

Cohomological Insulators



Also, Non-Symmorphic Fermions







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How Many Types Of Energy Fermions Are There in Nature?

HourGlass Fermions

Group extensions by Wilson loops

Generalizes spatial nonsymmorphism to the Brillouin zone

Bulk fermions with 3,6,8 -fold degeneracies

Degeneracies on planes and surfaces

Exotic Transport Response

<u>Chiral edge states</u> Do not rely on any symmetry.



<u>Symmetry-protected edge states</u> Time-reversal symmetry, spin-orbit coupling (Kane,Mele)







2D+ 3D Mollenkamp, Hassan and many others

C can be defined within a mirror subspace (Teo,Fu,Kane) e.g., SnTe, BiSb,CeBi (Hsieh, Fu, Suyang, Nasser, Hasan,

Or no edge states at all: Hughes Prodan BAB, Turner and Vishwanath 2011; Teo, Ryu, Turner, others

.)

Initial criterion for symmetry-protected edge states

Degeneracies at isolated points

- Two points (k_1, k_2) with enhanced degeneracy 1)
- Trivial degeneracy on the line bridging k_1 - k_2 2)





1





Better criterion for symmetry-protected edge states

Connectivity of submanifold (S) Degree of connectivity = D

- 1) Two submanifolds (S_1, S_2) with equal and enhanced connectivity $(D_1 = D_2 > 1)$.
- 2) S_3 bridges S_1 and S_2 , and has a connectivity (D_3) that nontrivially divides D_1 ,

i.e., D_1/D_3 = an integer greater than one.

Which symmetry groups have nontrivial connectivity?

More complete answer: *all* nonsymmorphic space groups.

Concept of connectivity: Zak

Example of Connectivity in Our New Top Ins









HourGlass

Fermion.

and Synthesized



Perfect termination

Modified surface potential

KHgX; X= As,Bi, Sb

KZnP: trivial phase

KHgSb: topological phase

Different quantum numbers under spatial transformations.

• Inversion of (screw) rotational eigenvalues: $\exp[-iJ_z\pi/3]$



 ΔJ_z = Mirror Chern number mod 6

Criterion for nontrivial topology in *any* space group with screw/rotational symmetry.

• generalizes previous criterion for symmorphic rotation (Chen Fang et al)

Cohomology and Crystals



 $\rightarrow z$ $M_{\chi}^2 = I$ How many ways can I make a 1D crystal that extends in z, and has also this reflection symmetry?

Obvious (for cohomologists, *trivial/split*; for crystallographers: **symmorphic**)

 $M_{\chi}^2 = I$



The two algebras differ only by insertion of spatial translations.



Group of the wavevector

 $\underline{Mx}^2 = -\exp(i k_z) \rightarrow 2$ branches of eigenvalues = +/- $i * \exp(i k_z/2)$



A degeneracy that is movable but unremovable.

010

100

Connectivity

Symmetries: $T, \underline{Mx},$ $(\overline{M}_x)^2 = t(\hat{z}) * (2\pi \text{ rotation}) = -e^{-ik_z}$



Group of the wavevector

$$(T^*\underline{Mx})^2 = -1$$

Kramers-like degeneracy at every wavevector, i.e., is two-fold connected.



Connectivity



Putting Everything Together



 $\mathbf{Mz}: \mathbf{Z} \to -\mathbf{Z}$

Mirror Chern number: (T) $\int \mathcal{F}(k) d^2k$ in the even subspace.

(Teo, Fu, Kane)

Hourglass-flow topology



Rest of this talk: how do we diagnose this topology in the bulk wavefunction? A non-abelian generalization of the theory of polarization.

ARPES on KHgSb



Bulk Indices And Wilson Group Extensions

Wilson Band Structures Have ALWAYS Provided Faithful Representations of Any Topological Insulator We Thought Of

Wilson loops: matrix representation of parallel transport around momentum loops.



$$\mathcal{W} = \exp(-\int A \, dk_y);$$

$$A_{mn} = \left\langle U_{m,k_y} \right| \partial_{k_y} U_{n,k_y} \rangle$$

 $\exp[i\theta_{n,\boldsymbol{k}_{\parallel}}].$



We Define A Wilson Group

Since Wilson loops winding gives correct surface symmetries, we define a wilson group

All elements g (spatial or time-reversal symmetries) such that

$$\hat{g} \, \mathcal{W} \, \hat{g}^{-1} = \mathcal{W}^{\pm 1}$$

$$\breve{T}(-\pi, \boldsymbol{k}_{\scriptscriptstyle ||}) \, \mathcal{W}(\boldsymbol{k}_{\scriptscriptstyle ||}) \, \breve{T}(-\pi, \boldsymbol{k}_{\scriptscriptstyle ||})^{-1} = \mathcal{W}(-\boldsymbol{k}_{\scriptscriptstyle ||})^{-1}$$



Cohomology and Crystals



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The two algebras differ only by insertion of spatial translations.

