} 1 - f_1 - f_2 & f_1 & f_2 \\ -f_1 & f_1 - f_3 & f_3 \\ -f_2 & f_3 & f_2 - f_3 \end{bmatrix}$$

Governing eigenvalues with multiplicity, the discriminant surface of its characteristic polynomial is a pair of *swallowtails* in the $f_1 f_2 f_3$-space:

The equation for this surface is a non-homogeneous real polynomial in f_1, f_2, f_3 of degree 6.



Swallowtail couple $\mathrm{sw2}$

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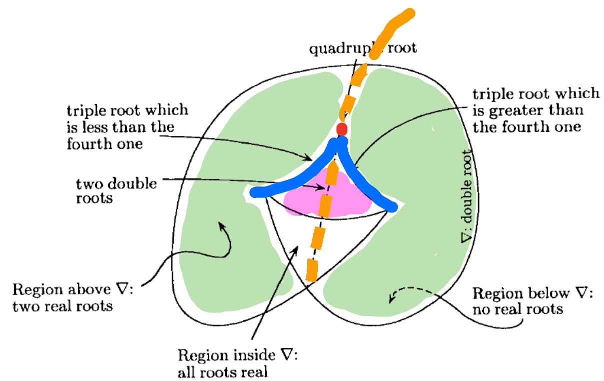


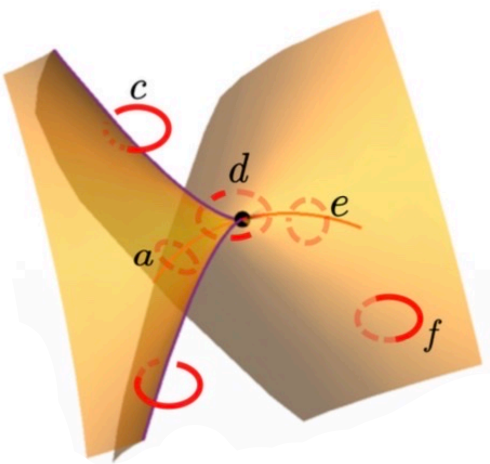
The space of polynomials $x^4 + ax^2 + bx + c$

Again, we aim to find computable algebraic invariants that systematically classify the evolutions of eigenvectors along loops in such stratified parameter spaces, including when they cross the discriminant surface resulting in degeneracies of various sorts.

Mathematical set-up: Eigenframe evolution of non-Hermitian systems

We have explicitly calculated the intersection homology of the swallowtail catastrophe, which appears locally in many 3-band non-Hermitian systems.

$$I^{\bar{p}}H_1(\text{swallowtail}) = \begin{cases} \mathbb{Z}e & \text{if } \bar{p}(1) < 0, \bar{p}(2) < 0 \\ \mathbb{Z}a \oplus \mathbb{Z}b \oplus \mathbb{Z}c & \text{if } \bar{p}(1) \geqslant 0, \bar{p}(2) < 0, \bar{p}(3) < 1 \\ \mathbb{Z}a \oplus \mathbb{Z}b \oplus \mathbb{Z}c/(a+b+c=0) & \text{if } \bar{p}(1) \geqslant 0, \bar{p}(2) < 0, \bar{p}(3) \geqslant 1 \\ 0 & \text{otherwise} \end{cases}$$



$\bar{p}$ = *perversity* (badness of loops/1-cycles in terms of intersection with strata)

$$a + b + c = d, \quad d = e$$

since the 2D chains that witness these equations are *allowable*.

Eigenframe rotation as vector bundles: Revisiting the Hermitian case

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Remarks on eigenvalues and eigenvectors of Hermitian matrices, Berry phase, adiabatic connections and quantum Hall effect, 1995.

Also: Polymathematics, 2000.

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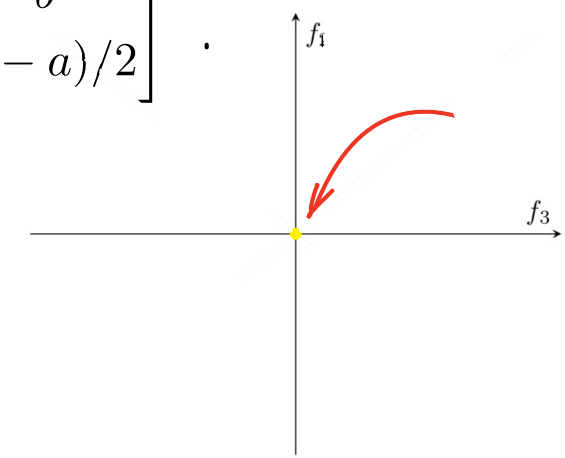

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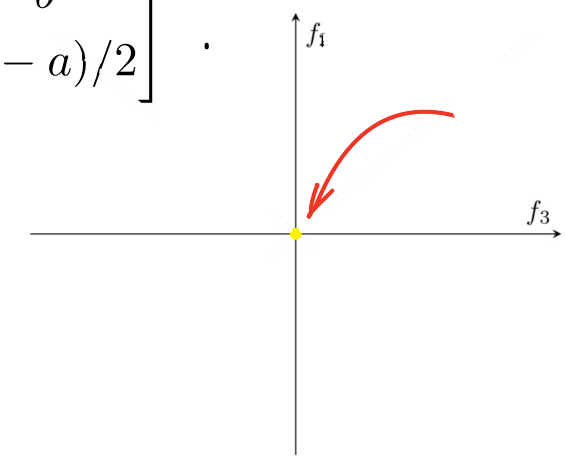

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The parameter $f_1 f_3$-plane thus has an isolated singular point $(0, 0)$ and is a particularly simple stratified space.

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Moreover, they obtained non-Abelian "topological charge" for *n*-band Hermitian systems when $n > 2$, such as

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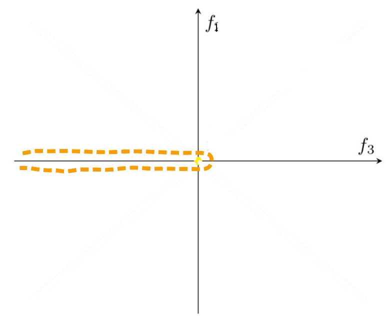

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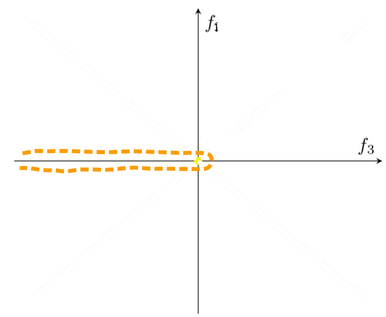

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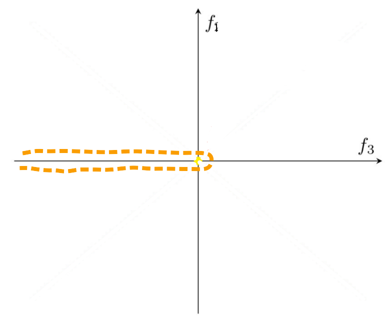

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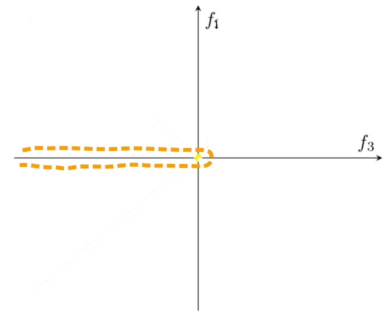

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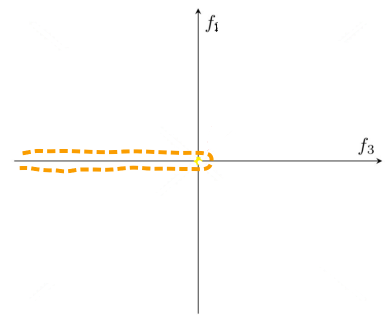

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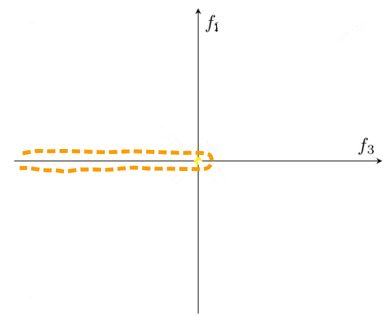

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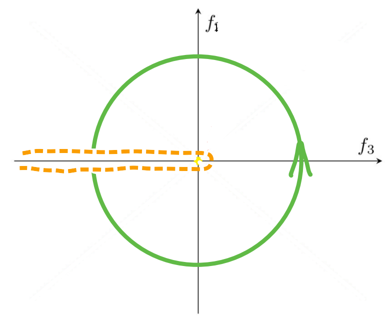

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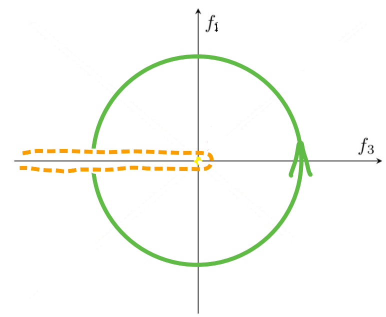

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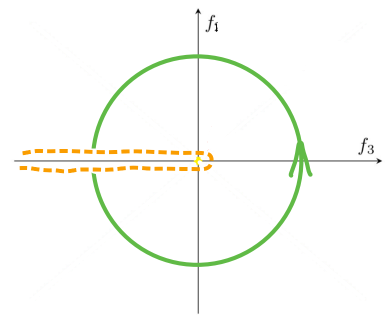

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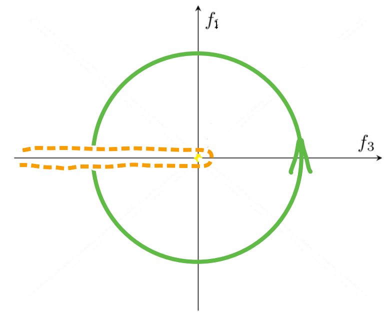

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We compute that

$$\lim_{\theta\to(-\pi)_+} \frac{v_+}{|v_+|} = \begin{bmatrix} 0 \\ -1 \end{bmatrix}$$

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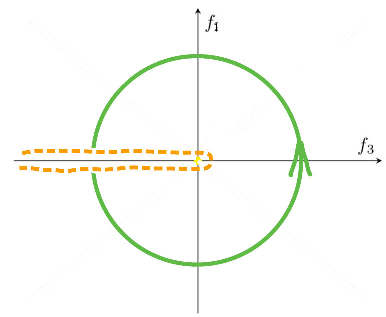

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$$\to \begin{bmatrix} 0 & 0 \\ f_1 & -f_3-\sqrt{} \end{bmatrix} \Rightarrow v_+ = \begin{bmatrix} f_3+\sqrt{f_1^2+f_3^2} \\ f_1 \end{bmatrix} \overset{\begin{cases} f_3=\cos\theta \\ f_1=\sin\theta \end{cases} \ -\pi<\theta<\pi}{=\!=\!=\!=\!=} \begin{bmatrix} \cos\theta+1 \\ \sin\theta \end{bmatrix}$$

Observe that when $\theta \to (-\pi)_+$, we have $\cos\theta + 1 \to 0_+$ and $\sin\theta \to 0_-$,

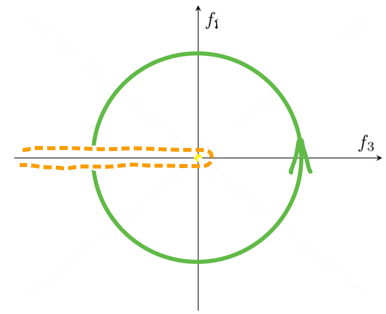
whereas when $\theta \to \pi_-$, we have $\cos\theta + 1 \to 0_+$ and $\sin\theta \to 0_+$.

We compute that

$$\left.\begin{aligned} \lim_{\theta\to(-\pi)_+} \frac{v_+}{|v_+|} &= \begin{bmatrix} 0 \\ -1 \end{bmatrix} \\ \lim_{\theta\to\pi_-} \frac{v_+}{|v_+|} &= \begin{bmatrix} 0 \\ 1 \end{bmatrix} \end{aligned}\right\} \text{Half Möbius band!}$$

Eigenframe rotation as vector bundles: Revisiting the Hermitian case

To solve for eigenvectors v_+ corresponding to ω_+, perform Gaussian elimination through elementary row operations:



$$\begin{bmatrix} f_3 - \sqrt{f_1^2 + f_3^2} & f_1 \\ f_1 & -f_3 - \sqrt{f_1^2 + f_3^2} \end{bmatrix} \xrightarrow{-f_3-\sqrt{f_1^2+f_3^2} \neq 0 \iff \cancel{f_1 = 0,\, f_3 \leq 0}}$$

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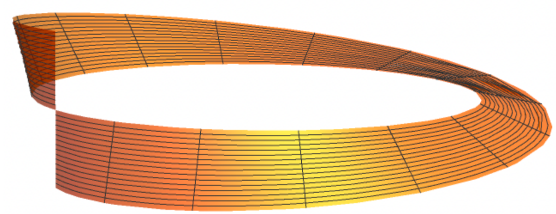

Eigenframe rotation as vector bundles: Revisiting the Hermitian case

Lemma. The universal rank-1 eigenbundle for Hermitian 2-band systems is given by the Hopf bundle

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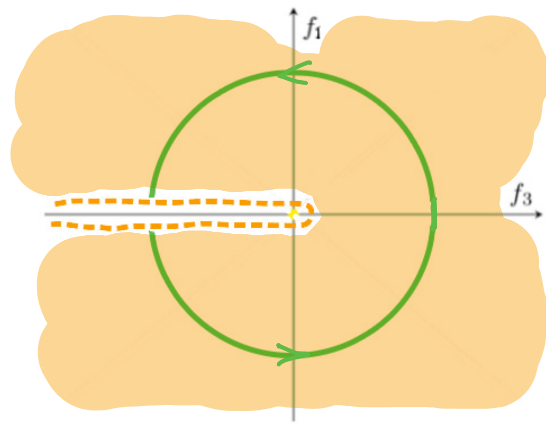

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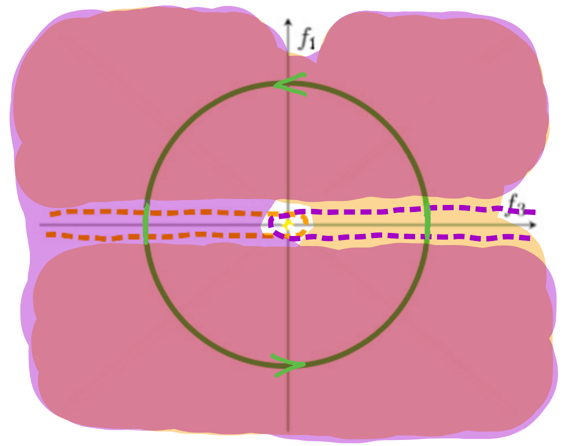

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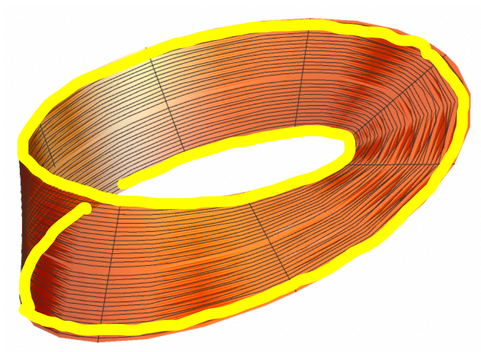

