Automatic generation and topological classification of low-energy Hamiltonians at multi-fold degeneracies

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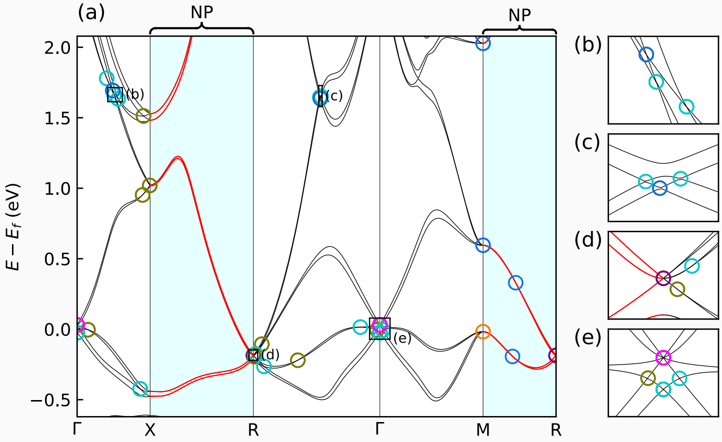
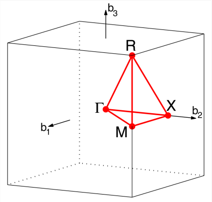
Topological band crossings



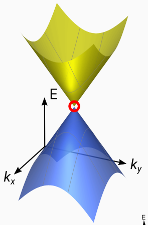
Band crossings of CoSi [Huber et al. 2022]

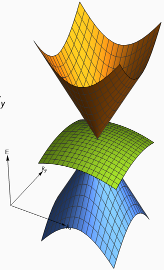


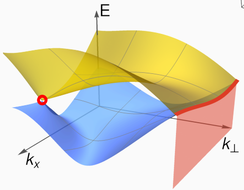
from [Setyawan et al. 2010]

Topological band crossings

Simplest is a **Weyl point** (WP):







- **Two band** crossings at single k-point
- Sources and sinks of Berry curvature $\boldsymbol{\Omega}_n$ (band n)
- $\boldsymbol{\Omega}_n = \nabla \times \boldsymbol{A}_n$ with Berry connection $\boldsymbol{A}_n = i \langle n|\nabla|n\rangle$
- Topological invariant/charge $\nu_n = \frac{1}{2\pi}\int_S \boldsymbol{\Omega}_n \cdot \mathrm{d}\boldsymbol{S} \in \mathbb{Z}$ over sphere S around Weyl point $\neq 0 \implies$ Weyl point **stable** against perturbations
- Can only be removed by annihilation with WP of opposite charge

Physical implications: Anomalous Hall effect, Fermi arc-states, non-linear optic responses, quantum oscillation

Other kinds of topological crossings are possible:

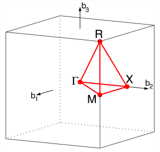
- **Multi-fold crossings** (crossings of >2 bands)
- **Higher dimensional crossings** (crossings on lines or planes in the BZ)

Today: **Multi-fold crossings**. Goal: Classify (compute ν_n) all multi-fold crossings in all space groups

Space groups: collection of symmetries of lattices (example: rotations C_n)

Irreducible representations

Multi-fold crossings at **high-symmetry points** possible (where $gk = k$). Example: R



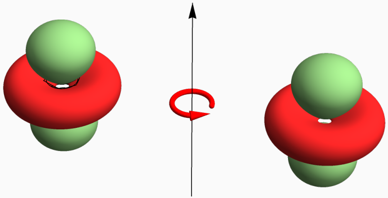
from [Setyawan et al. 2010]

Need build local Hamiltonian to compute $\boldsymbol{\Omega}$ and ν

Low-energy Hamiltonian must be **symmetric** in the little group G

$$\forall g \in G : H(g\boldsymbol{k}) = D(g)H(\boldsymbol{k})D(g^{-1}) \tag{1}$$

Representation $D(g)$ simple example of C_2 with two orbitals (no lattice)



