22nd Westlake Math Colloquium | Yifei Zhu: Topology of stratified singular moduli spaces for gapless quantum mechanical systems

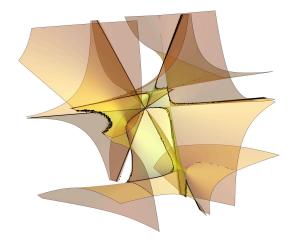
Time: 16:00-17:00, Friday, Nov 11, 2022 Venue: E4-233, Yungu Campus & ZOOM ZOOM ID: 863 6606 6486 PASSCODE: 738489

Host: Dr. Xing Gu, Institute for Theoretical Sciences, Westlake University

Speaker: Dr. Yifei Zhu, an assistant professor at the Department of Mathematics of the Southern University of Science and Technology. His research interests are in algebraic topology and related fields, particularly in its connections to algebraic geometry and number theory via objects such as formal groups, elliptic curves, and modular forms.

Title: Topology of stratified singular moduli spaces for gapless quantum mechanical systems **Abstract:** This talk presents an external application of the algebraic topology of moduli spaces. In condensed matter physics, the Hamiltonian of a quantum mechanical system takes a mathematical form of a square matrix, with parameters functions on the 3D momentum space. Such a matrix satisfies the Hermitian symmetry, so that its eigenvalues are real and represent observed energies. We will discuss this space of parameters for Hamiltonians, especially its degeneracy locus where eigenvalues occur with multiplicities. Such a locus gives rise to exceptional properties in the larger scale, with applications to the design of sensing and absorbing devices. We focus on certain non-Hermitian Hamiltonians, the imaginary parts of whose eigenvalues model energy exchange of open systems. Their parameter space possesses intriguing topology, with a stratification of non-isolated singularities, which affords interesting phenomena such as the so-called bulk-edge correspondence. The associated algebraic invariants enable classifications and predictions for phases of matter. This work is in collaboration with C. T. Chan, Jing Hu, Hongwei Jia, Xiaoping Ouyang, Yixiao Wang, Yixin Xiao, Ruo-Yang Zhang, and Zhao-Qing Zhang.

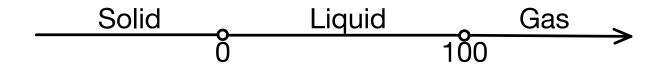
Topology of stratified singular moduli spaces for gapless quantum mechanical systems



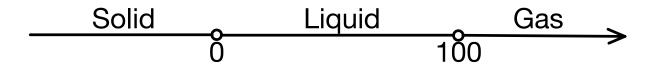
Yifei Zhu (SUSTech)

Westlake Math Colloquium, November 2022

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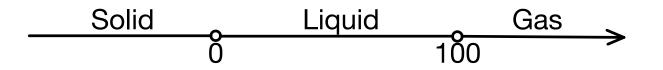


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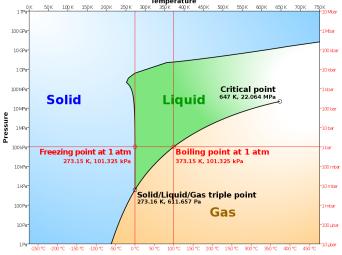
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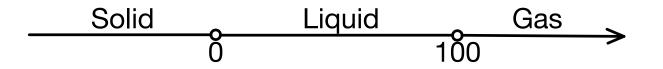


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If we also allow pressure to vary, then there are only two phases of H_2O .



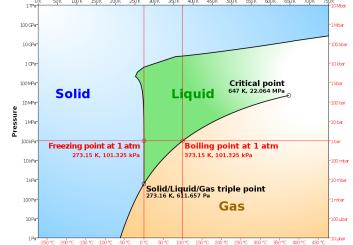
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A mathematical framework



There is a space \mathcal{M} of "systems" with a "singular" locus $\Delta \subset \mathcal{M}$, and we are interested in $\pi_0(\mathcal{M} - \Delta)$ or, more generally, the homotopy type of $\mathcal{M} - \Delta$.