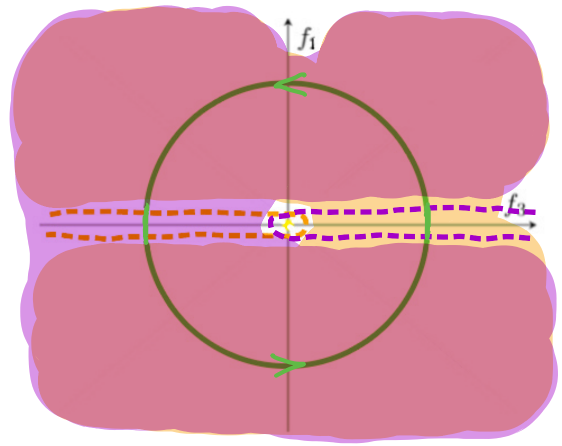

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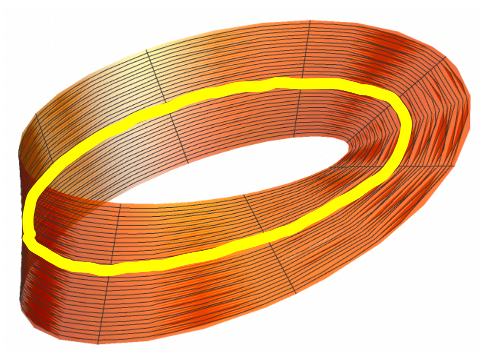

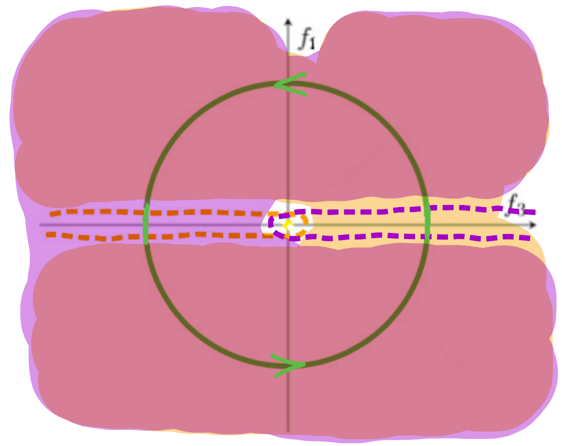

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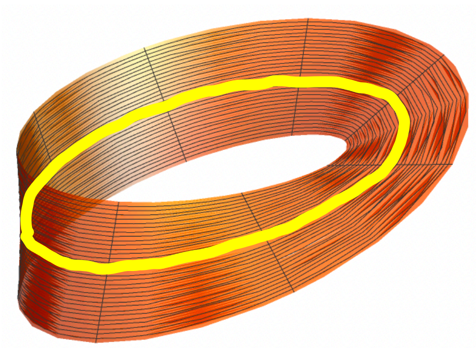

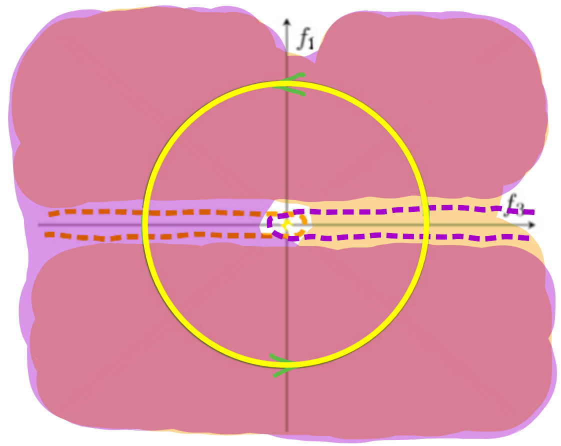

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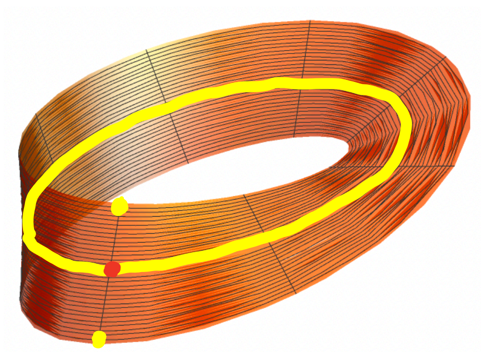

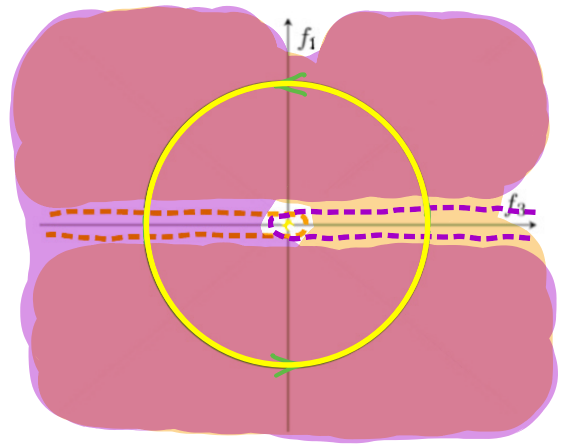

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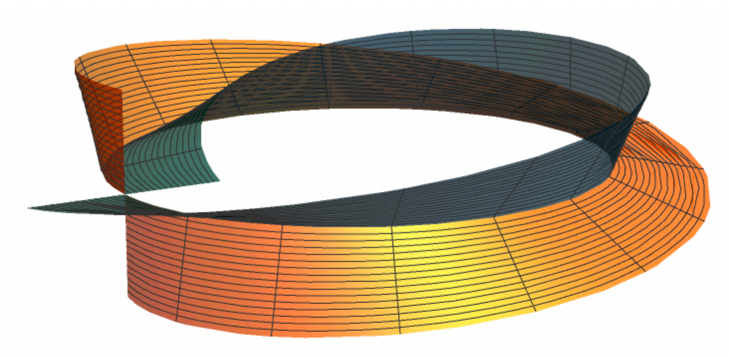

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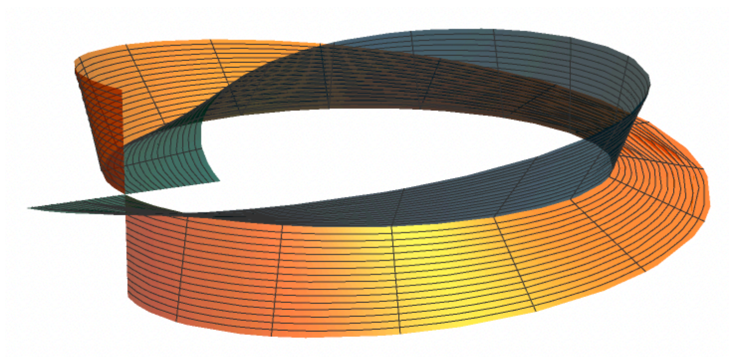

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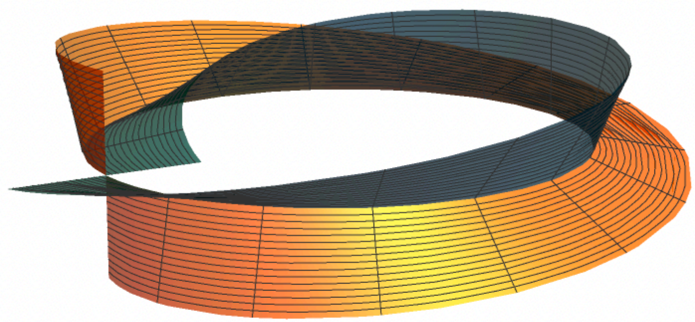

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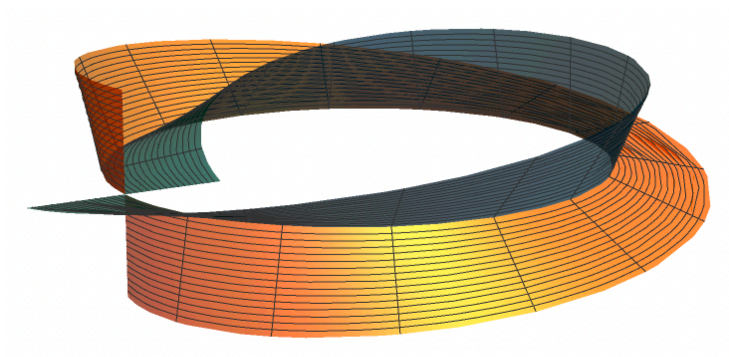

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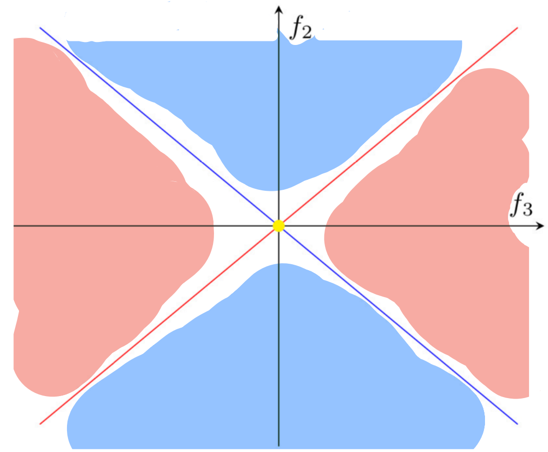

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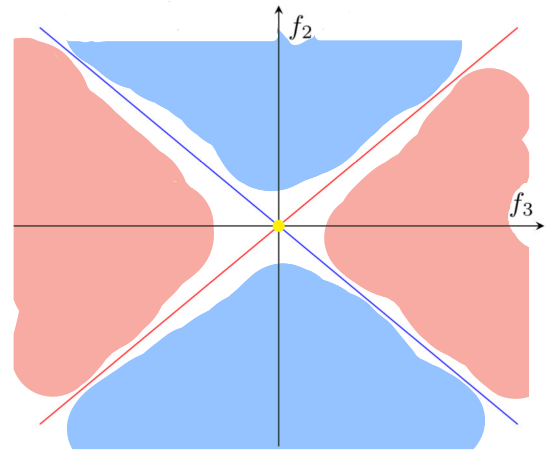

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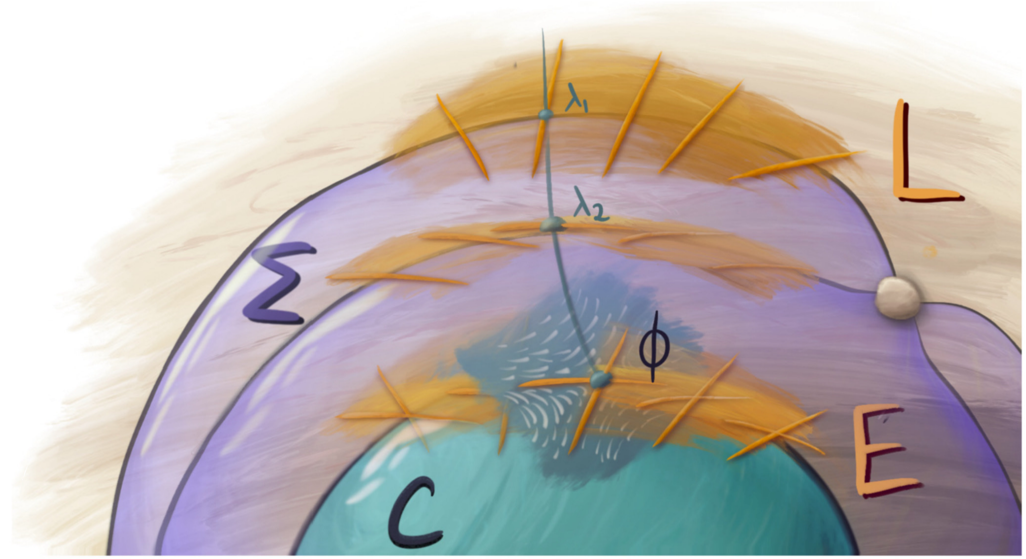
A *Higgs bundle* $(E, \phi) \to C$ is essentially a family of matrices



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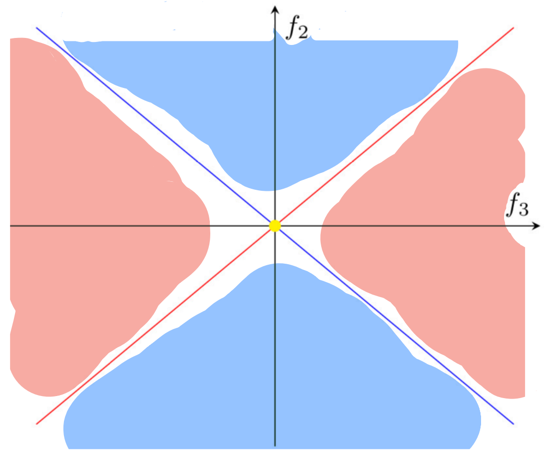

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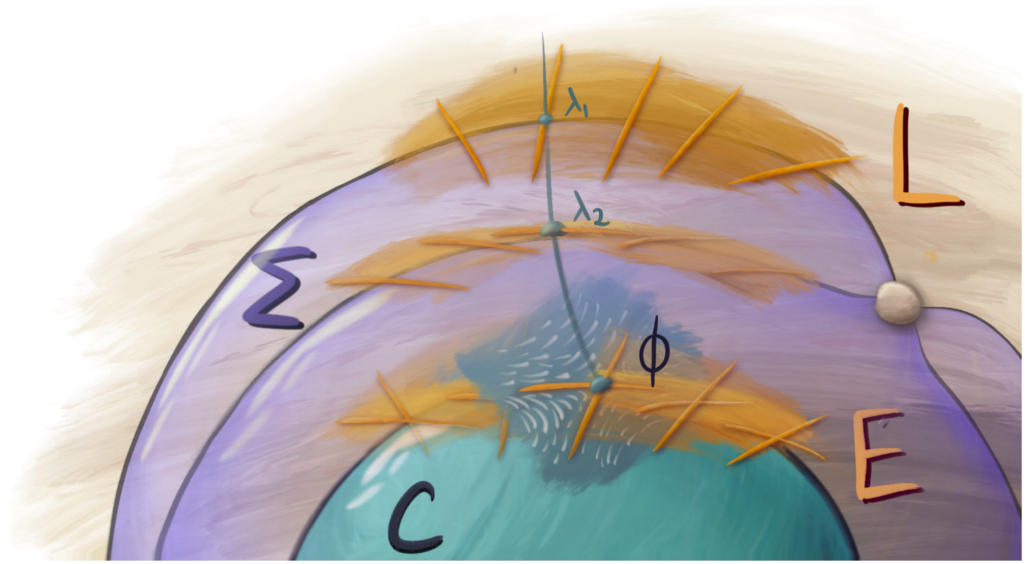
Peter Higgs (bosons)



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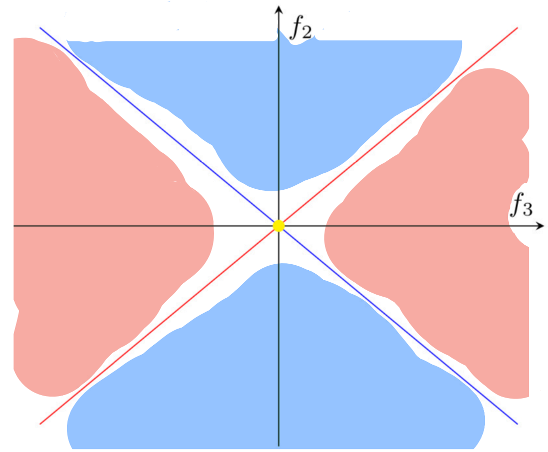