Group Extensions <u>Cohomology in crystallography</u>

Different extensions are classified by the second cohomology group:

$$H^{2}(G_{p}, \mathcal{T}) = \mathbb{Z}_{2}$$

$$G_{p} = \{1, M_{x}\} \xrightarrow{f} \mathcal{T} = \{ t(\hat{z})^{n} \mid n \in \mathbb{Z} \}$$

- each extension corresponds to a different crystal order / space group.

In essence, this is how one determines there are

1) 17 space groups in two spatial dimensions,

2) 219 in 3D,

3) 4783 in 4D, and

4) a finite number in any finite spatial dimension.

(Hilbert's 18'th problem, 1900)

Most groups nonsymmorphic

Nonsymmorphicity exists only in real space, why not in momentum space?

Group Extensions

Topological Insulators exist because of a nontrivial extension of the time - reversal symmetry group with that of spin.

With Spin, We can have two situations:

T^2=1 (spinful, but no spin-orbit coupling)

T^2=-1 (spinful, with spin-orbit coupling, nontrivial TI possible)

New Topological Classes Wilson Group Can Be Extended Nontrivially

$$\hat{g}\,\mathcal{W}\,\hat{g}^{-1}=\mathcal{W}^{\pm 1}$$

 $\bar{M}_x \mathcal{W}_{-\pi}(\pi, k_z) \bar{M}_r^{-1} = \mathcal{W}_0(\pi, k_z)$

For kx=Pi, the Mirror is NOT part of the Wilson Group - translates the origin of the Wilson line.



 $-\pi$

Can Build a Nontrivial Mirror:

$$\bar{\mathcal{M}}_x \, \mathcal{W}_{-\pi} \, \bar{\mathcal{M}}_x^{-1} = \mathcal{W}_{-\pi}, \text{ with } \bar{\mathcal{M}}_x = \mathcal{W}_{-\pi \leftarrow 0} \, \bar{\mathcal{M}}_x. \qquad \qquad \bar{\mathcal{M}}_x^2 = \bar{E} \, t(\vec{z}) \, \mathcal{W}_{-\pi}^{-1}$$

There exists an extension by the Wilson loop!

Gives the correct prediction of the possible surface modes, Gives the equivalent of spatial nonsymmorphic symmetries to the **Brillouin zone**

The two glide-invariant planes in our case study correspond to different representations of the same symmetries – by deducing the possible Wilson 'bandstructures' in both planes, we demonstrated that one plane allows for a glide-spin-Hall subtopology, and the other does not.



Different extensions lead to different 2D topologies.

Cohomological Insulators

$$\overline{M}_{x} \mathcal{W} \overline{M}_{x}^{-1} = \mathcal{W}$$

$$T \mathcal{W} T^{-1} = \mathcal{W}^{-1}$$

Ordinary representation

$$\overline{M}_{x}^{2} = (2\pi \text{ rot.})(\text{spatial trans.})$$
$$= -\mathbf{t}(\hat{z})$$
$$T^{2} = -I$$

 $\overline{M}_{\chi}T = T\overline{M}_{\chi}$

Identical to the algebra of the surface symmetries

 \rightarrow surface prediction is valid.



$$ar{\mathcal{M}}_x = \mathcal{W}_{-\pi \leftarrow 0} \, ar{M}_x$$
 $ar{\mathcal{M}}_x \mathcal{W} ar{\mathcal{M}}_x^{-1} = \mathcal{W}$
 $\mathcal{T} \mathcal{W} \mathcal{T}^{-1} = \mathcal{W}^{-1}$

 $\frac{\text{Projective representation}}{\overline{\mathcal{M}}_{x}^{2}} = -t(\hat{z})\mathcal{W}^{-1}$ $\mathcal{T}^{2} = -I$ $\overline{\mathcal{M}}_{x}\mathcal{T} = \mathcal{T}\overline{\mathcal{M}}_{x}\mathcal{W}$

 $\overline{\mathcal{M}}_x, \mathcal{T}$ are generalized symmetries that encode parallel transport.