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Let $\Delta \subset \mathcal{M}_n$ be the locus of *n*-tuples $x = (x^1, ..., x^n)$ in which not all x^i are distinct. Configurations in $\mathcal{M}_n - \Delta$ satisfy a "gap condition," and now there *is* nontrivial topology: $\mathcal{M}_n - \Delta$ has *n*! contractible components.

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A gapped configuration $x \in \mathcal{M}_n - \Delta$ determines a permutation $\sigma(x) \in \text{Sym}_n$. In fact, σ induces an isomorphism $\pi_0(\mathcal{M}_n - \Delta) \cong \text{Sym}_n$ of *groups*.

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- There is a complete invariant of the path component, which is an isomorphism to a known or computable set.
 Such a complete invariant is not present in all situations.

Why do we care about moduli spaces for physical systems?



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Design materials that can "do wonders", which cannot be found in nature, e.g., invisibility cloaks.

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where **1** is the identity matrix and $\vec{\sigma} = (\sigma_1, \sigma_2, \sigma_3)$ are the Pauli matrices $\sigma_1 = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$ $\sigma_2 = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$ $\sigma_3 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$

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We compute for which values of parameters H_2 has a doubled eigenvalue.

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$$\Rightarrow H_{2} = \mathbf{1} - 2|\phi_{-}\rangle\langle\phi_{-}|$$

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Thus the moduli space $\mathcal{M}_2 = SO(2)/\mathbb{Z}_2 \cong S^1$ and its "topological charge" (a homotopy invariant) is $\pi_1(\mathcal{M}_2) \cong \mathbb{Z}$.

Taking

$$f_1(\overrightarrow{k}) = k_x k_z$$

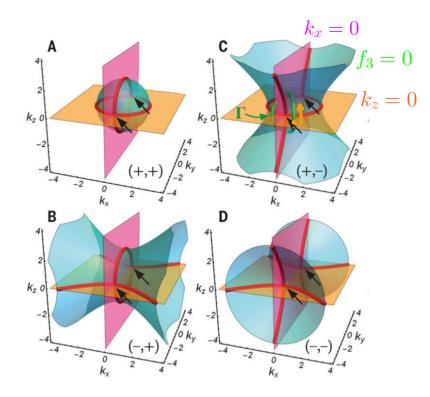
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Wu et al., Science 365, 1273-1277 (2019)

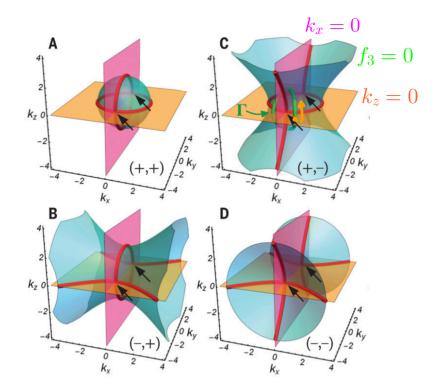
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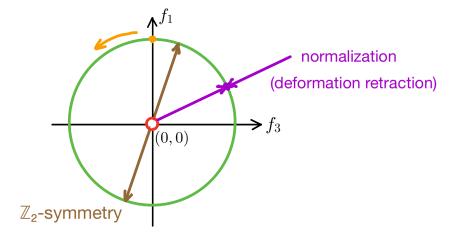
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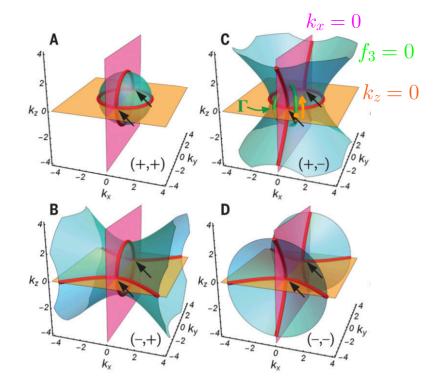
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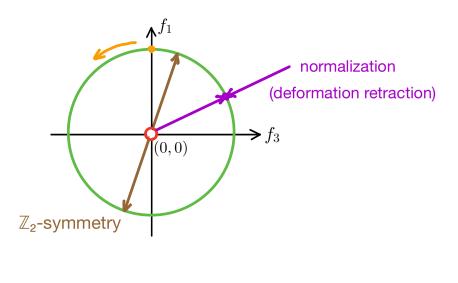
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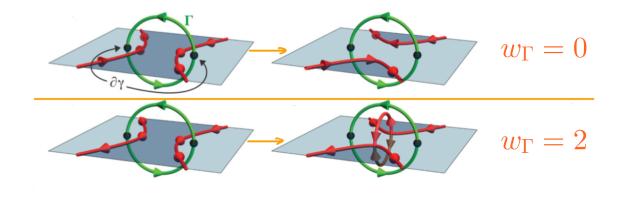
and in the moduli space



