# 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: 86366066486
PASSCODE: 738489


#### Abstract

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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## A mathematical framework



There is a space $\mathscr{M}$ 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 $\mathcal{M}-\Delta$.

## Moduli problems: a basic example

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

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A gapped configuration $x \in \mathscr{M}_{\mathrm{n}}-\Delta$ determines a permutation $\sigma(x) \in \operatorname{Sym}_{\mathrm{n}}$. In fact, $\sigma$ induces an isomorphism $\pi_{0}\left(\mathcal{M}_{\mathrm{n}}-\Delta\right) \cong$ Sym $_{\mathrm{n}}$ 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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H_{2}(\vec{k})=f_{0}(\vec{k}) \mathbf{1}+\vec{f}(\vec{k}) \cdot \vec{\sigma}
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where $\mathbf{1}$ is the identity matrix and $\vec{\sigma}=\left(\sigma_{1}, \sigma_{2}, \sigma_{3}\right)$ are the Pauli matrices

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\sigma_{1}=\left[\begin{array}{ll}
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f_{0}+f_{3} & f_{1} \\
f_{1} & f_{0}-f_{3}
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& \text { (complex conjugation) }
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\omega_{-}=-\sqrt{ } & \vec{\phi}_{-}=\left[\begin{array}{c}
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Observe that $\quad\left|\phi_{-}\right\rangle \mapsto-\left|\phi_{-}\right\rangle \quad$ does not change $H_{2}$.
Thus the moduli space $\mathbb{M}_{2}=S O(2) / \mathbb{Z}_{2} \cong S^{1}$ and its "topological charge" (a homotopy invariant) is $\pi_{1}\left(\mathcal{M}_{2}\right) \cong \mathbb{Z}$.

## Moduli spaces for quantum mechanical systems

Taking

$$
\begin{aligned}
f_{1}(\vec{k}) & =k_{x} k_{z} \\
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Wu et al., Science 365, 1273-1277 (2019)

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The winding number $w_{\Gamma}$ of the loop 「 equals 2.

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where $\quad D_{2}=$ the three-dimensional "dihedral" crystallographic point group
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(We have $\pi_{1}(\mathrm{SO}(3)) \cong \pi_{1}\left(\mathbb{R} P^{3}\right) \cong \mathbb{Z}_{2}, \mathrm{SU}(2) \cong S^{3}$ its 2 -fold universal cover.)

## Moduli spaces for non-Hermitian Hamiltonians

Beyond the well-studied Hermitian symmetry, non-Hermitian Hamiltonians possess eigenvalues with imaginary part that represents energy exchanges with surrounding environment.

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Joint with the physics group at HKUST led by Che Ting Chan, especially Hongwei Jia and Jing Hu, we investigated moduli spaces for 2-band and 3band Hamiltonians with the following symmetries:

$$
\eta H \eta^{-1}=\overline{H^{t}} \quad \text { and } \quad[P T, H]=0
$$

pseudo-Hermiticity
parity-time symmetry
where

$$
\eta=\left[\begin{array}{cc}
I_{n-1} & 0 \\
0 & -1
\end{array}\right] \quad \text { is a Riemannian metric form }
$$

$P T=$ complex conjugation operator

## Moduli spaces for non-Hermitian Hamiltonians

Beyond the well-studied Hermitian symmetry, non-Hermitian Hamiltonians possess eigenvalues with imaginary part that represents energy exchanges with surrounding environment.

Joint with the physics group at HKUST led by Che Ting Chan, especially Hongwei Jia and Jing Hu, we investigated moduli spaces for 2-band and 3band Hamiltonians with the following symmetries:

$$
\eta H \eta^{-1}=\overline{H^{t}} \quad \text { and } \quad[P T, H]=0
$$

pseudo-Hermiticity
parity-time symmetry
where

$$
\eta=\left[\begin{array}{cc}
I_{n-1} & 0 \\
0 & -1
\end{array}\right] \quad \text { is a Riemannian metric form }
$$

$P T=$ complex conjugation operator
Here emerge non-isolated, stratified singular loci, making our systems gapless and their topology much intriguing.

## Moduli spaces for non-Hermitian Hamiltonians: 2-band systems

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

$$
H_{2}=\left[\begin{array}{cc}
f_{3} & f_{2} \\
-f_{2} & -f_{3}
\end{array}\right] \quad \text { Recall Hermitian }\left[\begin{array}{cc}
f_{3} & f_{1} \\
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\end{array}\right] \text { ) }
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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): $\eta$-orthogonal eigenstates (non-defective degeneracy)


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The moduli space $\mathscr{M}_{2}$ can be identified as $S^{1} \vee$ $S^{1} \vee S^{1}$ doubly covering $S^{1} \vee S^{1}$. Thus $\pi_{1}\left(\mathscr{M}_{2}\right)$ is a free subgroup of $F(a, \beta)$ on 3 generators. This gives the gapless system a physically meaningful, non-Abelian topological charge.