Exchange of orbitals: σ_x in orbital position space

Project rotated orbital onto original basis: $\exp(-i\phi\boldsymbol{J})$ rotation with angular momentum operator

So: $D(g) = \sigma_x \otimes \exp(-i\pi\boldsymbol{J})$

Irreducible representations

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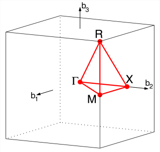

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Simultaneous **block-diagonalization** of all $D(g)$ in little group G:

Representations $D(g)$ can be decomposed into **irreducible representations** (irreps) $D(g) = D_1(g) \oplus D_2(g)$...

d_g is the dimension of an irrep $D_n(g)$

mass terms are not allowed by $D_n(g)$

$\implies$ H is d_g **degenerate**

Look up irreps in all space groups (BILBAO [Aroyo et al. 2006]), search for all $d_g > 2$ (multi-fold degeneracy)

General low-energy **Hamiltonian** at high-symmetry points (expansion in k) $n, m \leq d_g$:

$$H_{nm}(\boldsymbol{k}) = \sum_{hp_1} \alpha_{h,1} H^1_{hp_1 nm} k_{p_1} + \sum_{hp_1 p_2} \alpha_{h,2} H^2_{hp_1 p_2 nm} k_{p_1} k_{p_2} + \mathcal{O}(k^3) \tag{2}$$

The algorithm: generation of symmetric Hamiltonians

We only look at linear k terms H^1

Input: **Space group**, **Irrep**

Output: All possible terms of a general low-energy **Hamiltonian**

- Start by generating some number (30) **random** hermitian matrices $\tilde{H}^1_{hpnm}$ $(0 \leq h < 30)$
- Symmetrize with [Gresch et al. 2018]

$$H^1_{hvij} = \frac{1}{|G|} \sum_{g \in G} g^{-1}_{vp} D(g)_{in} \tilde{H}^1_{hpnm} D(g^{-1})_{mj} \tag{3}$$

- Find all **linearly independent** terms via Gram-Schmidt orthogonalization
  Discard all other terms
- Problem: H^1 is ugly. Random numerical values.
  Solution: New terms from **superpositions** of old terms. Matrix of all nonzero entries in H^1_h per h M_{hq} with $q = (v, i, j)$. Reduce q entries such that M is invertible and quadratic. Build up new H terms

$$H^1_{h'pnm} = \sum_h M^{-1}_{h'h} H^1_{hpnm} \tag{4}$$

(redefinition $\alpha_h = \sum_{h'} \alpha_{h'} M^{-1}_{h'h}$)

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  Example

$$\begin{aligned} H = \alpha_0(0.41 k_x\sigma_x + 0.2 k_y\sigma_z) + \\ \alpha_1(-0.2 k_x\sigma_x + 0.41 k_y\sigma_z) \end{aligned} \implies M = \begin{bmatrix} 0.41 & 0.2 \\ -0.2 & 0.41 \end{bmatrix} \implies \begin{aligned} M^{-1}M = \\ \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \end{aligned} \implies \begin{aligned} H = \alpha_0 k_x\sigma_x + \\ \alpha_1 k_y\sigma_z \end{aligned}$$

Input to the algorithm

Example: Irrep $\bar{\Gamma}_6\bar{\Gamma}_7$ with **dimension 4** of space group 198

Input (from BILBAO [Aroyo et al. 2006]):

	$\{2_{001}\|1/2,0,1/2\}$	$\{2_{010}\|0,1/2,1/2\}$
$\bar{\Gamma}_6\bar{\Gamma}_7$	$\begin{pmatrix} -i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \end{pmatrix}$	$\begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$

	$\{3^+_{111}\|0,0,0\}$	Time-reversal $\mathcal{T}$
$\bar{\Gamma}_6\bar{\Gamma}_7$	$\begin{pmatrix} e^{i5\pi/12} & e^{-i\pi/12} & 0 & 0 \\ e^{i5\pi/12} & e^{i11\pi/12} & 0 & 0 \\ 0 & 0 & e^{-i5\pi/12} & e^{i\pi/12} \\ 0 & 0 & e^{-i5\pi/12} & e^{-i11\pi/12} \end{pmatrix}$	$\begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$