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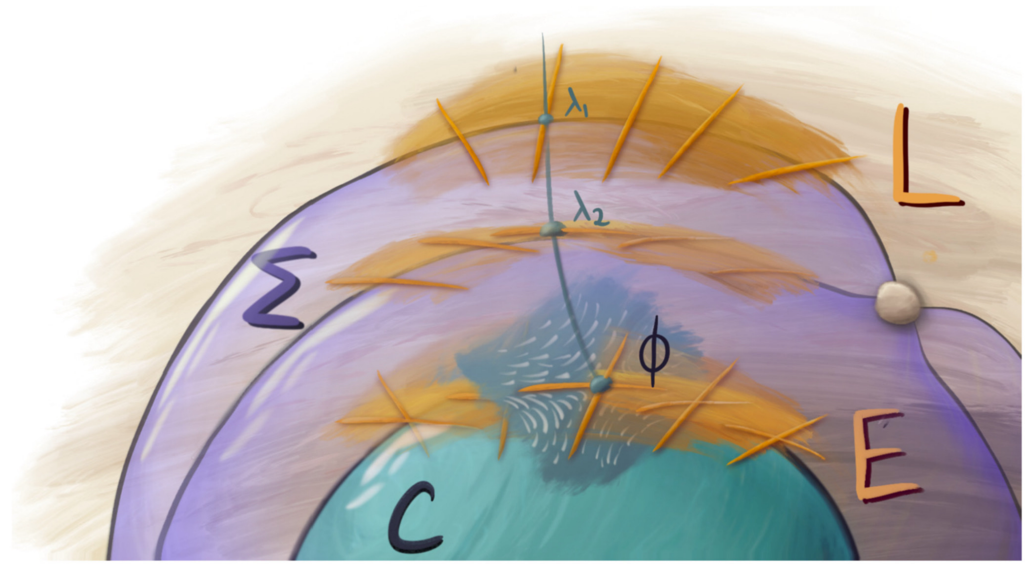
Nigel Hitchin 1987



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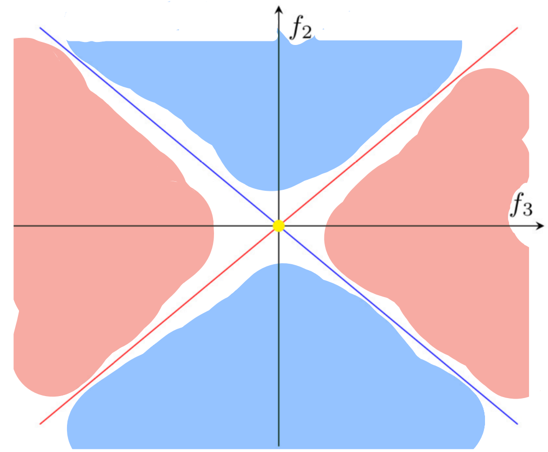

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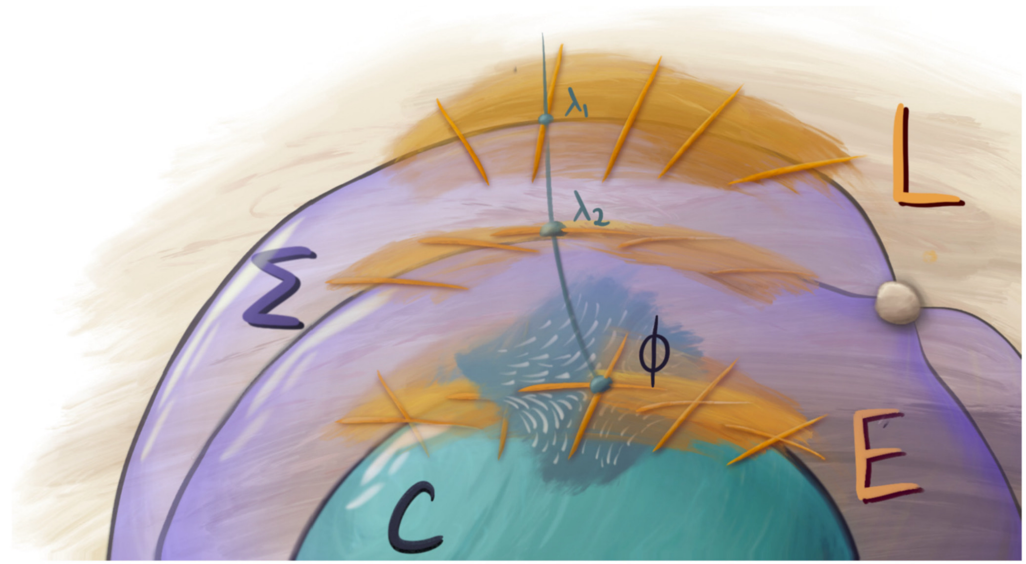
Nigel Hitchin 1987

C compact Riemann surface



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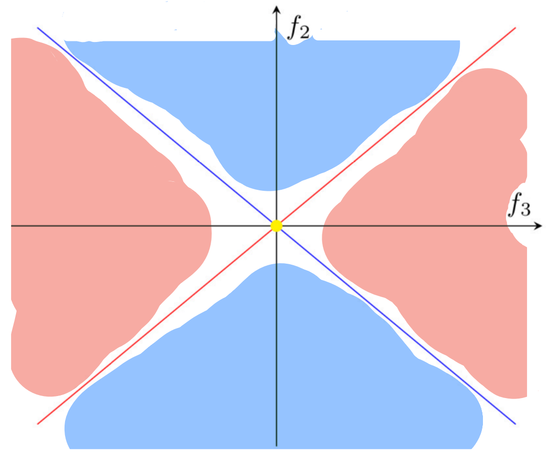

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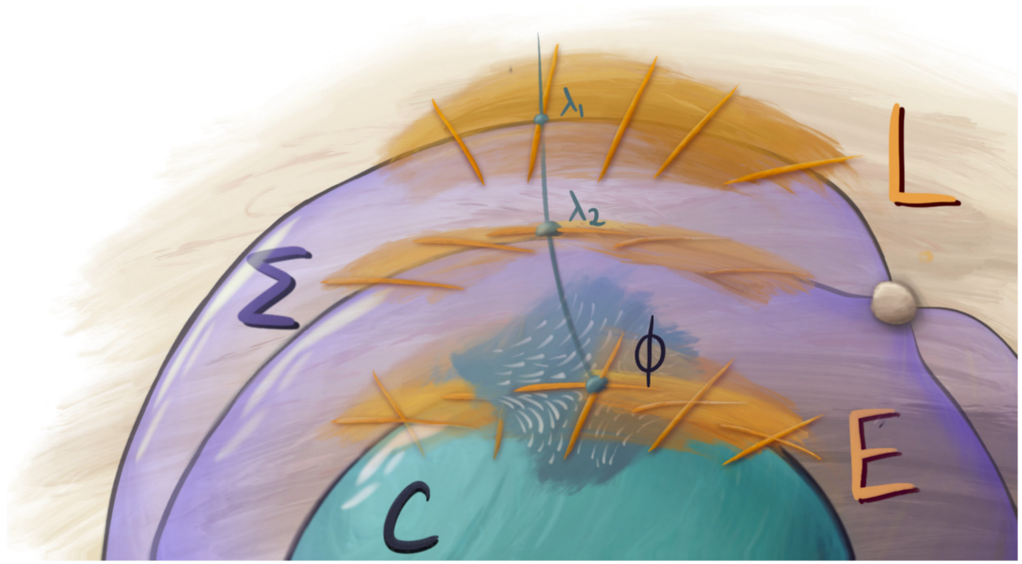

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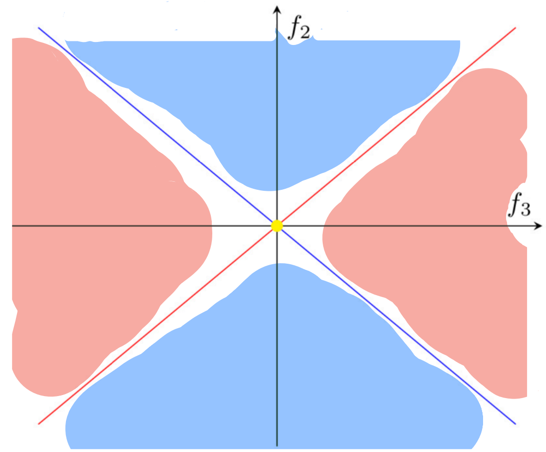

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Nigel Hitchin 1987

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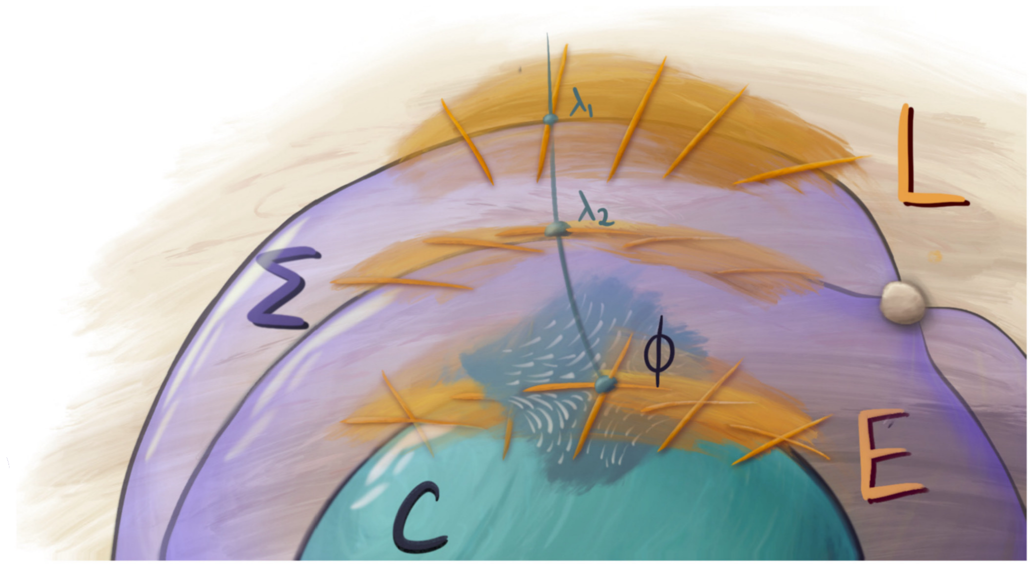

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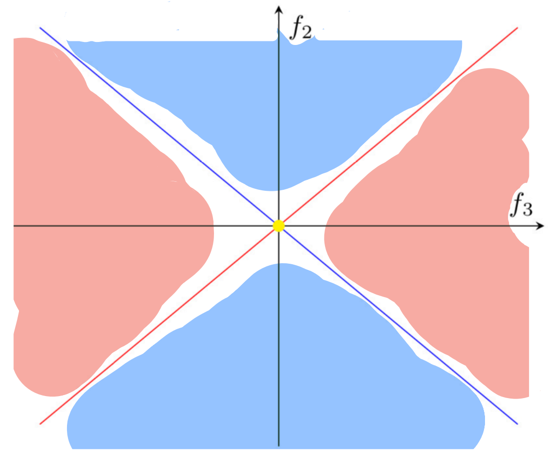

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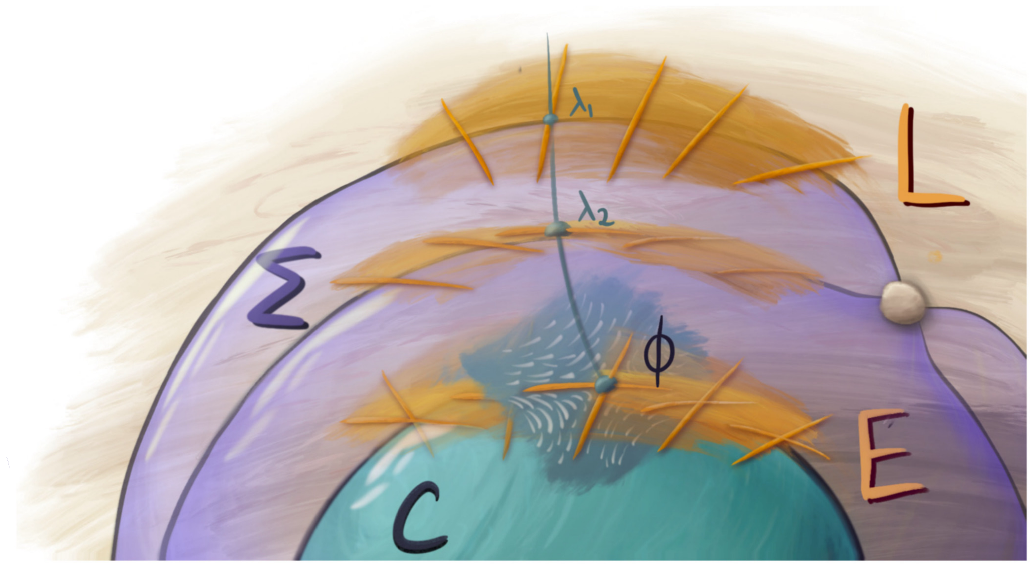

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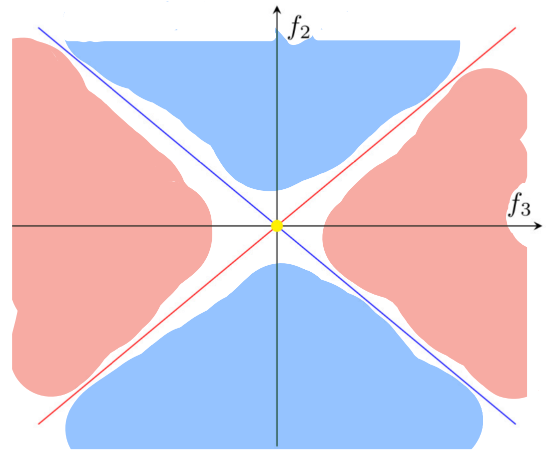

0. Over $\{(0, 0)\}$, H has a double eigenvalue, whose eigenspace is 2-dimensional.
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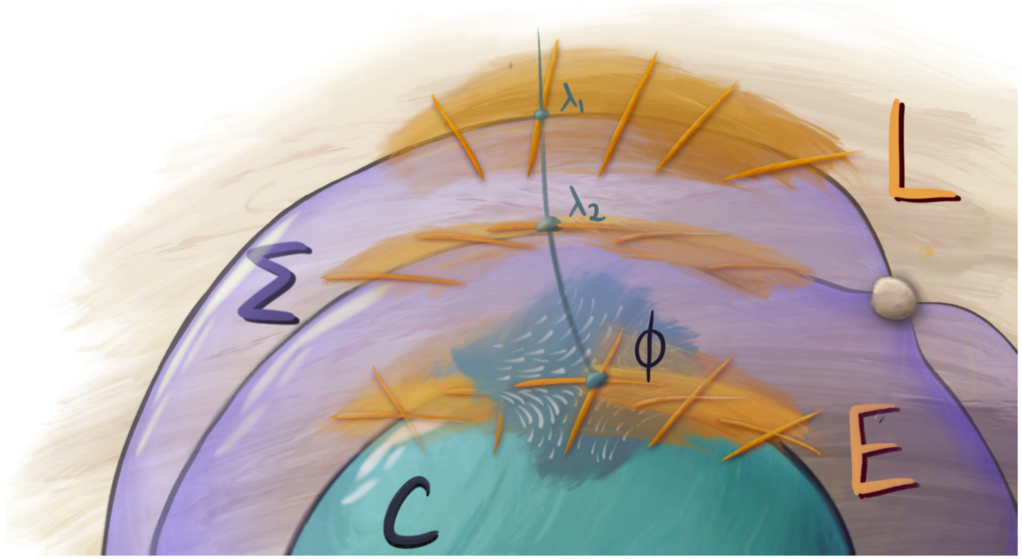
A *Higgs bundle* $(E, \phi) \to C$ is essentially a family of matrices



Peter Higgs (bosons)

Nigel Hitchin 1987
Carlos Simpson

C compact Riemann surface (or more generally Kähler manifold)
E holomorphic vector bundle
ϕ Higgs field: a holomorphic 1-form taking values in the bundle of endomorphisms of E such that $\phi \wedge \phi = 0$