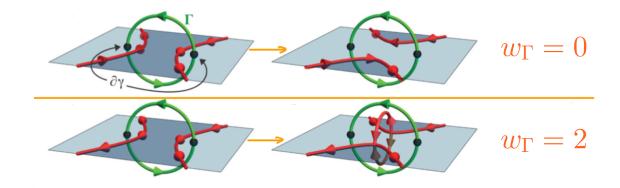
The winding number w_{Γ} of the loop Γ equals 2.

Wu et al., Science 365, 1273-1277 (2019)

The winding number serves as a topological classifier:

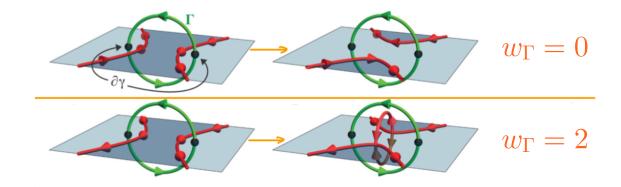


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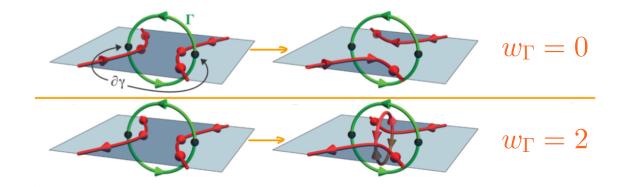


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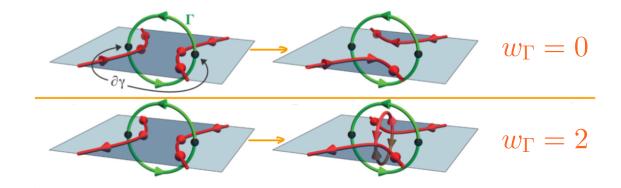
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and $\pi_1(\mathcal{M}_3) \cong Q = \{\pm 1, \pm i, \pm j, \pm k\}$, the quaternion group.

The winding number serves as a topological classifier:



More generally, for all $n \ge 2$, Wu et al. computed topological charges for *n*-band Hermitian Hamiltonians with PT symmetry and found that $\pi_1(\mathcal{M}_n)$ is non-Abelian when $n \ge 3$. For example,

$$\mathcal{M}_3 = \mathrm{SO}(3)/D_2$$

where D_2 = the three-dimensional "dihedral" crystallographic point group \cong the Klein four-group

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(We have $\pi_1(SO(3)) \cong \pi_1(\mathbb{R}P^3) \cong \mathbb{Z}_2$, $SU(2) \cong S^3$ its 2-fold universal cover.)