Different from the algebra of the surface symmetries.

The Wilsonian algebra determines the possible topologies of the Wilson bands along $\mathbf{X} \ \mathbf{U}$.

 $H_2(G_{\circ}, N) \qquad \qquad \mathcal{N} = \{ \, \bar{E}^a \, t(\vec{z})^b \, \mathcal{W}^c \mid a \in \mathbb{Z}_2, b, c \in \mathbb{Z} \, \}$

Cohomology determines the band sub-topology



 $\mathcal{W}|\theta,k_z\rangle = e^{i\theta}|\theta,k_z\rangle, \qquad \mathbf{t}(\hat{z})|\theta,k_z\rangle = e^{-ik_z}|\theta,k_z\rangle$

Energy- and momentum-dependent quantum numbers: $\operatorname{eig}[\overline{\mathcal{M}}_{x}] = \pm i \ e^{-i(k_{z}+\theta)/2}$

Hypothetical Glide Spin Hall Effect



$$\begin{split} k_z &\to k_z + 4\pi \\ \theta &\to \theta + 2\pi \\ \mathrm{eig}[\overline{\mathcal{M}}_x] &\to -\mathrm{eig}[\overline{\mathcal{M}}_x] \end{split}$$

Assumption: Wilson bands come in multiples of four.

Multiplication rules in the group extension,

e.g., $\overline{\mathcal{M}}_{\chi}^2 = -\mathbf{t}(\hat{z})\mathcal{W}^{-1}$,

constrain the Wilson energies.





Distinct connectivities of the Wilson energies correspond to topologically inequivalent groundstates.

Summary and outlook

- □ We introduced a criterion for symmetry-protected band topologies. The idea is to generalize symmetry-protected degeneracy by connectivity.
- □ This motivates nonsymmorphic crystals which have nontrivial connectivity.
- □ While the surface analysis gets many things right, the sure-fire method to classify band topology is through the Wilson loop. The connectivity criterion should be applied to the Wilson 'bands'.

Spin-off: There exists further of the 230 Space Group topologies!

Wang, Alexandradinata, Cava, BAB, Nature Alexandradinata, Wang, BAB, PRX

Semimetals: Why Are They Interesting?

See Ali's Talk Tomorrow

2-fold

Weyl, Dirac: Experimentally Discovered materials first theoretically predicted.

Two - types of "Dirac" Semimetal: 1. Two 2-fold irreps crossing linearly (CdAs):



Topological Semimetals: weird transport

Dirac Semimetals generically break into Weyl (due to symmetry) and can have negative magneto-resistance.

Ong Felser Cava Hasan Ding Chen Yazdani Mollenkamp

Volovik, Murakami, Burkov, Balents, Moore, Vishwanath, Savrasov, Kane, Fu, Grushin, Zhang, Qi, Hosur, Bardarson, Weng, Dai, Soluyanov, Bergholtz, Fang, Yao, Nagaosa, Vanderbilt, Sachdev and others



New Types of Fermions

Barry Bradlyn, Jennifer Cano, Zhijun Wang, Maia Vergniory, Claudia Felser, Bob Cava, BAB, submitted

3-fold Degeneracy (in several symmetry groups)

Violates spin 2S+1 degeneracy (always even)

Linear crossing, but Chern number 2 bands.

 $\vec{k} \cdot \vec{S}$

Spin 1, 3/2



arXiv:1509.00861

Dirac Cone Protected by Non-Symmorphic Symmetry: 4 fold nonsymmorphic

Leslie M. Schoop, Mazhar N. Ali, Carola Straßer, Viola Duppel, Stuart S. P. Parkin, Bettina V. Lotsch, Christian R. Ast

3-fold, 6-fold, 8-fold Crossings: All Different Fermions

For 8-fold see also Benjamin J. Wieder, Youngkuk Kim, A. M. Rappe, C. L. Kane, arXiv:1512.00074

k dot p models

1.0 0.5 $\epsilon(\mathbf{k})$ 0.0 -0.5 -1.0 -0.10 -0.05 0.00 SK 2 0.15 0.05 Sky 0.10 0.05 0.10 0.00 Sk. -0.05 0.15 -0.10(b) SG 220