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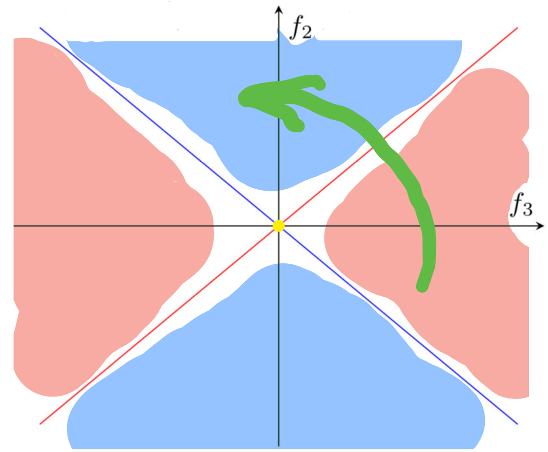

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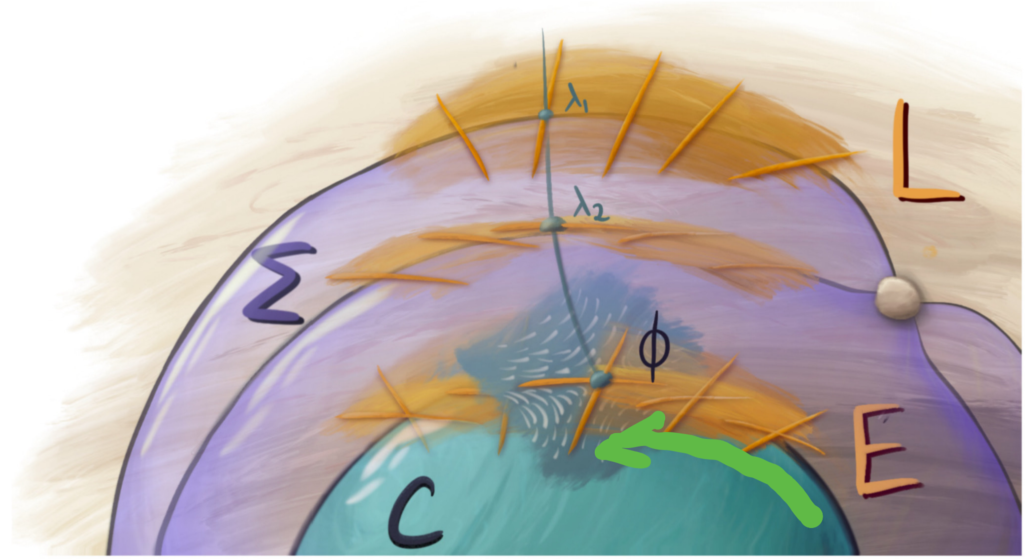
$$\phi_x \in \mathrm{End}(E_x), x \in C$$



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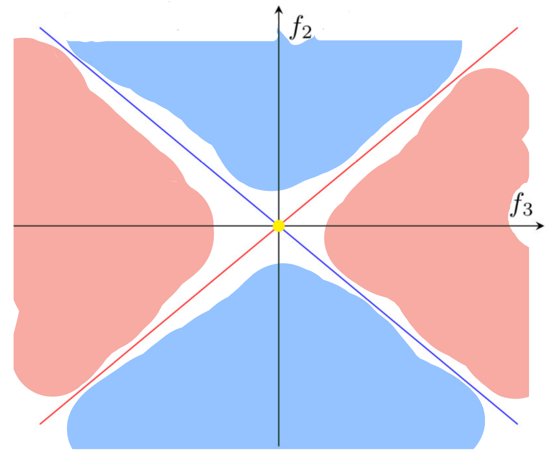

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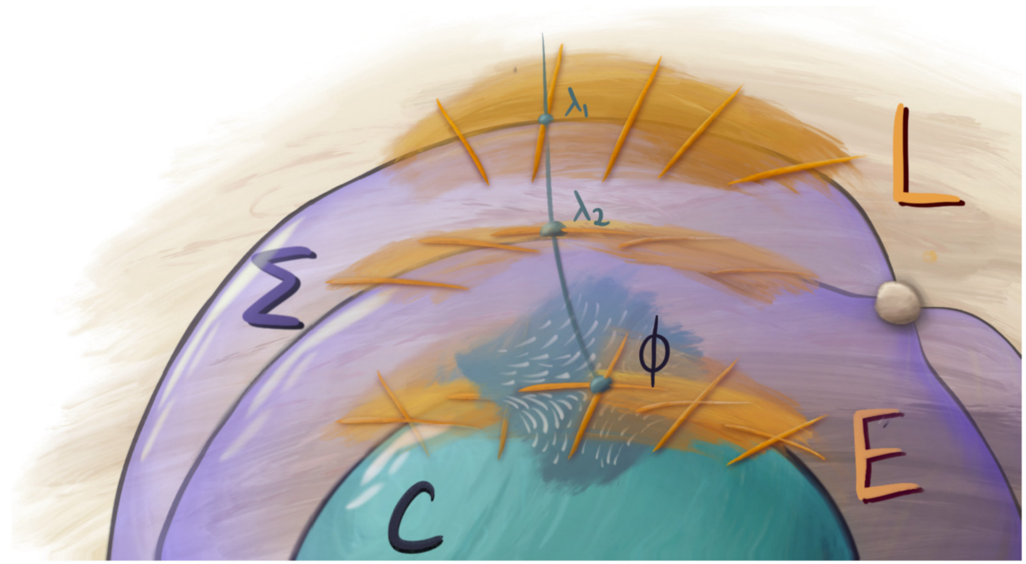

Portrait from Kienzle and Rayan, *Hyperbolic band theory through Higgs bundles*, ***Adv. Math.***, 2022.

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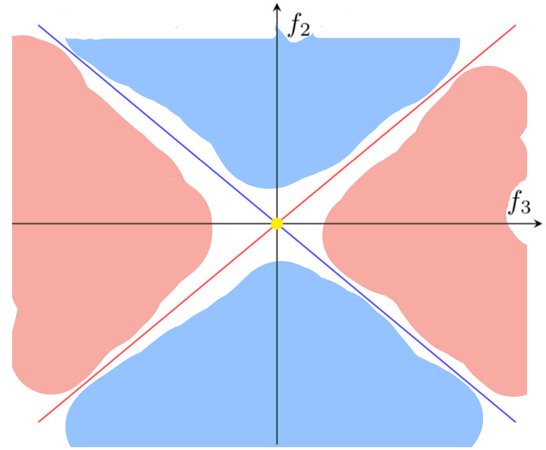

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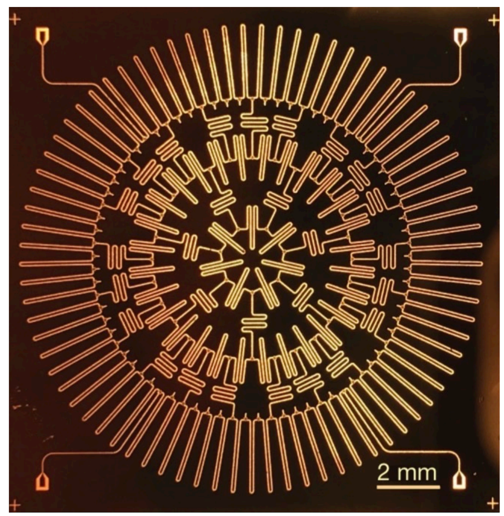

*Hyperbolic metric on the base C. Kollár et al., **Nature**, 2019.*

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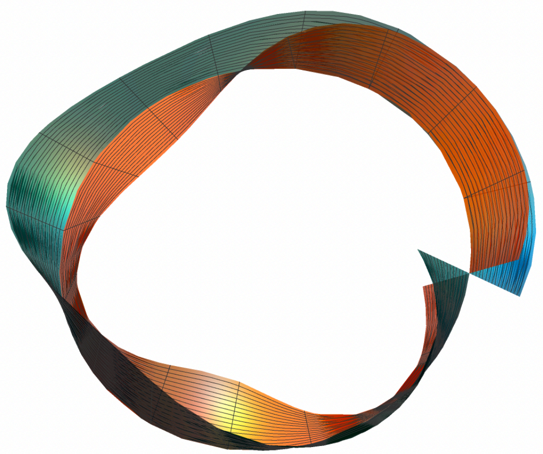
Proposition. The universal eigenbundle for non-Hermitian 2-band systems is given by a pair of kissing half Möbius bands



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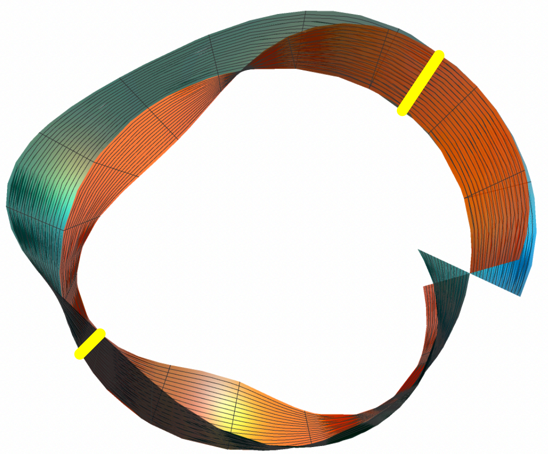

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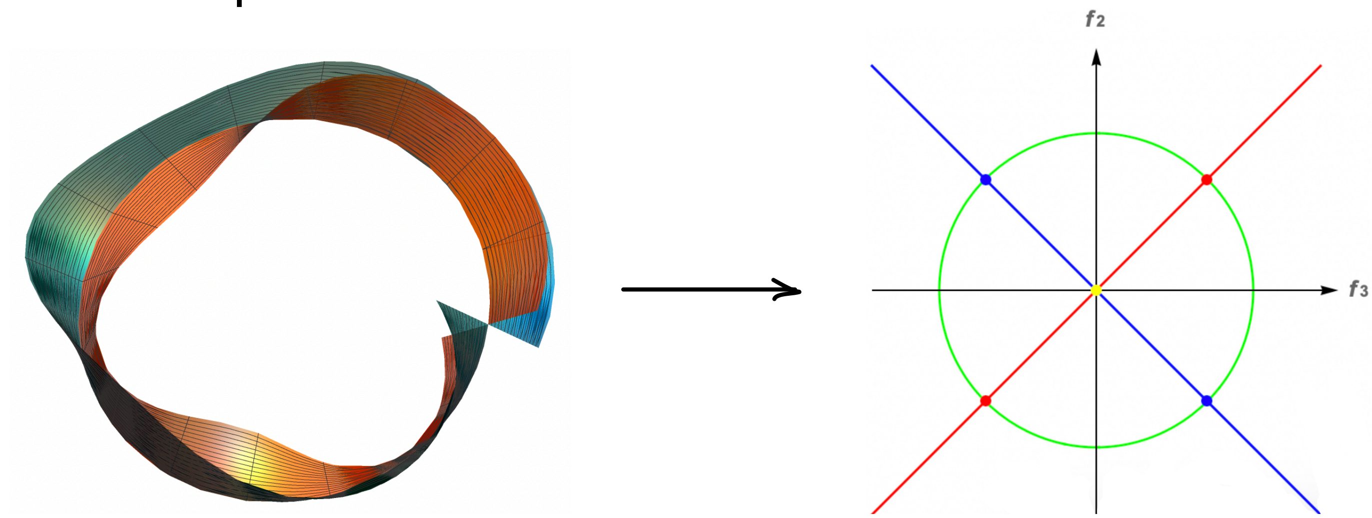

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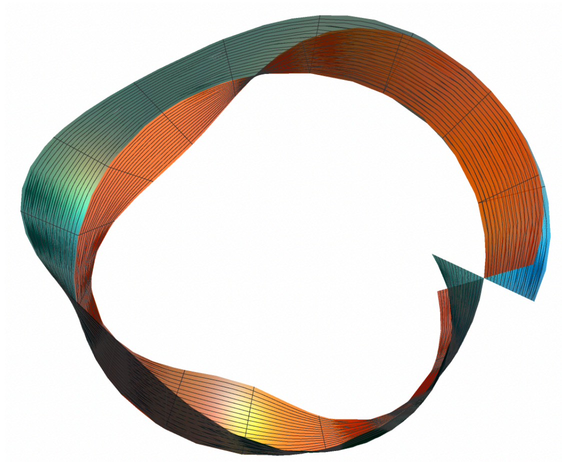

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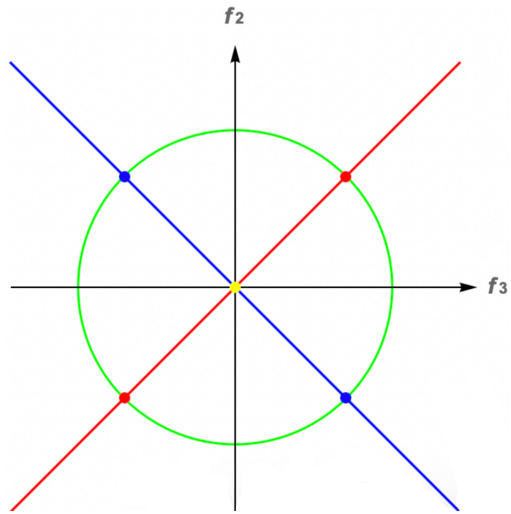

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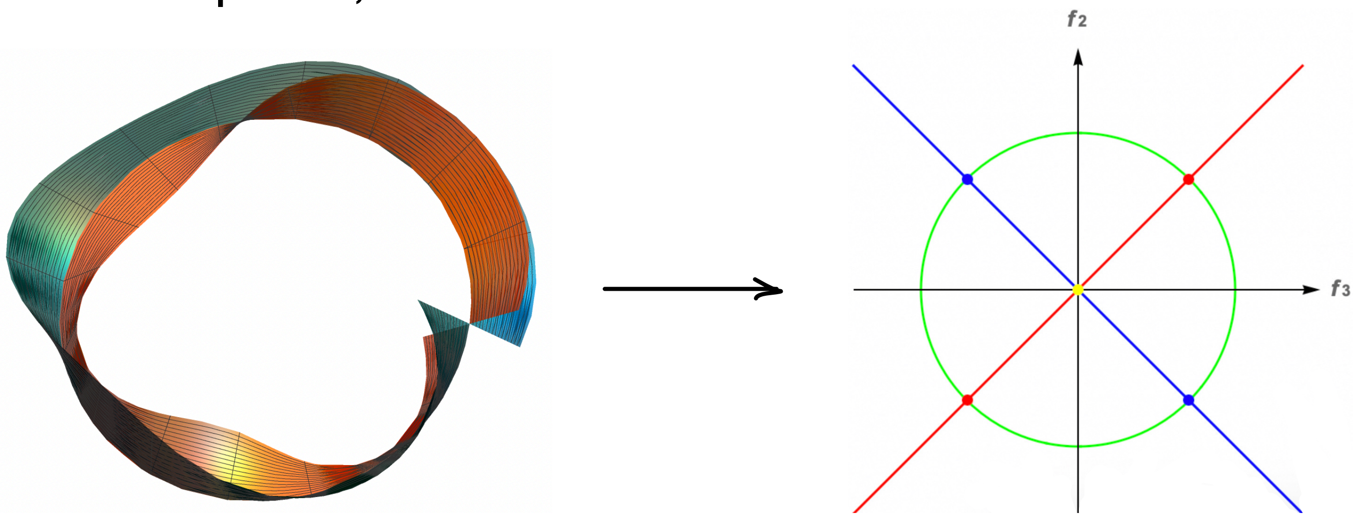

Note. In the non-Hermitian case, since the eigenvectors are in $\mathbb{C}^2$, we have adopted (a variant of) the *Hermitian angle* to properly characterize the eigenframe rotation and deformation:

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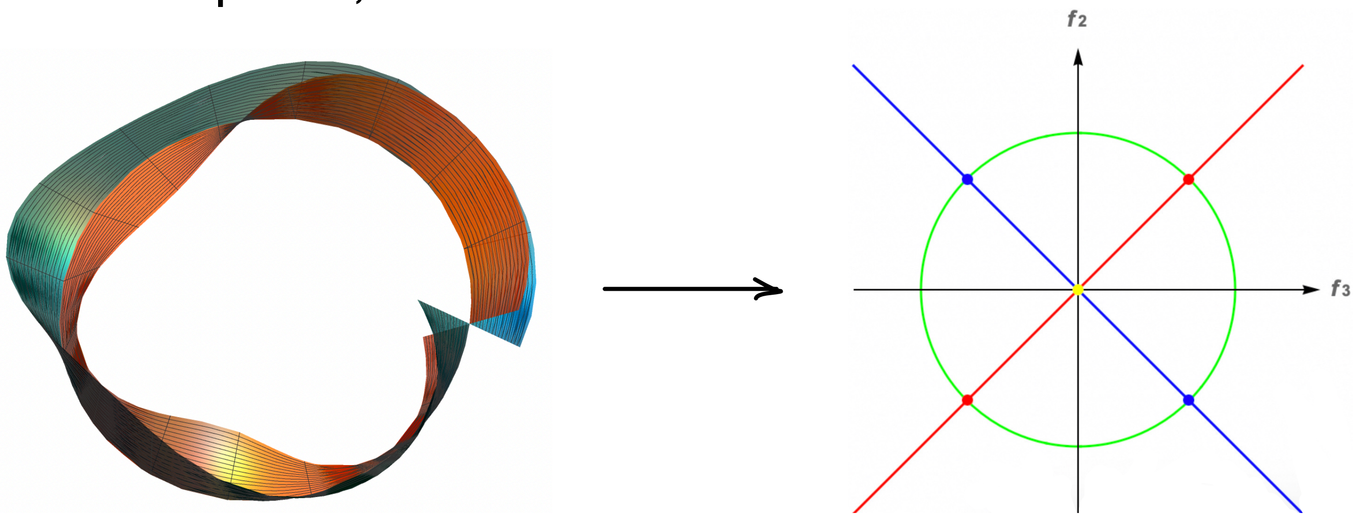

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The intrinsic geometry should be independent of real/complex coordination, though.