## Moduli spaces for non-Hermitian Hamiltonians: 3-band systems

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


$$
\left[\begin{array}{ccc}
1 & f_{1} & f_{2} \\
-f_{1} & -1 & f_{3} \\
-f_{2} & f_{3} & -1
\end{array}\right]\left[\begin{array}{ccc}
1-f_{1}-f_{2} & f_{1} & f_{2} \\
-f_{1} & f_{1}-f_{3} & f_{3} \\
-f_{2} & f_{3} & f_{2}-f_{3}
\end{array}\right]
$$


$\left[\begin{array}{cccc}0 & -f_{1} & -f_{2} & -f_{3} \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0\end{array}\right]$

A mechanical wave system

$$
\left[\begin{array}{lll}
f_{1} f_{2} & f_{1} & f_{2} \\
-f_{1} & f_{1} & f_{3} \\
-f_{2} & f_{3} & f_{2}
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A mechanical wave
The central figure within these configurations is the so-called swallowtail catastrophe.

$$
\left[\begin{array}{ccc}
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-f_{1} & f_{1} & f_{3} \\
-f_{2} & f_{3} & f_{2}
\end{array}\right]
$$

## Moduli spaces for non-Hermitian Hamiltonians: 3-band systems

The singularity of a swallowtail arises in the discriminant surface of a generic degree-4 polynomial. Here, it is the characteristic polynomial of $H\left(f_{1}, f_{2}, f_{3}\right)$.

$$
\left|\begin{array}{cccc}
-\omega & -f_{1} & -f_{2} & -f_{3} \\
1 & -\omega & 0 & 0 \\
0 & 1 & -\omega & 0 \\
0 & 0 & 1 & -\omega
\end{array}\right|=\omega^{4}+f_{1} \omega^{2}+f_{2} \omega+f_{3}
$$



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$$
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-\omega & -f_{1} & -f_{2} & -f_{3} \\
1 & -\omega & 0 & 0 \\
0 & 1 & -\omega & 0 \\
0 & 0 & 1 & -\omega
\end{array}\right|=\omega^{4}+f_{1} \omega^{2}+f_{2} \omega+f_{3} \\
\Delta\left(f_{1}, f_{2}, f_{3}\right)=4 f_{1}^{3} f_{2}^{2}+27 f_{2}^{4}-16 f_{1}^{4} f_{3}-144 f_{1} f_{2}^{2} f_{3}+128 f_{1}^{2} f_{3}^{2}-256 f_{3}^{3} \\
\text { https:///yifeizhu.github.io/swtl.mp4 }
\end{array}
$$



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$\left|\begin{array}{cccc}-\omega & -f_{1} & -f_{2} & -f_{3} \\ 1 & -\omega & 0 & 0 \\ 0 & 1 & -\omega & 0 \\ 0 & 0 & 1 & -\omega\end{array}\right|=\omega^{4}+f_{1} \omega^{2}+f_{2} \omega+f_{3}$

$$
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\end{array}
$$

Discriminant surfaces are ruled (in fact, developable).


1908 quadratic $\left(\Delta=b^{2}-4 a c\right)$

cubic



$$
\left[\begin{array}{cccc}
0 & -f_{1} & -f_{2} & -f_{3} \\
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0
\end{array}\right]
$$

Illustration from Klein's lecture notes by Hellinger.

## Moduli spaces for non-Hermitian Hamiltonians: 3-band systems

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.

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

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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,


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Reg I and Reg II: PT-exact phases Reg III: PT-broken phase close and open of gaps).

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


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a2, b2: trajectories of eigenvalues a3, b3: trajectories of eigenframe, experimental (above) and theoretical (below)

## Implications and ramifications

- Our $S^{1} \vee S^{1} \vee S^{1}$ classification for 2-band systems predicts a new kind of nonHermitian gapless phase of matter, with topologically protected edge states.


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The unfurled swallowtail over the ordinary swallowtail

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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

- Daniel S. Freed, Lectures on field theory and topology, American Mathematical Society, 2019
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- Quadric surfaces diagrams for $\vec{k}$-spaces of Hermitian systems and winding number comparison diagrams adapted from
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- 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.
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- Spherical swallowtail plot, loop transition video and diagrams from

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- 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