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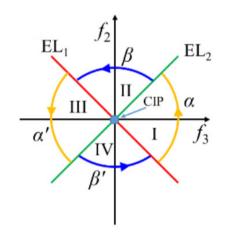
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Here emerge non-isolated, stratified singular loci, making our systems gapless and their topology much intriguing.

$$H_2 = \begin{bmatrix} f_3 & f_2 \\ -f_2 & -f_3 \end{bmatrix}$$
 (Recall Hermitian $\begin{bmatrix} f_3 & f_1 \\ f_1 & -f_3 \end{bmatrix}$)

In the generic 2-band case, we give complete invariants.

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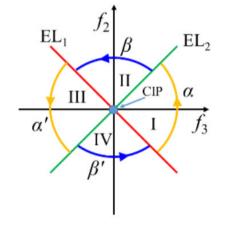


I, III: real eigenstates

II, IV: complex eigenstates

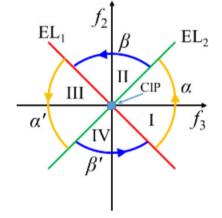


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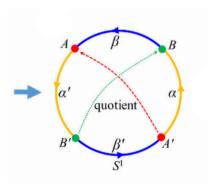


- I, III: real eigenstates II, IV: complex eigenstates Stratified singular locus:
- EL (exceptional line): doubled eigenstate (defective degeneracies)
- CIP (complete intersection point): η-orthogonal eigenstates (non-defective degeneracy)

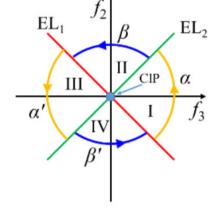
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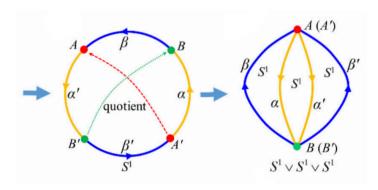
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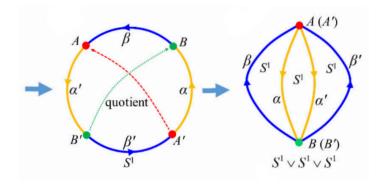


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 EL_2

CIP

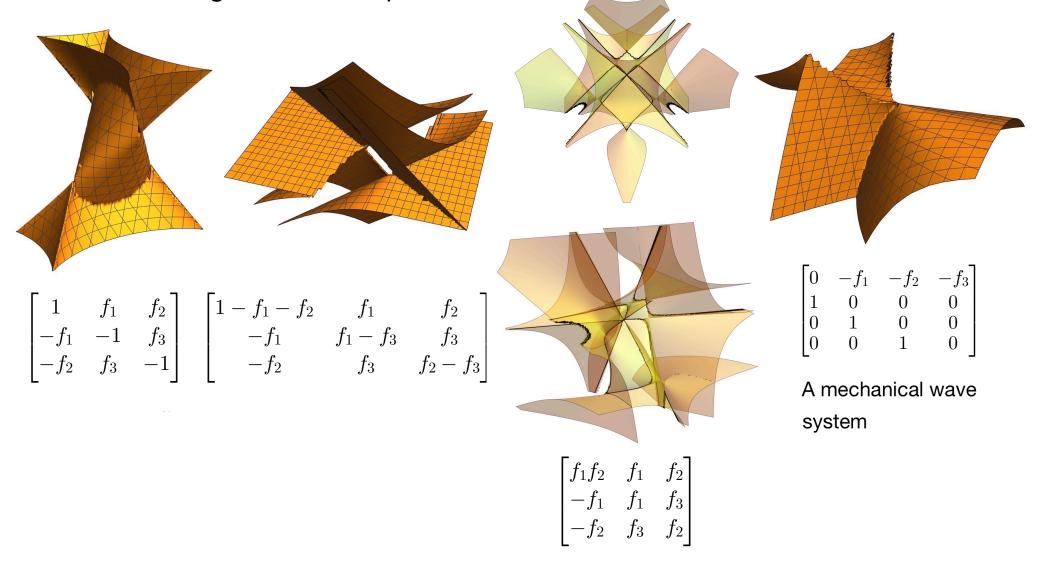
EL₁

 α'