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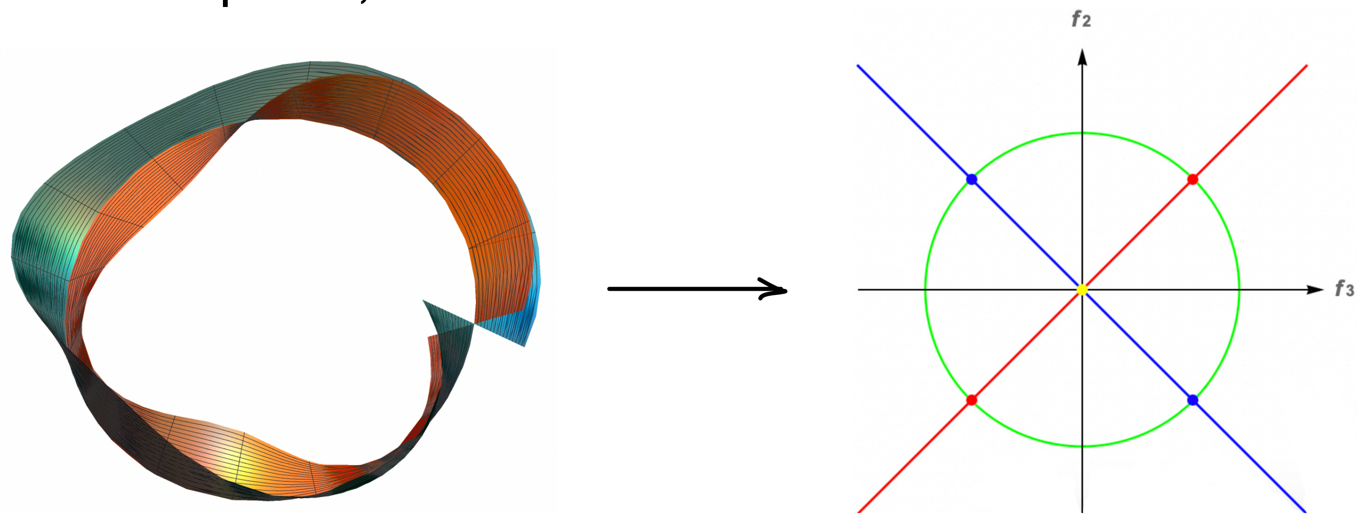

Note. Recently, we have observed that, with respect to the Minkowski-like inner product from the “pseudo-Hermiticity”, the eigenframe behaves the same way as that in the Hermitian system with the usual Euclidean metric, regardless of the degeneracy lines. This indicates that a change of geometry in the moduli space may lead to new understanding both mathematically and physically.

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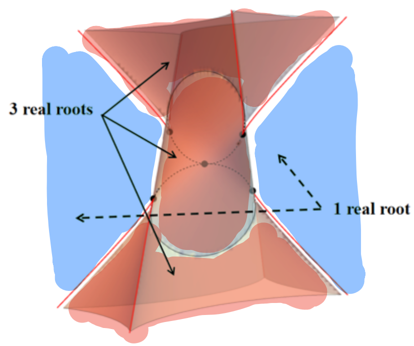

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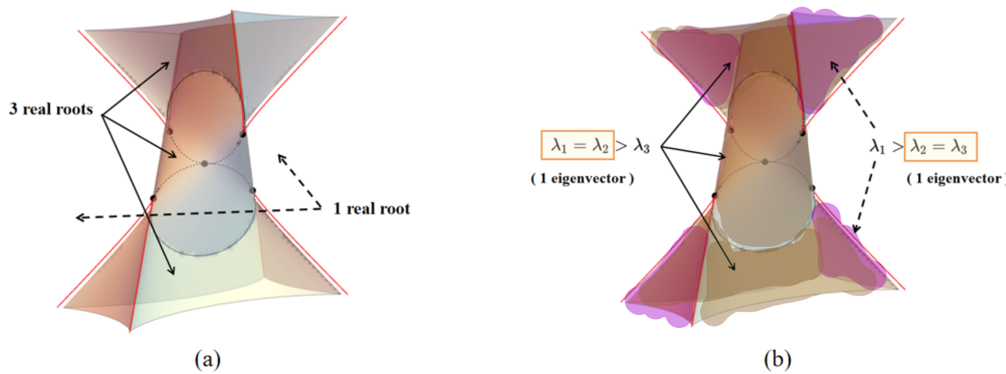

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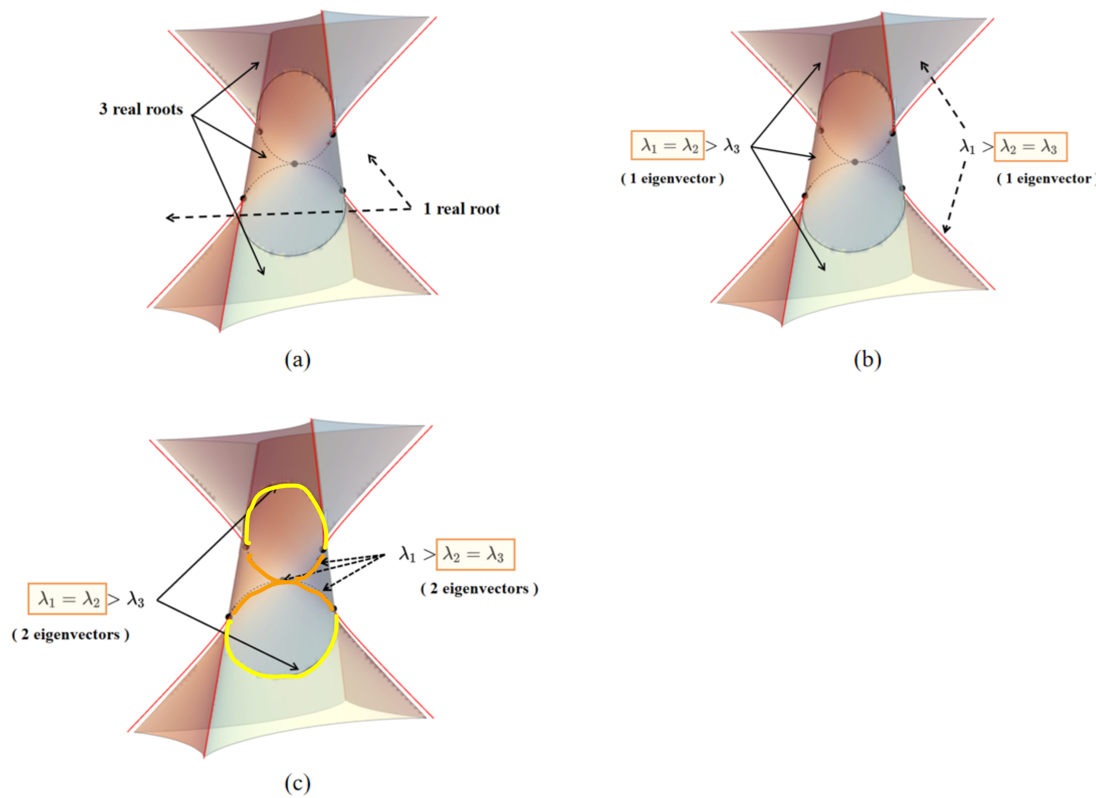

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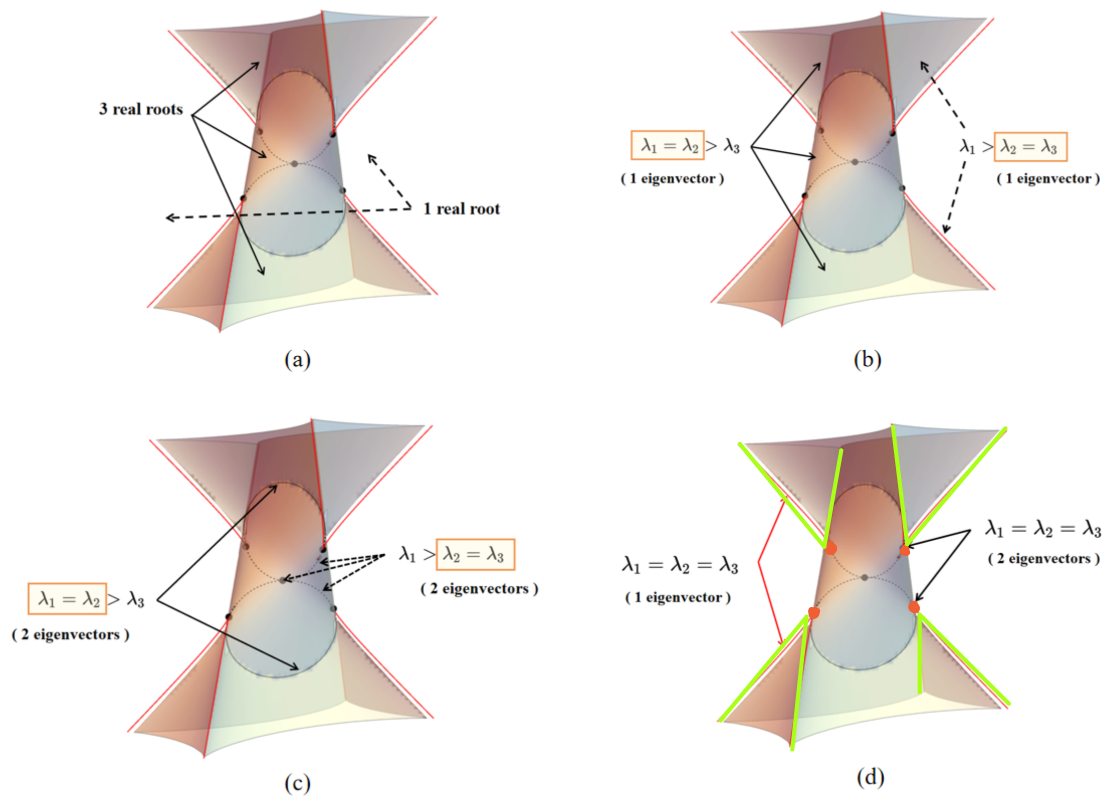

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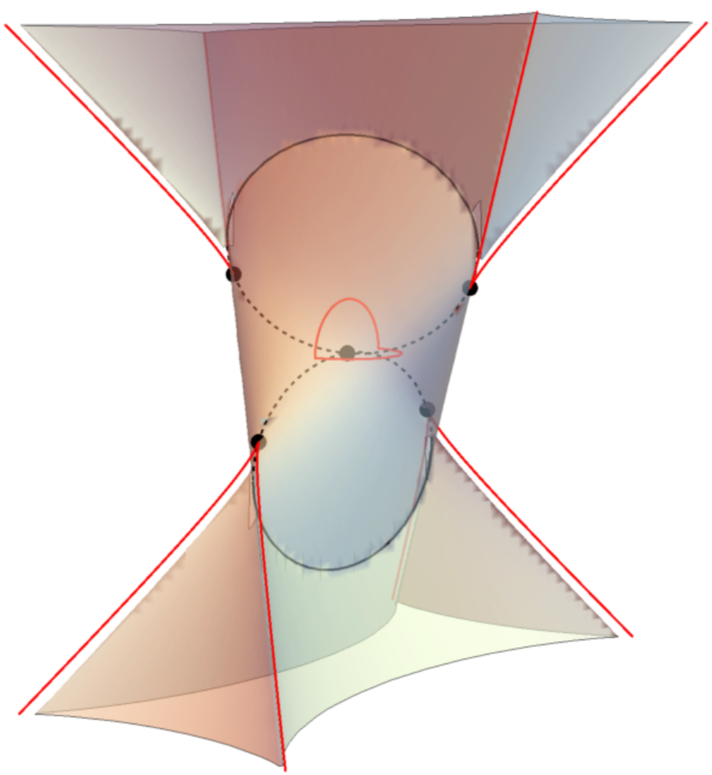

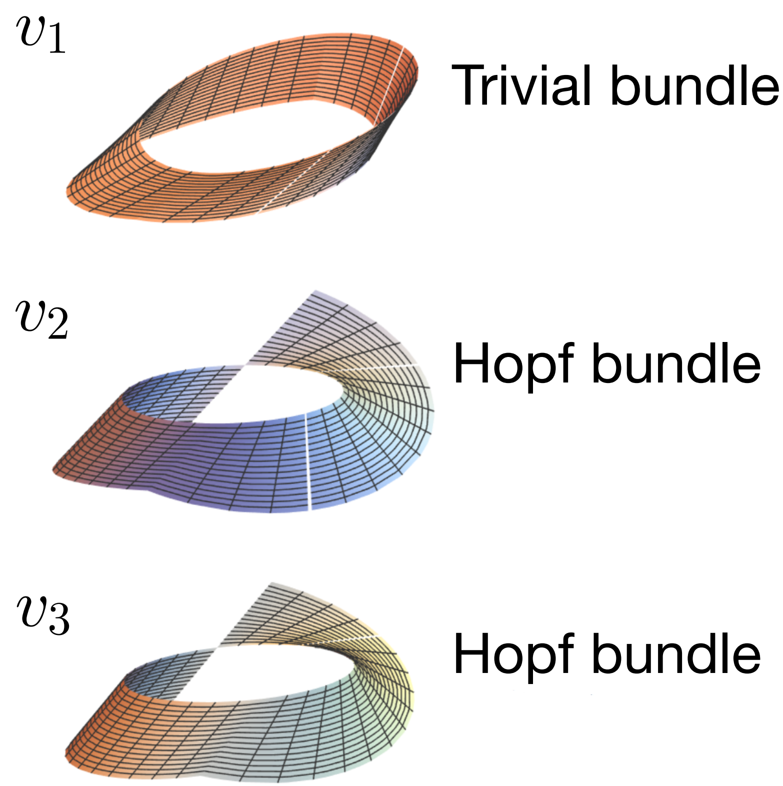

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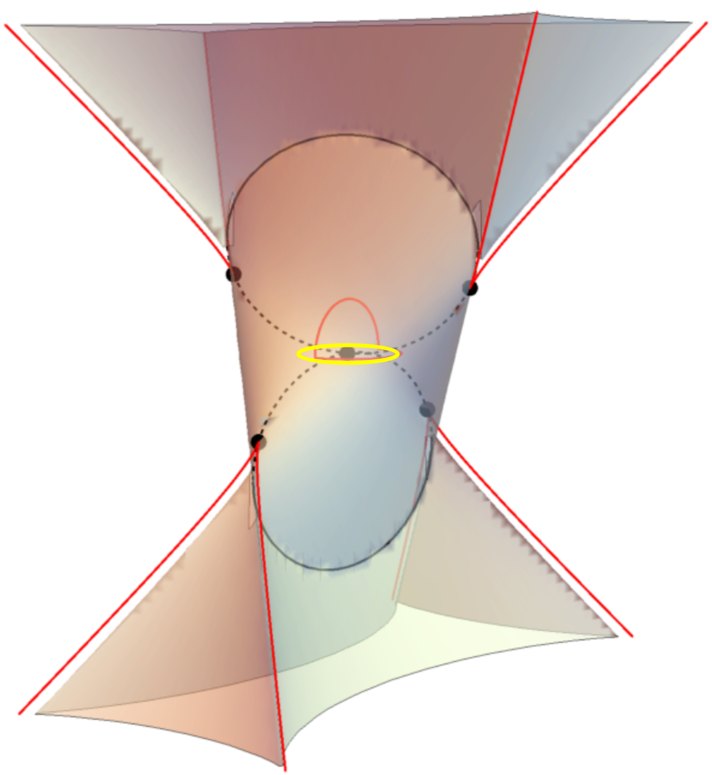