Output of the algorithm

Example: Irrep $\bar{\Gamma}_6\bar{\Gamma}_7$ with **dimension 4** of space group 198

α_n are parameters

σ and τ are **Pauli matrices**

$$
\begin{aligned}
H =&\alpha_0 \Big[2k_x\sigma_x\tau_z + k_y\left(-\sqrt{3}\sigma_x\tau_0 - \sigma_y\tau_0\right) + \\
&k_z\left(\sigma_x\tau_x + \sqrt{3}\sigma_y\tau_x\right)\Big] + \\
&\alpha_1\Big[-2k_x\sigma_y\tau_z + k_y\left(-\sigma_x\tau_0 + \sqrt{3}\sigma_y\tau_0\right) + \\
&k_z\left(\sqrt{3}\sigma_x\tau_x - \sigma_y\tau_x\right)\Big] + \\
&2\alpha_2\Big[k_x\sigma_z\tau_x + k_y\sigma_0\tau_y + k_z\sigma_z\tau_z\Big]
\end{aligned}
$$

Topological classification

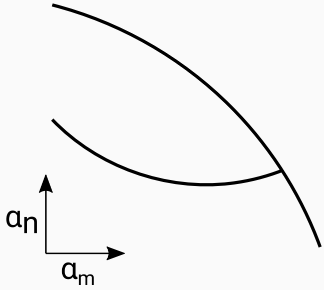
What now? Find an **analytical mapping** from parameters α to topological invariant $\nu : \alpha_0, ..., \alpha_N \to \nu \implies$ **topological phase diagram**

Problems:

- Classification must be done **manually** :(
- Can not analytically integrate $\nu = \frac{1}{2\pi} \int_S \Omega(k, H) \cdot \mathrm{d}S$ in general

Strategy:

- Need to only find points in parameter space with H **gapless** away form $\boldsymbol{k} = 0$ analytically. Only places where **topological phase transition** can happen.
- Color spaces in between with computed Chern number at **one single point**



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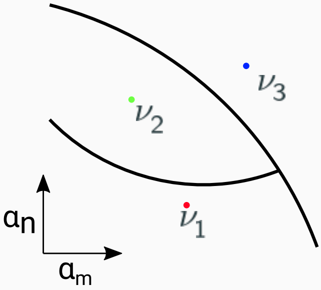

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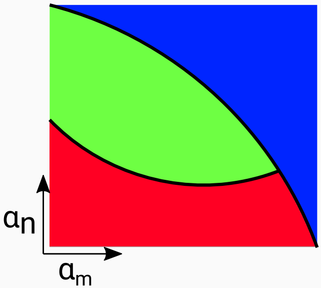
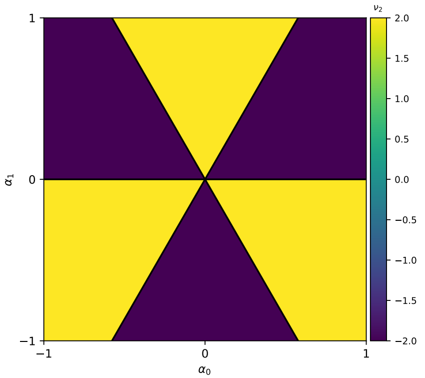


Topological classification of all multi-fold crossings

3-fold crossings: points are all equivalent in all space groups.