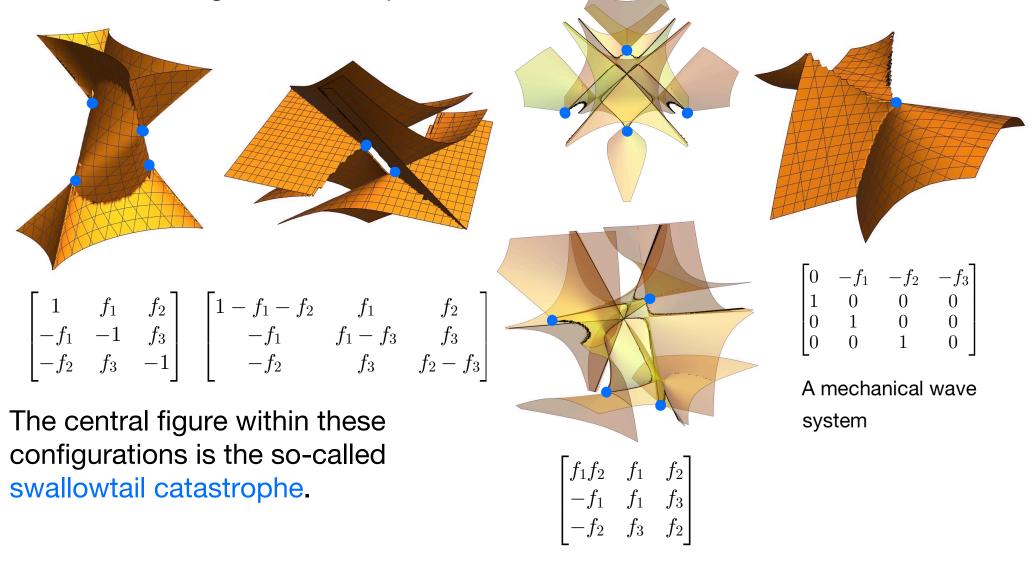
III

The moduli space \mathcal{M}_2 can be identified as $S^1 \vee S^1 \vee S^1$ doubly covering $S^1 \vee S^1$. Thus $\pi_1(\mathcal{M}_2)$ is a free subgroup of $F(a, \beta)$ on 3 generators. This gives the gapless system a physically meaningful, non-Abelian topological charge.

The 3-band case is more complex and exotic. Here is a sample of portraits for the stratified singular moduli spaces.

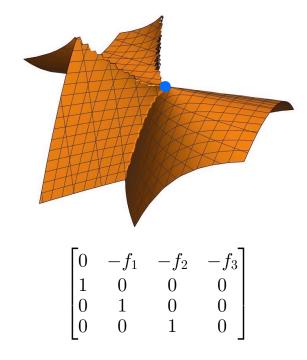


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The singularity of a swallowtail arises in the discriminant surface of a generic degree-4 polynomial. Here, it is the characteristic polynomial of $H(f_1, f_2, f_3)$.

$$\begin{vmatrix} -\omega & -f_1 & -f_2 & -f_3 \\ 1 & -\omega & 0 & 0 \\ 0 & 1 & -\omega & 0 \\ 0 & 0 & 1 & -\omega \end{vmatrix} = \omega^4 + f_1 \omega^2 + f_2 \omega + f_3$$

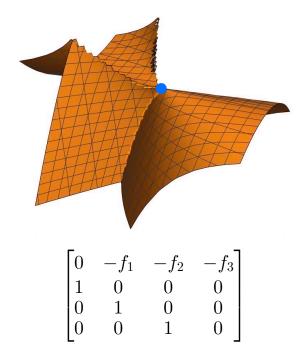


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https://vifeizhu.github.io/swtl.mp4