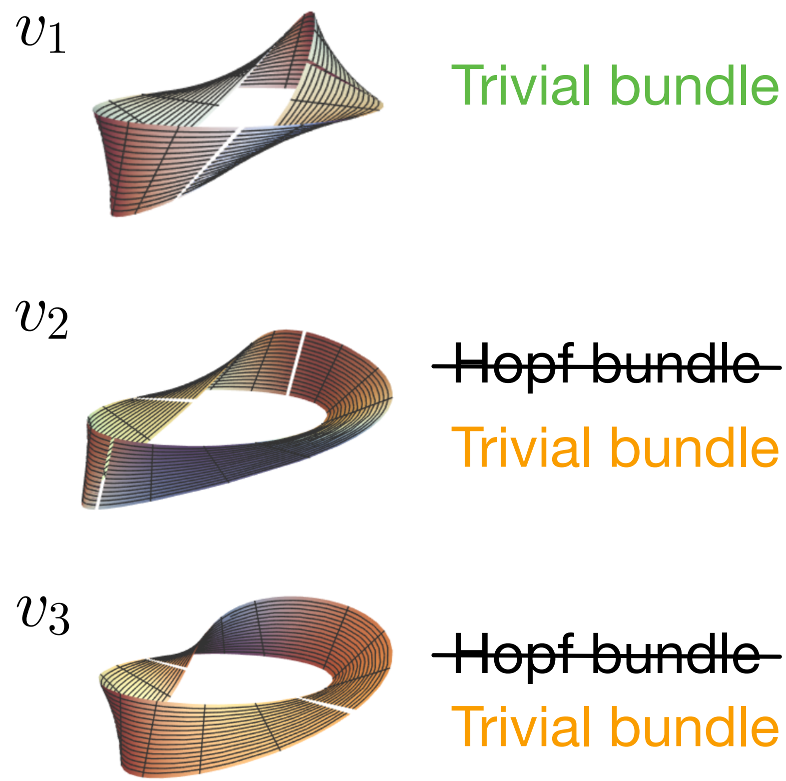

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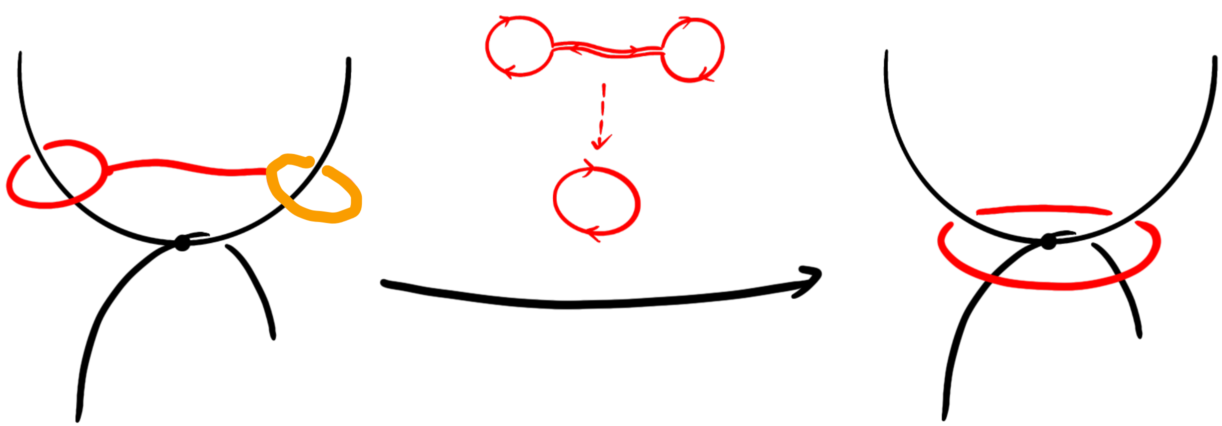

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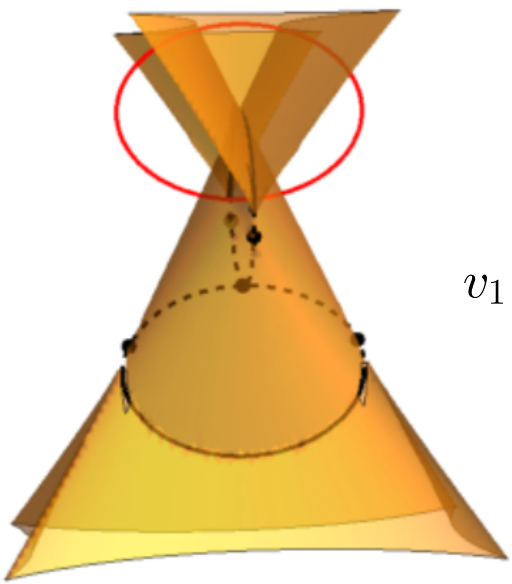

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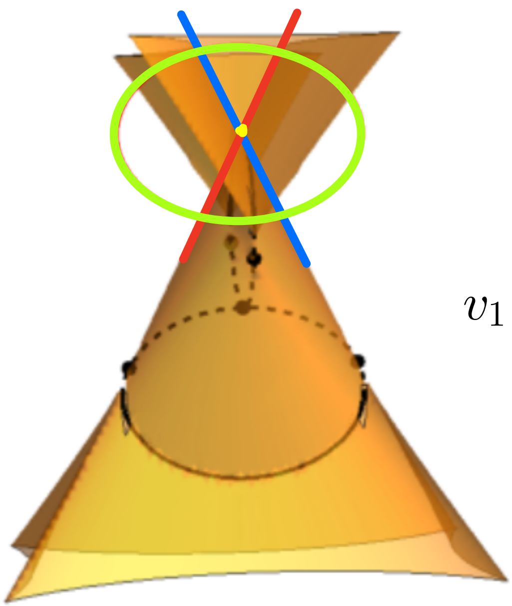

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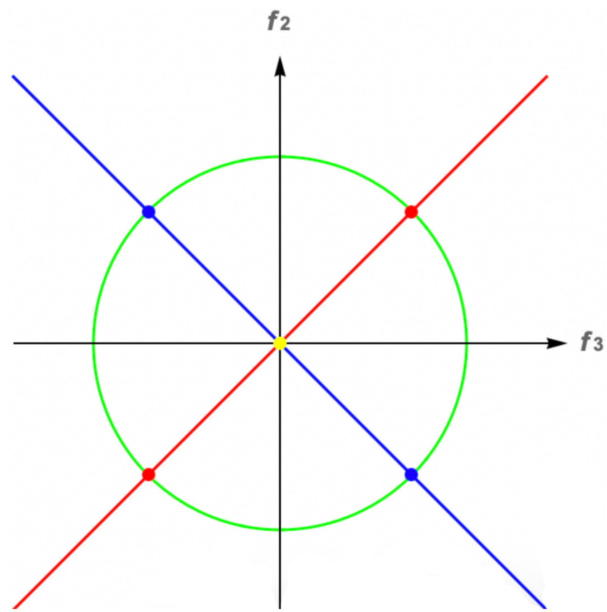

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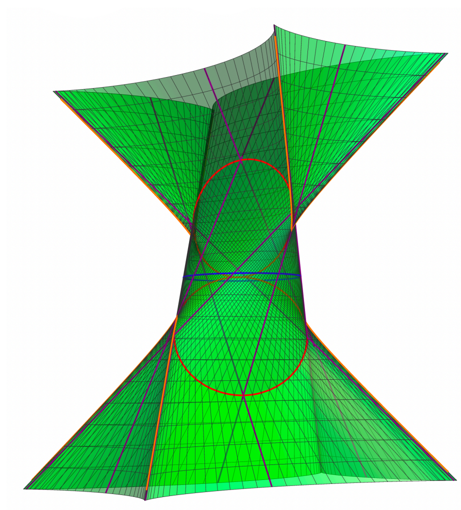

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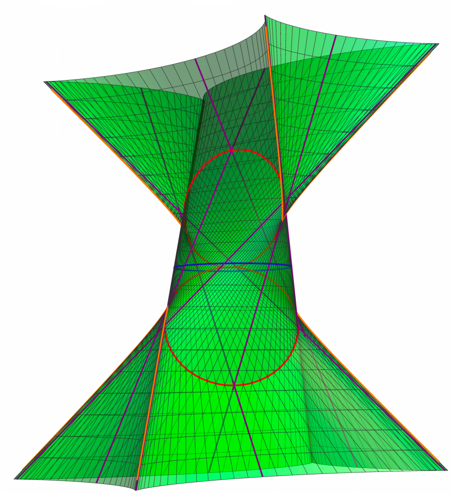

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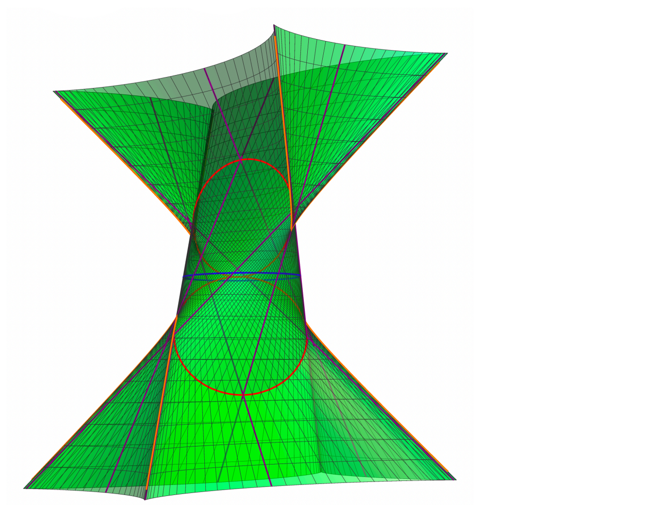

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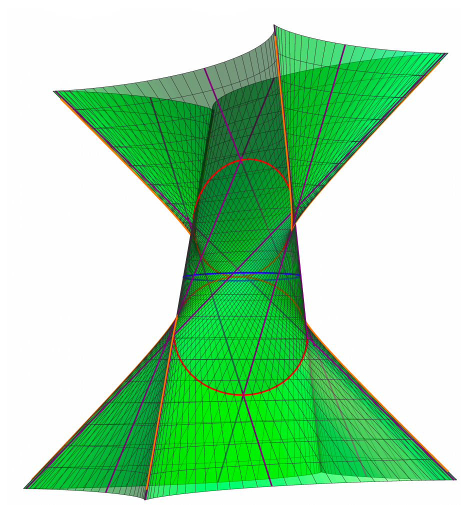

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  ⇒ boundary of a hyperbolic 3-manifold?

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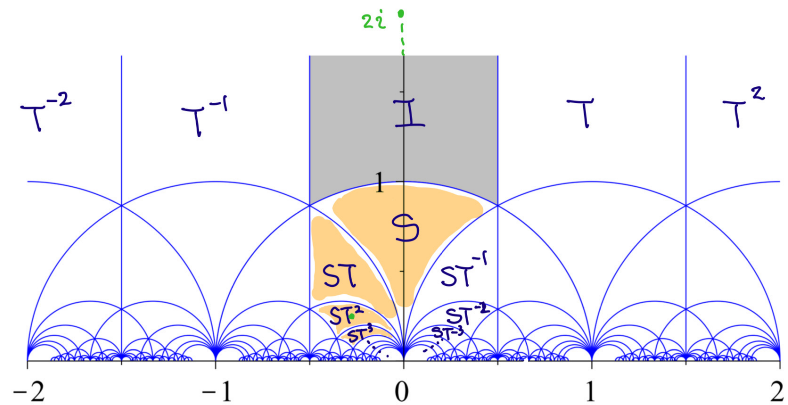

A prototypical 2D hyperbolic lattice with a straight-line boundary

Implications of ruledness:

- Improved precision with graphing and engineering
- In fact, developable ⇒ Gaussian curvature = 0

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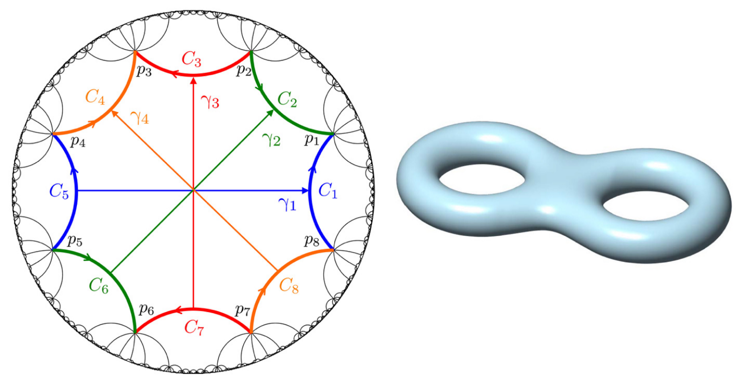

Another basic example of a hyperbolic lattice associated to a genus-2 surface
(from Maciejko and Rayan, *Hyperbolic band theory*, ***Sci. Adv.***, 2021)

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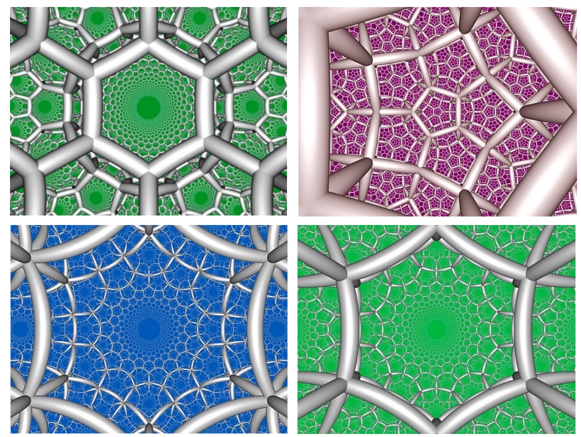

Four 3D hyperbolic lattices tiling up the hyperbolic 3-space $\mathbb{H}^3$ (from John Baez's blog)

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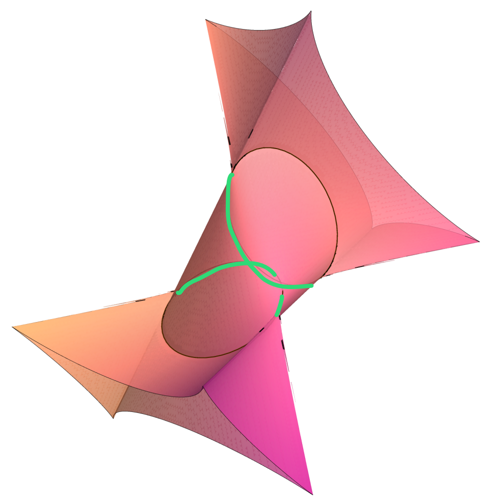

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Existence of nodal curves inside also gives evidence, supporting nontrivial loops around (generating a free group on 3 letters) acting on a 3D hyperbolic lattice.