Hamiltonian consistent with [Bradlyn et al. 2016]. $\nu = \pm 2$



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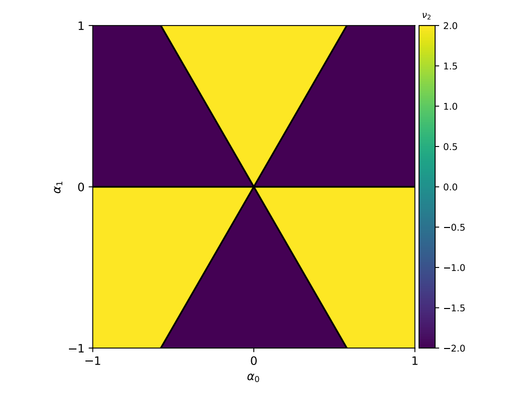

https://www.safetyemporium.com/01614

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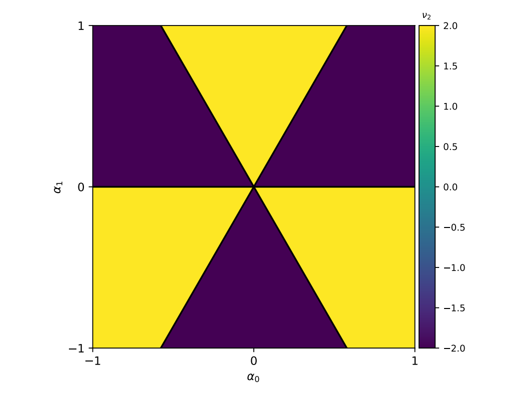

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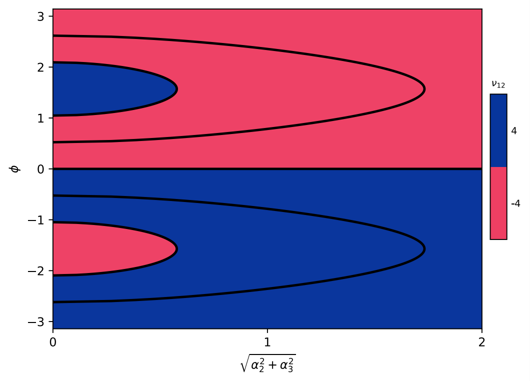
Topological classification of all multi-fold crossings

6-fold crossings: all crossings are equivalent. Hamiltonian consistent with [Bradlyn et al. 2016]. $\nu_{12} = \pm 4$



Topological classification of all multi-fold crossings

4-fold crossings: many different models.

Without SOC:

Space group	Irrep	ν_1	ν_2	ν_{12}	Model	Transformation
19	R_1R_1	-	-	± 2	9	-
92	A_1A_2	-	-	± 2	7	$k_x \to k_y, k_y \to -k_x, \alpha_2 = 0, \alpha_3 = 0$
96	A_1A_2	-	-	± 2	7	$k_y \to -k_y, \alpha_2 = 0, \alpha_3 = 0$
198	R_1R_3/R_2R_2	-	-	± 2	5	-
212/213	R_1R_2	-	-	± 2	5	-
212/213	R_3	-	-	± 2	6	-

Topological classification of all multi-fold crossings

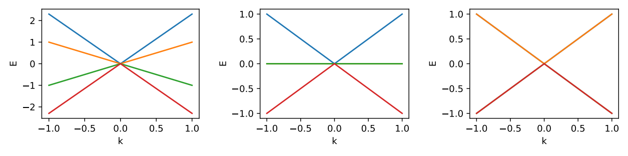
4-fold crossings: many different models.

With SOC:

Space group	Irrep	ν_1	ν_2	ν_{12}	Model	Transformation
18	$\bar{S}_5\bar{S}_5/\bar{R}_5\bar{R}_5$	-	-	± 2	3	-
19	$\bar{S}_5\bar{S}_5$	-	-	± 2	3	-
19	$\bar{T}_5\bar{T}_5$	-	-	± 2	3	$k_x \to k_y, k_y \to k_z, k_z \to k_x$
19	$\bar{U}_5\bar{U}_5$	-	-	± 2	3	$k_y \to k_z, k_z \to k_y$
90	$\bar{A}_6\bar{A}_7/\bar{M}_6\bar{M}_7$	-	-	± 2	7	-
92/94/96	$\bar{M}_6\bar{M}_7$	-	-	± 2	7	-
92/96	$\bar{R}_5\bar{R}_5$	-	-	± 2	3	$k_x \to k_y, k_y \to k_z, k_z \to k_x$
92/96	$\bar{A}_7\bar{A}_7$	-	-	± 4	8	-
94	$\bar{A}_6\bar{A}_7$	-	-	± 2	7	$k_x \leftrightarrow k_y$
195/196/197/198/199	$\bar{\Gamma}_6\bar{\Gamma}_7$	± 3	$\pm 1, \mp 5$	$\pm 4, \mp 2$	1	-
195	$\bar{R}_6\bar{R}_7$	± 3	$\pm 1, \mp 5$	$\pm 4, \mp 2$	1	-
197	$\bar{H}_6\bar{H}_7$	± 3	$\pm 1, \mp 5$	$\pm 4, \mp 2$	1	-
198	$\bar{M}_5\bar{M}_5$	-	-	± 2	3	-
199	$\bar{H}_6\bar{H}_7$	± 3	$\pm 1, \mp 5$	$\pm 4, \mp 2$	1	$U = \sigma_z \tau_x$
207/208/209/210 /211/212/213/214	$\bar{\Gamma}_8$	± 3	$\pm 1, \mp 5$	$\pm 4, \mp 2$	2	-
207/208	$\bar{R}_8$	± 3	$\pm 1, \mp 5$	$\pm 4, \mp 2$	2	-
211	$\bar{H}_8$	± 3	$\pm 1, \mp 5$	$\pm 4, \mp 2$	2	-
212	$\bar{M}_6\bar{M}_7$	-	-	± 2	4	-
213	$\bar{M}_6\bar{M}_7$	-	-	± 2	4	$k_y \to -k_y$
214	$\bar{H}_8$	± 3	$\pm 1, \mp 5$	$\pm 4, \mp 2$	2	$U = \sigma_0 \tau_x, \gamma \to -\gamma$

Finding topological phase transitions

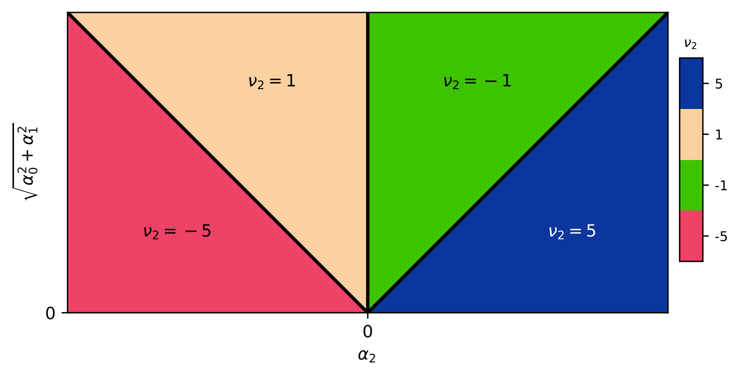
Example: Irrep $\bar{\Gamma}_6\bar{\Gamma}_7$ with **dimension 4** of space group 198
Main points of derivation:



- Characteristic polynomial of H is $\chi(E) = E^4 + aE^2 + \det(H) \implies$ spectrum is **particle-hole symmetric**
- $\implies$ can become **gapless** when $E_2 = E_3 = -E_2 = 0$ or $E_1 = E_2$
- Happens when $\det(H) = E_1 E_2(-E_1)(-E_2) = E_1^2 E_2^2 = 0$ or $\mathcal{Q} = a^2 - 4\det(H) = 0$
- $\chi(E)$ is **rotationally invariant** in phase space around the α_2 axis $\implies$ topological phase diagram is **rotationally invariant**
- $\det(H) \geq 0 \implies$ Don't find $\det(H) = 0$. Easier, find **minimum** with $\nabla_\alpha \det(H) = 0$
- Same can be shown for $\mathcal{Q}$
- Use **scale-invariance** of H in α and $\boldsymbol{k}$ (H is linear)

Topological phase diagram of $\bar{\Gamma}_6\bar{\Gamma}_7$

Example: Irrep $\bar{\Gamma}_6\bar{\Gamma}_7$ with **dimension 4** of space group 198. $\nu_2 \in \{-5, -1, 1, 5\}$