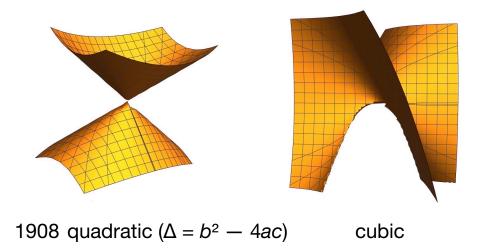
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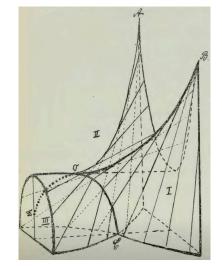
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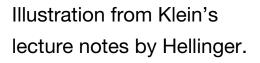
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Discriminant surfaces are ruled (in fact, developable).







 $\begin{bmatrix} 0 & -f_1 & -f_2 & -f_3 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}$

As the singular loci of moduli spaces for polynomials, swallowtail and other catastrophes are important and well-studied objects in dynamical systems and algebraic geometry. Arnold famously related their complements to braid groups and computed their cohomology, establishing a connection to topology as well.

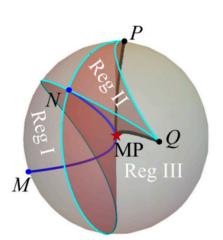


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However, moduli spaces for Hamiltonians carry additional structures and are more complex:

 Physicists desire classifications for the behavior of eigenstates along a loop across/encircling the stratified non-isolated singularity (e.g., Berry phase of adiabatic transformation, close and open of gaps).



Reg I and Reg II: PT-exact phases Reg III: PT-broken phase



V. I. Arnold's tombstone at the Novodevichy Cemetery in Moscow

• Over the reals, we know less even on the mathematical side.

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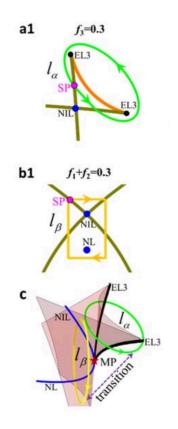
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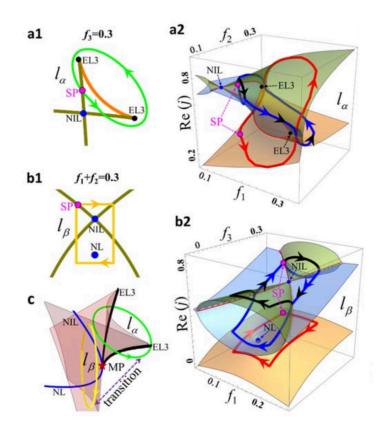
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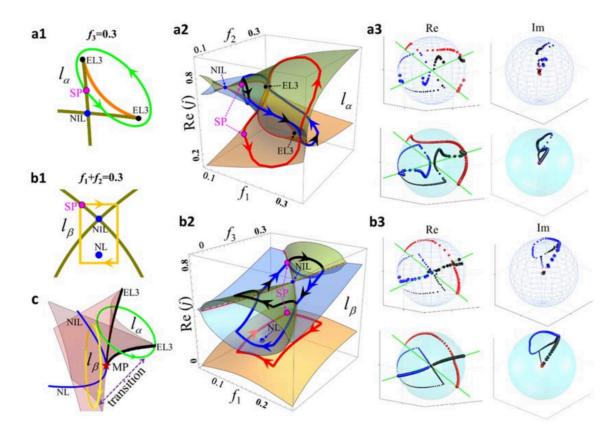
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- a3, b3: trajectories of eigenframe, experimental (above) and theoretical (below)