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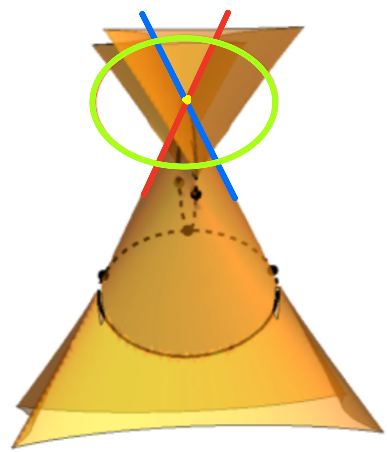

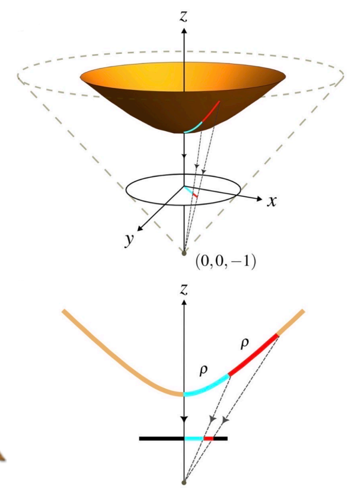

Pictures on the right adapted from Patino, Rasmussen, Ruzzene, ***Phys. Rev. Applied***, 2024

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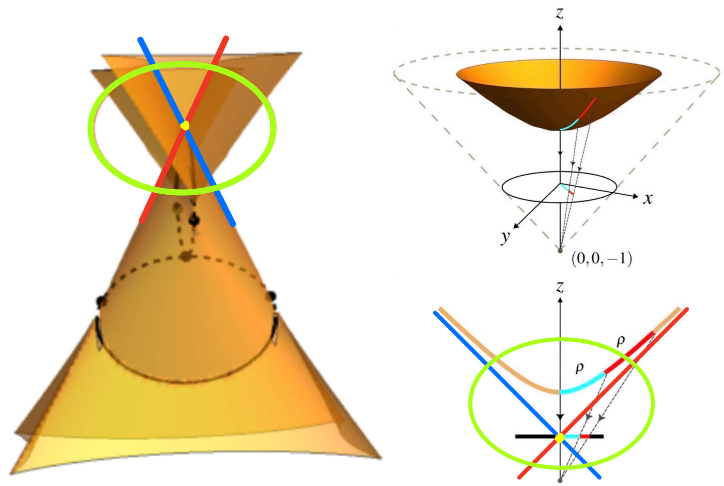

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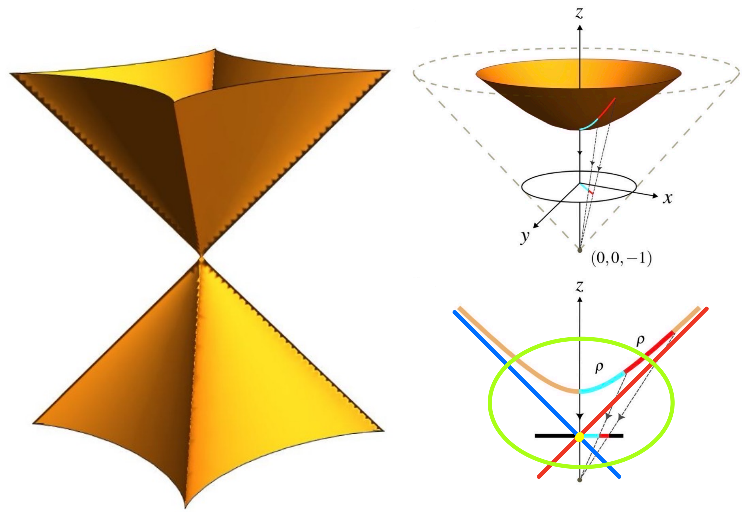

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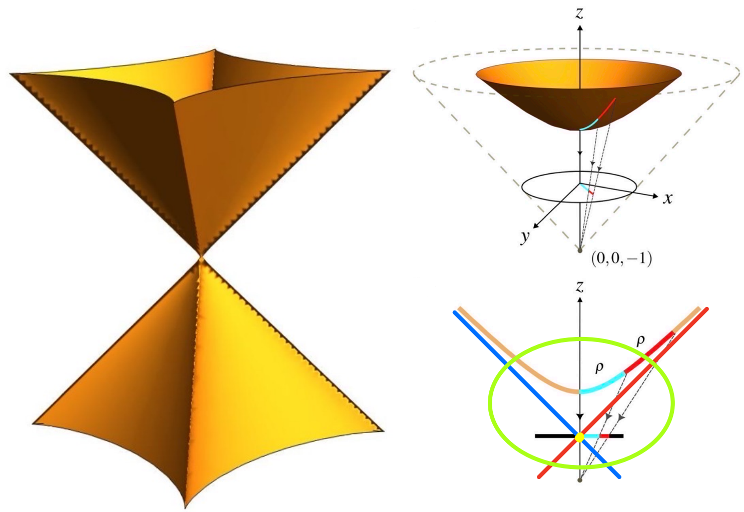

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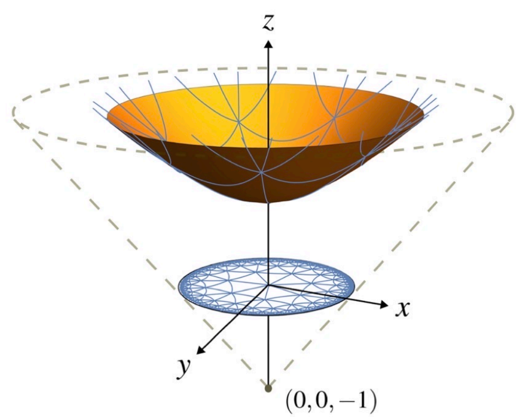

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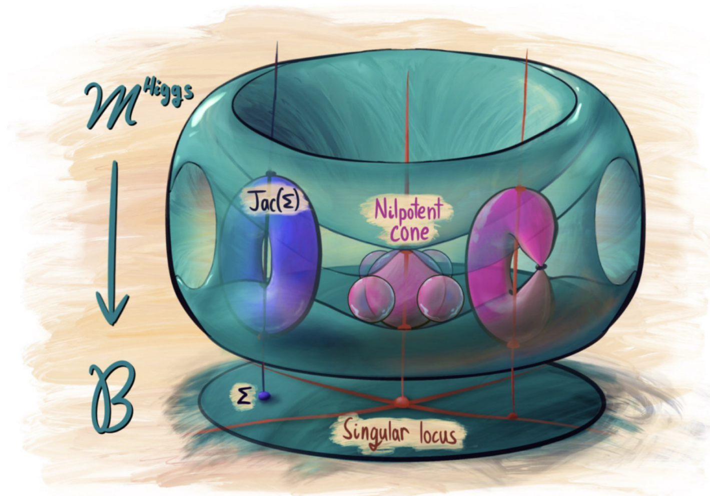

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$$h\colon \mathscr{M}^{\mathrm{S}}_{\mathrm{Higgs}}\big(\mathrm{SL}_n(\mathbb{C})\big) \longrightarrow \bigoplus_{i=2}^{n} H^0(\Sigma; K^i) =: \mathscr{B}$$

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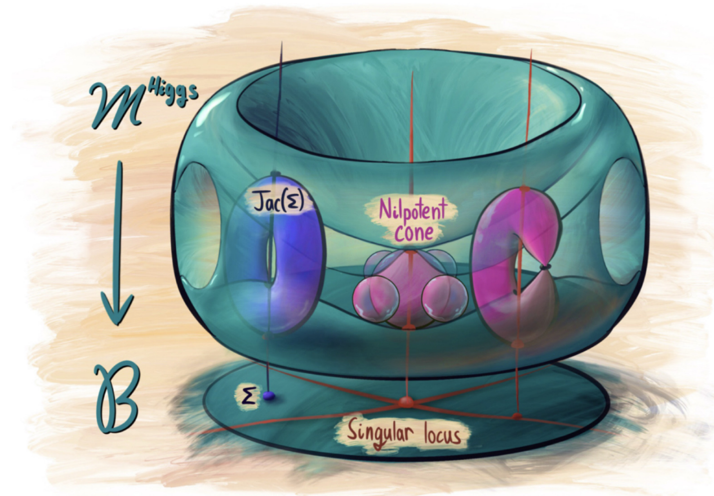

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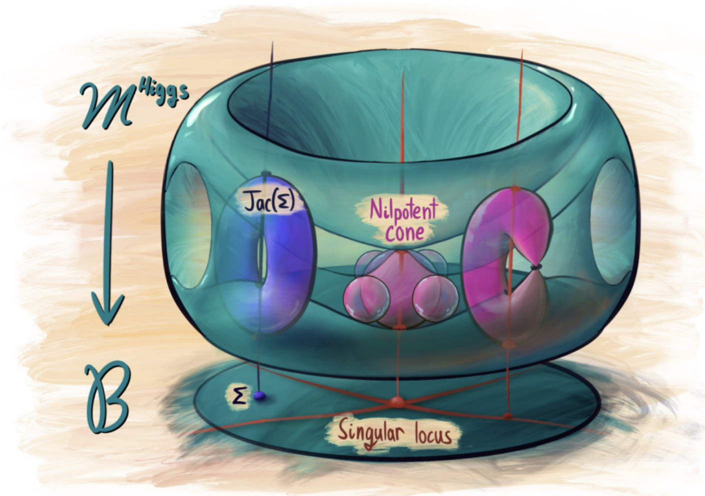

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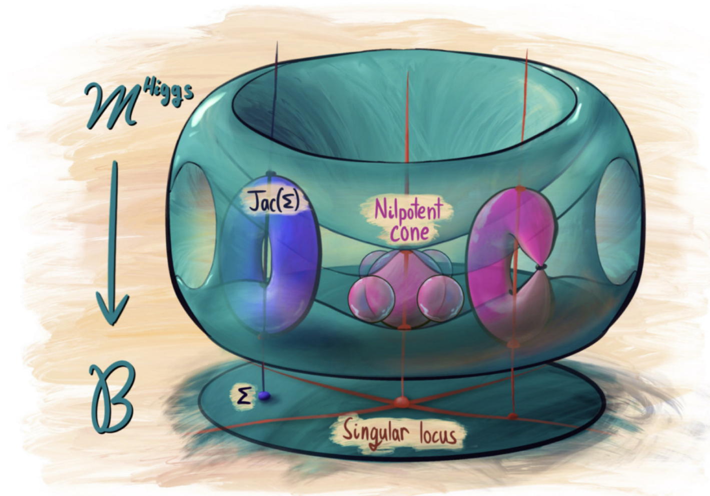

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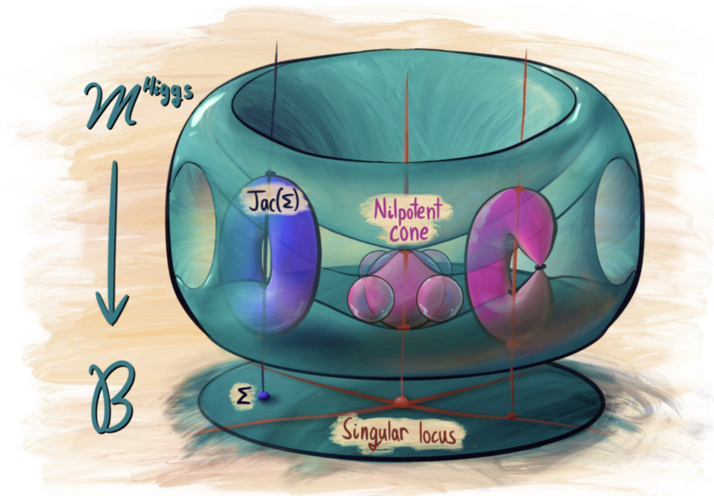

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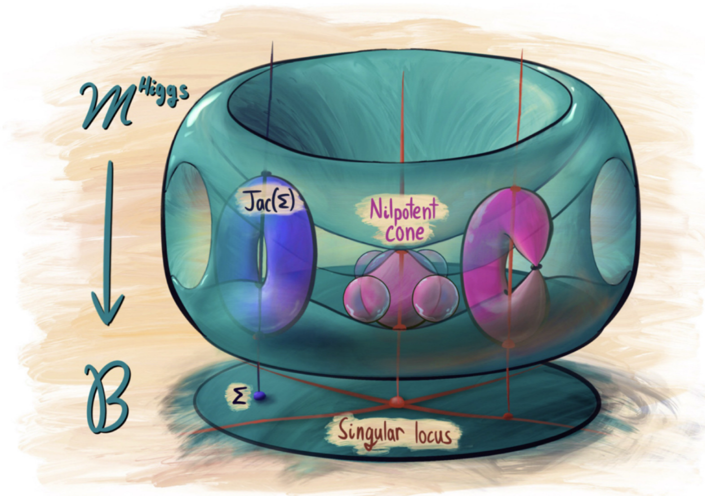

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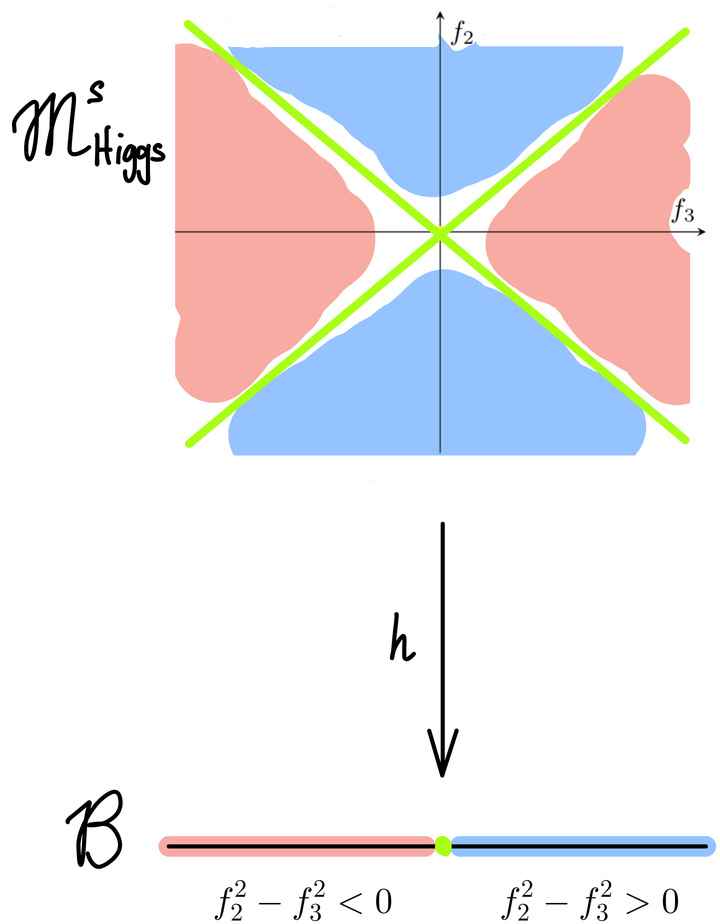