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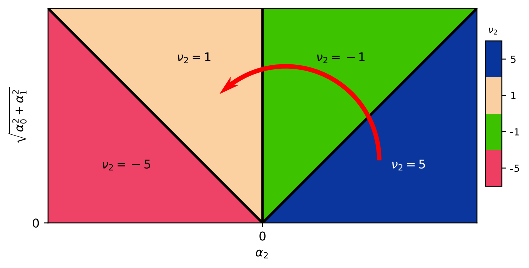
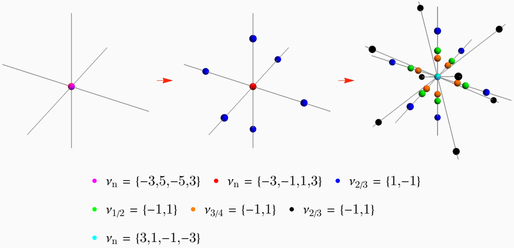
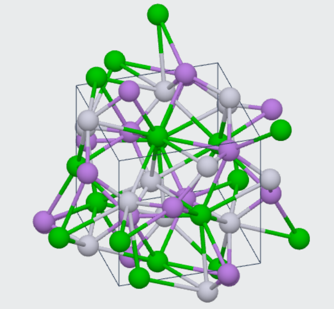
Weyl point production via phase transitions



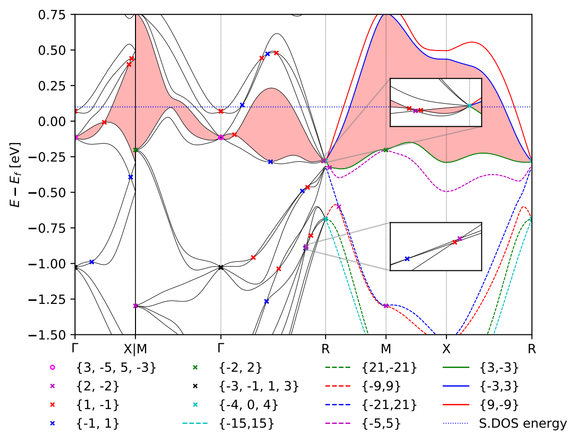


Creation of total of 26 WPs

Material search was performed to find $\nu = 5$ phase near E_{fermi}



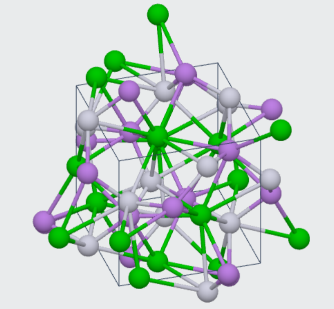
BaAsPt in SG 198



Full topological classification of BaAsPt with $\bar{\Gamma}_6\bar{\Gamma}_7$ in $\nu = 5$ phase

$\nu = 5$ phase material search

Material search was performed to find $\nu = 5$ phase near E_{fermi}



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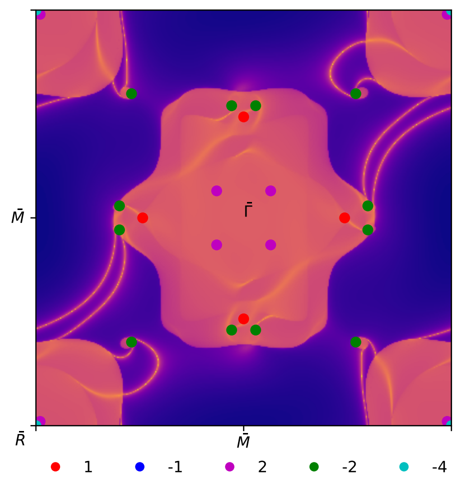

Surface DOS with Fermi arcs and projected charges

Conclusion

- Automatic generation of low-energy Hamiltonian at multi-fold crossings
- Analytical tools for topological phase diagrams
- Applied to all space groups
- Found unusually high Chern number of $\nu = 5$
- Material BaAsPt

References i

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