3-fold degeneracy, Line-nodes on $|\delta k_x| = |\delta k_y| = |\delta k_z|$



4-fold degenerate at corner of BZ: Dirac Line Nodes





Four non-degenerate and two doubly degenerate pairs of bands on $|\delta k_x| = |\delta k_y| = |\delta k_z|$

NonSymmorphicity, Degeneracies, and Group Cohomology

(8-fold crossings example, everything else is similar)

Start With Non-Symmorphic 4-Fold

$$\begin{array}{c} T, R_1, R_2 & \xrightarrow{T_1 = T \\ T_2 = -1 \\ R_1^2 = R_2^2 = -1 \\ [T, R_1] = [T, R_2] = 0 \\ R_1 R_2 = e^{i(\theta_{12} + \theta_{13} + \theta_{31})} R_2 R_1 \\ \text{If } \{R_1, R_2\} = 0 \\ \text{only 4-fold degeneracy} \end{array} \xrightarrow{T_1, T_2, T_3 \\ 3 \text{ antiunitaries} \\ T_i T_j, T_i \\ e^{i\frac{\theta_{13}}{3}R_2 \cdot T} \\ T_i^2 = -1 \\ T_i T_j = e^{i\theta_{ij}} T_j T_i \\ e^{i(\theta_{12} + \theta_{23} + \theta_{31})} \neq 1 \\ 4 \text{-dim irrep, projective} \end{array}$$

available

NonSymmorphicity, Degeneracies, and Group Cohomology

SG 130 $T_1 = \mathcal{T}; T_2 = \mathcal{T}\overline{I}\overline{C}_{2x}; T_3 = \mathcal{T}\overline{I}\overline{C}_{2y}$

To obtain an 8-fold, we need another unitary

$$C_{4z}|\varphi\rangle = \lambda \cdot |\varphi\rangle$$



All other Fermions 3, 6, 8 fold, here also have projective representations

All distinct, all different responses

New Fermions: Classification And Surface/Line Degeneracies

Barry Bradlyn, Jennifer Cano, Zhijun Wang, Maia Vergniory, Claudia Felser, Bob Cava, BAB

Bravais lattice	Lattice vectors	Reciprocal lattice vectors
Primitive cubic	(a, 0, 0), (0, a, 0), (0, 0, a)	$\frac{2\pi}{a}(1,0,0), \frac{2\pi}{a}(0,1,0), \frac{2\pi}{a}(0,0,1)$
Body-centered cubic	$\frac{a}{2}(-1,1,1), \frac{a}{2}(1,-1,1), \frac{a}{2}(1,1,-1)$	$\frac{2\pi}{a}(0,1,1), \frac{2\pi}{a}(1,0,1), \frac{2\pi}{a}(1,1,0)$
Primitive tetragonal	(a, 0, 0), (0, a, 0), (0, 0, c)	$\frac{2\pi}{a}(1,0,0), \frac{2\pi}{a}(0,1,0), \frac{2\pi}{c}(0,0,1)$