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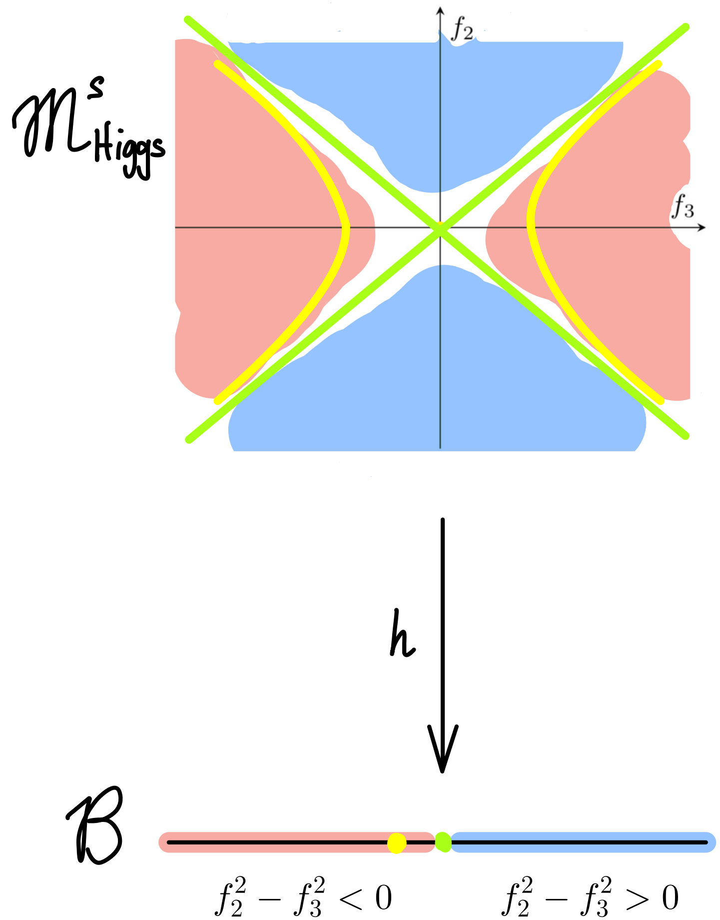

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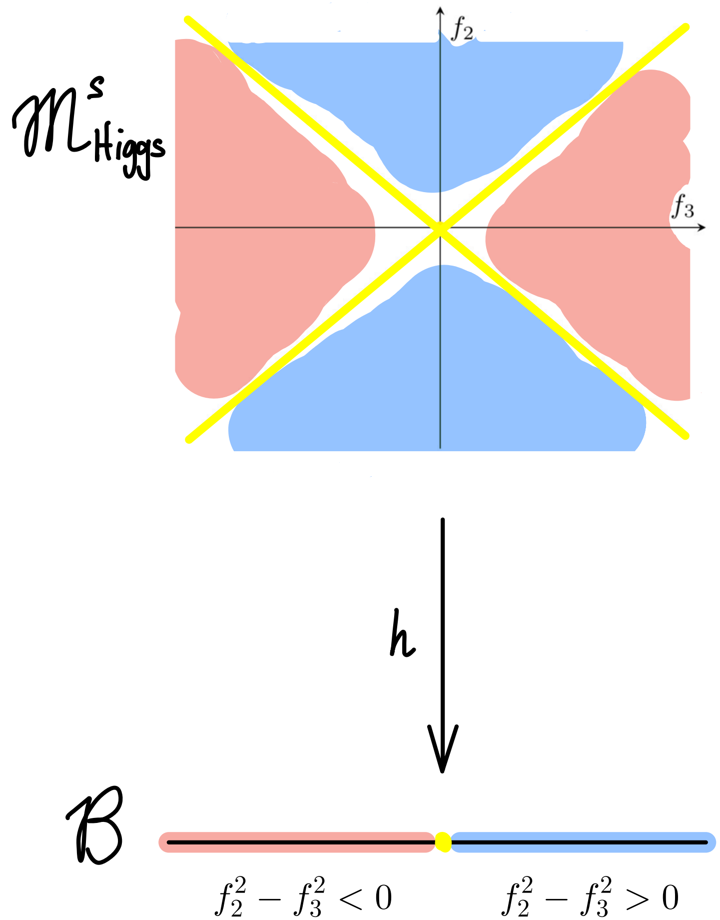

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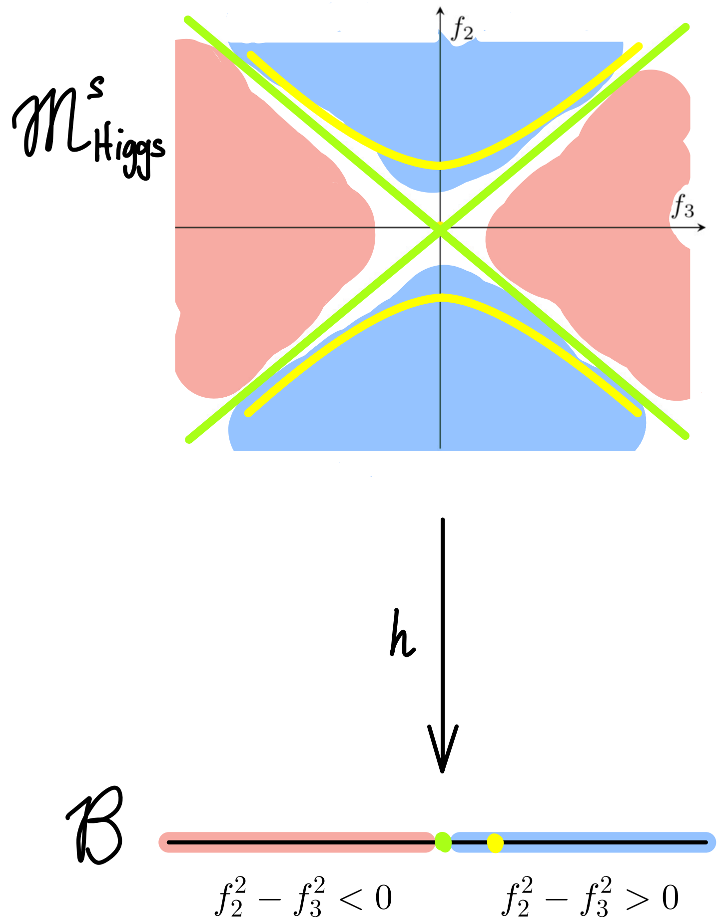

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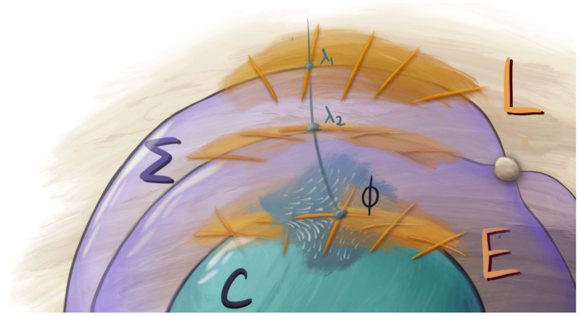

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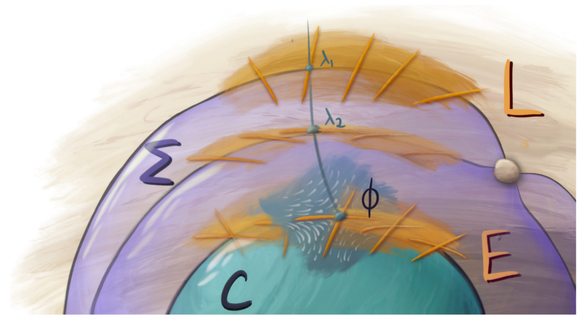

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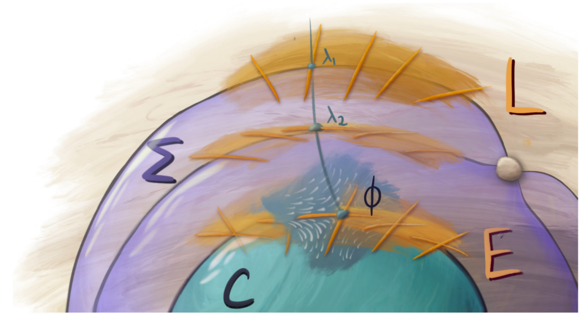

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Thus, given a Higgs bundle (E, ϕ), we get a harmonic map $f\colon \widetilde{C} \to \mathrm{SL}_n(\mathbb{C})/\mathrm{SU}(n)$.

Portrait by Elliot Kienzle

Moduli of Higgs bundles

Hyperbolic metric. Higgs bundles naturally sit over hyperbolic base spaces. The non-Euclidean metric form η in the definition of our non-Hermitian symmetry is compatible with this hyperbolicity through eigenframe deformation.

In fact, the non-Abelian Hodge correspondence gives analytic isomorphisms

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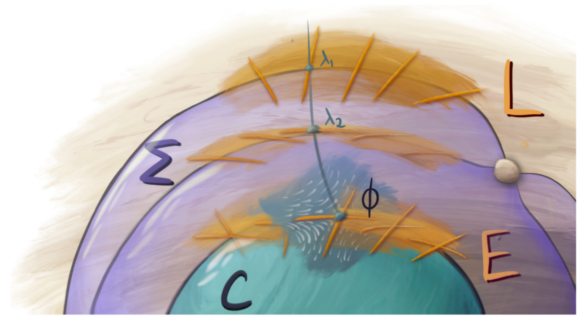

where $\mathscr{H}$ is the space of equivariant harmonic maps from the universal cover $\widetilde{C}$ to $\mathrm{SL}_n(\mathbb{C})/\mathrm{SU}(n)$, modulo isometries. Here, the equivariance is with respect to a representation $\rho\colon \pi_1(C) \to \mathrm{SL}_n(\mathbb{C})$.

Thus, given a Higgs bundle (E, ϕ), we get a harmonic map $f\colon \widetilde{C} \to \mathrm{SL}_n(\mathbb{C})/\mathrm{SU}(n)$. The negative semi-definite Killing form on the Lie algebra $\mathfrak{sl}_n(\mathbb{C})$ gives rise to a metric on $\mathrm{SL}_n(\mathbb{C})/\mathrm{SU}(n)$, which then pulls back along f and descends to C.

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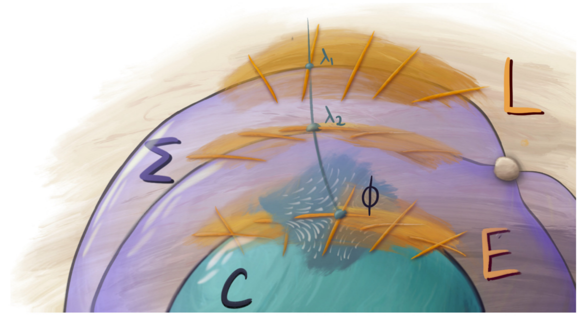

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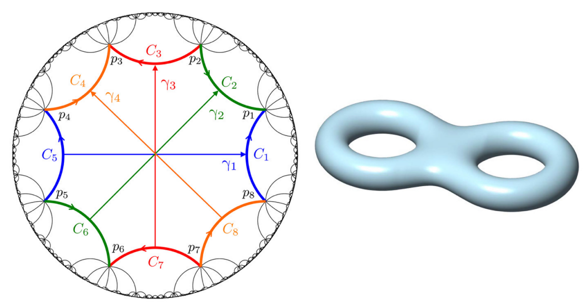

Maciejko–Rayan '21

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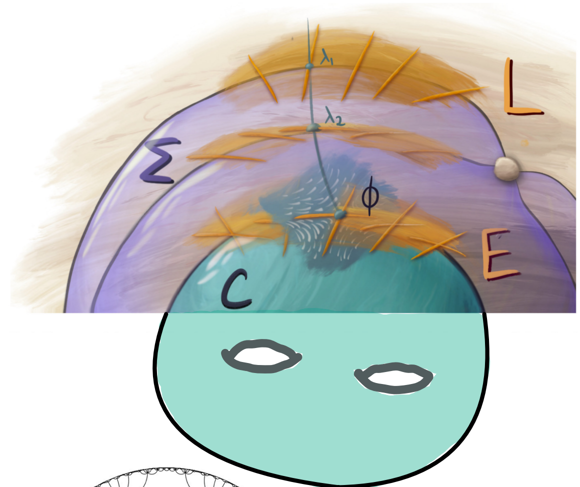

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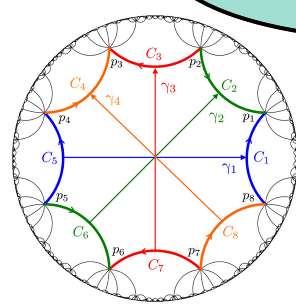

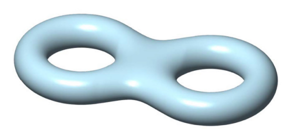

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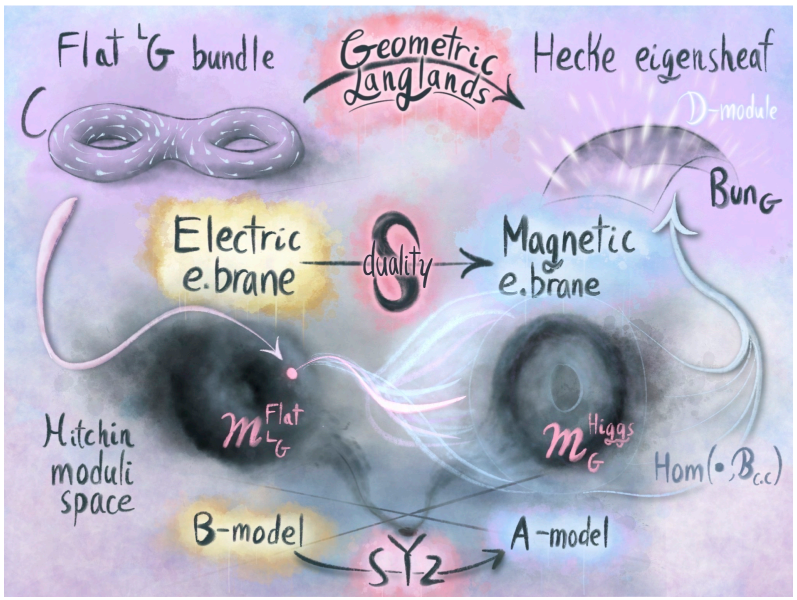

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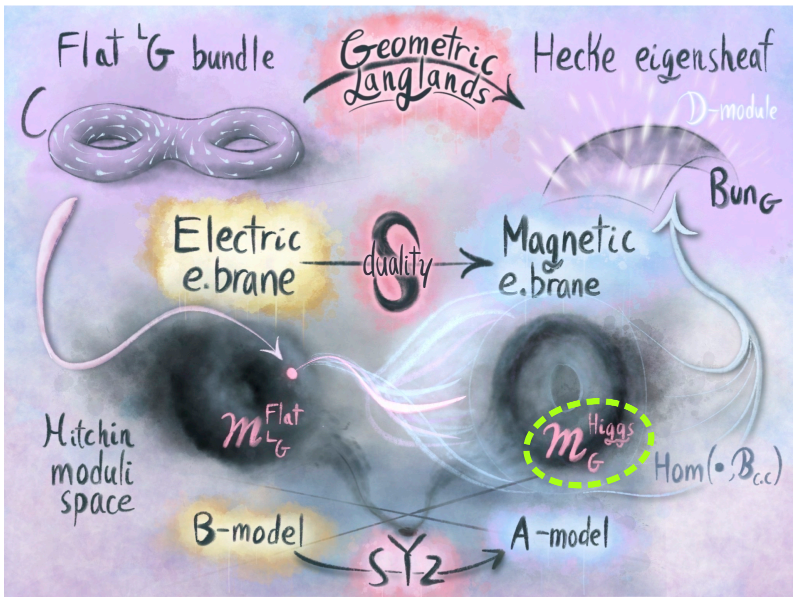

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Thank you.