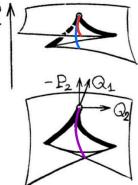
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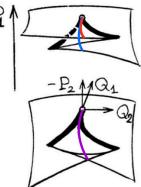
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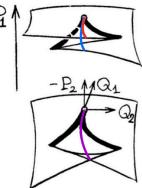
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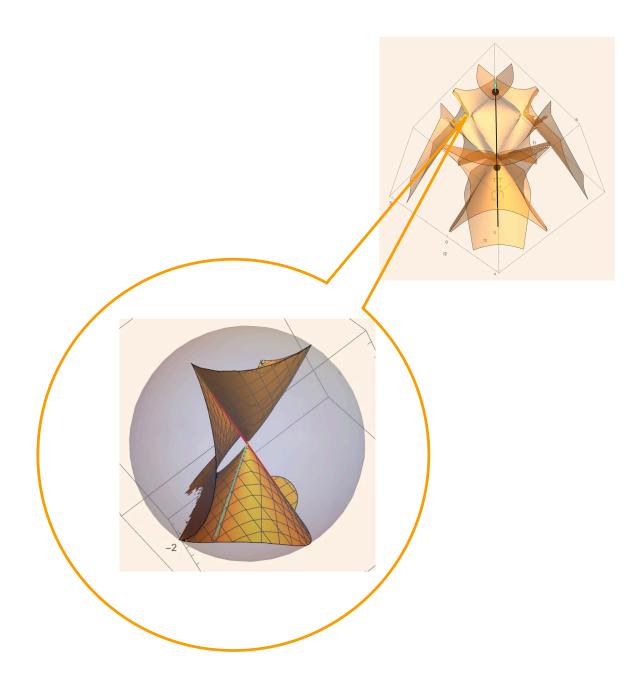
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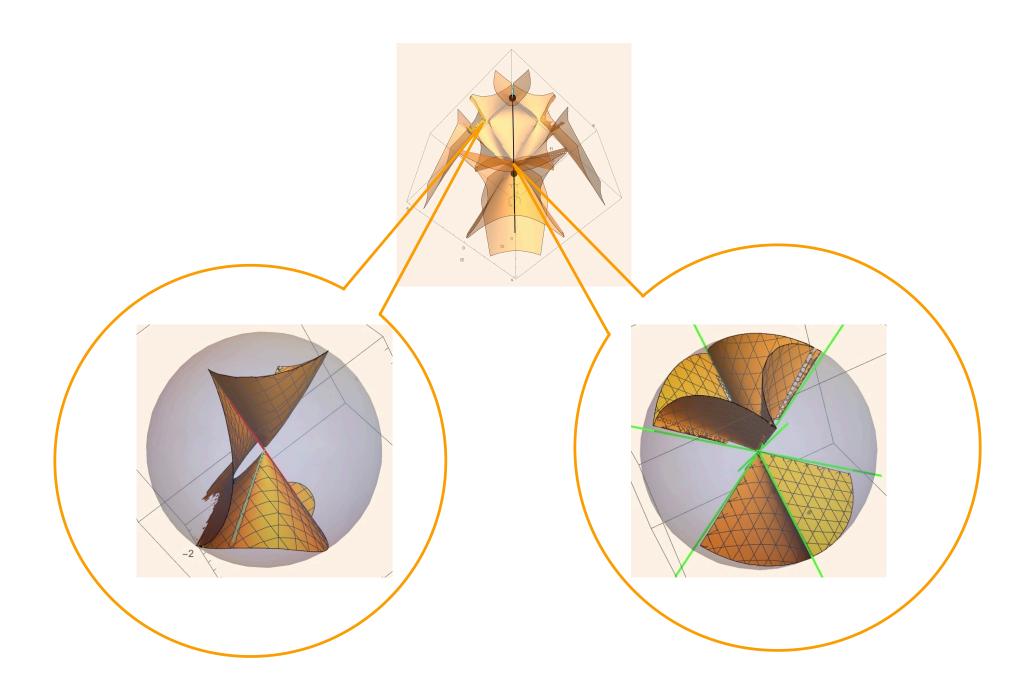
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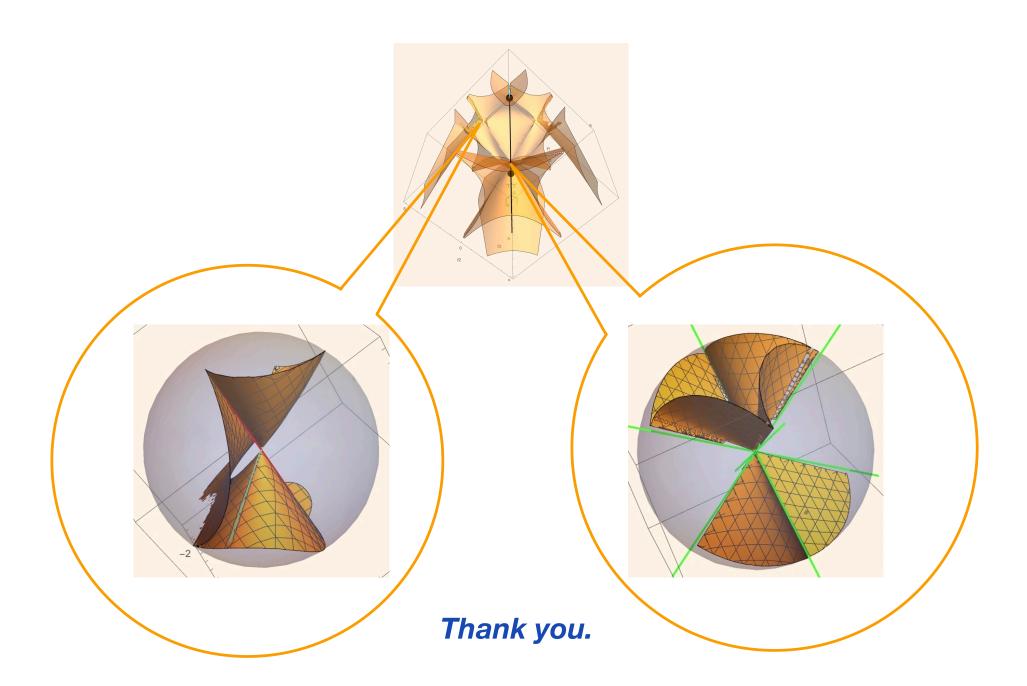