SG |La| k |d| Generators

198 cP R 6 $\{C_{3,111}^{-}|010\}, \{C_{2x}|\frac{1}{2}\frac{3}{2}0\}, \{C_{2y}|0\frac{3}{2}\frac{1}{2}\}$ 199 cI P 3 $\{C_{3,111}^{-}|101\}, \{C_{2x}|\frac{1}{2}\frac{1}{2}0\}, \{C_{2y}|0\frac{1}{2}\frac{1}{2}\}$ $205 \left| cP \right| R \left| 6 \right| \{ C_{3,111}^{-} | 010 \}, \{ C_{2x} | \frac{1}{2} \frac{3}{2} 0 \}, \{ C_{2y} | 0 \frac{3}{2} \frac{1}{2} \}, \{ I | 000 \}$ $206 \left| \mathbf{cI} \right| \mathbf{P} \left| 6 \left| \{ C_{3,111}^{-} | 101 \}, \{ C_{2x} | \overline{\frac{1}{2}} \overline{\frac{1}{2}} 0 \}, \{ C_{2y} | 0 \overline{\frac{1}{2}} \overline{\frac{1}{2}} \} \right|$ $212 \left| cP \right| R \left| 6 \right| \{ C_{2x} | \frac{1}{2} \frac{1}{2} 0 \}, \{ C_{2y} | 0 \frac{1}{2} \frac{1}{2} \}, \{ C_{3,111}^{-} | 000 \}, \{ C_{2,1\bar{1}0} | \frac{1}{4} \frac{1}{4} \frac{1}{4} \}$ $213 \left| cP \right| R \left| 6 \right| \{ C_{2x} | \frac{1}{2} \frac{1}{2} 0 \}, \{ C_{2y} | 0 \frac{1}{2} \frac{1}{2} \}, \{ C_{3,111}^{-} | 000 \}, \{ C_{2,1\bar{1}0} | \frac{3}{4} \frac{3}{4} \frac{3}{4} \}$ 214 $| cI | P | 3 | \{ C_{3,111}^{-1} | 101 \}, \{ C_{2x} | \frac{\overline{1}}{2} \frac{1}{2} 0 \}, \{ C_{2y} | 0 \frac{1}{2} \frac{\overline{1}}{2} \}$ $220 \left| \mathbf{cI} \right| \mathbf{P} \left| 3 \left| \{ C_{3,\bar{1}\bar{1}1} | 0\frac{1}{2}\frac{1}{2} \}, \{ C_{2y} | 0\frac{1}{2}\frac{1}{2} \}, \{ C_{2x} | \frac{3}{2}\frac{3}{2}0 \}, \{ IC_{4x}^{-} | \frac{1}{2}11 \} \right.$ $230 \left| \mathbf{cI} \right| \mathbf{P} \left| 6 \left| \{ C_{3,\bar{1}\bar{1}1} | 0\frac{1}{2}\frac{1}{2} \}, \{ C_{2y} | 0\frac{1}{2}\frac{1}{2} \}, \{ C_{2x} | \frac{3}{2}\frac{3}{2}0 \}, \{ IC_{4x}^{-} | \frac{1}{2}11 \} \right|$ 130 tP A 8 $\{C_{4z}|000\}, \{\sigma_{\bar{x}y}|00\frac{1}{2}\}, \{I|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$ 135 $|\text{tP}| A | 8 | \{ C_{4z} | \frac{1}{2} \frac{1}{2} \frac{1}{2} \}, \{ \sigma_{\bar{x}y} | 00 \frac{1}{2} \}, \{ I | 000 \}$ 218 cP R 8 $\{C_{2x}|001\}, \{C_{2y}|000\}, \{C_{3,111}^{-}|001\}, \{\sigma_{\bar{x}y}|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$ $220 \left| \text{cI} \right| \text{H} \left| 8 \left| \{ C_{2x} | \frac{1}{2} \frac{1}{2} 0 \}, \{ C_{2y} | 0 \frac{1}{2} \frac{3}{2} \}, \{ C_{3,111}^{-} | 001 \}, \{ \sigma_{\bar{x}y} | \frac{1}{2} \frac{1}{2} \frac{1}{2} \} \right\}$ 222 cP R 8 $\{C_{4z}^{-}|000\}, \{C_{2x}|000\}, \{C_{3,111}^{-}|010\}, \{I|\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\}$ 223 cP R 8 $\{C_{4z}^{-}|\frac{1}{2}\frac{1}{2}\frac{1}{2}, \{C_{2x}|000\}, \{C_{3,111}^{-}|010\}, \{I|000\}$ $230 | cI | H | 8 | \{ C_{4z} | 0\frac{1}{2}0 \}, \{ C_{2y} | 1\frac{1}{2}\frac{1}{2} \}, \{ C_{3,111} | 111 \}, \{ I | 000 \}$



(c) Dirac line nodes in SGs 130 and 135

(d) Line nodes in SG 218

R

 $\mathcal{T}C_{2y}$

 $\sigma_{x\bar{z}}$

For 8-fold see also Benjamin J. Wieder, Youngkuk Kim, A. M. Rappe, C. L. Kane



Results

New Types of Fermions in Nature!

Large Degeneracy Fermions, but degeneracy point not their exotic only property

Degeneracies on surfaces

Transport, localization, superconductors, interaction behaviors when large degeneracies are involved

New Types of Fermi Arcs

New Types of Dirac Lines

Measuring Projective Representations - physical consequences