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 We have been zooming in to local details of combinations of swallowtails (and other basic types of singularities) in order to pass from local invariants to global (and complete) invariants via fuller power of algebraic topology.







Credits and references

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- Phase diagram of water (simplified) from Wikipedia (author of the original work: Cmglee)
- Beijing Winter Olympics picture: http://en.kremlin.ru/events/president/news/67715
- Quadric surfaces diagrams for \vec{k} -spaces of Hermitian systems and winding number comparison diagrams adapted from

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- Order parameter space diagrams for non-Hermitian systems from Hongwei Jia, Ruo-Yang Zhang, Jing Hu, Yixin Xiao, Yifei Zhu, and C. T. Chan, *Topological classification for intersection singularities of exceptional surfaces in pseudo-Hermitian systems*, preprint, 2022
- 3D plots for 3-band-system moduli spaces drawn with Mathematica, middle-right pair by Hongwei Jia
- Swallowtail 3D video: Oliver Labs, https://yifeizhu.github.io/swtl.mp4
- Sketch of ruled swallowtail surface from Felix Klein's lecture notes by Ernst David Hellinger, 1907–1909.
- Photo of Arnold's tombstone from Boris A. Khesin and Serge L. Tabachnikov, ed., Arnold: Swimming against the tide, American Mathematical Society, 2014
- Spherical swallowtail plot, loop transition video and diagrams from Jing Hu, Ruo-Yang Zhang, Yixiao Wang, Xiaoping Ouyang, Yifei Zhu, Hongwei Jia, and C. T. Chan, Non-Hermitian swallowtail catastrophe revealing transitions across diverse topological singularities, preprint, 2022
- Unfurled swallowtail plot from

V. I. Arnold, Singularities of caustics and wave fronts, Springer, 1990

Swallowtail ensemble and detail plots drawn with Mathematica by Pingyao Feng