Flat bands of surface states via index theory of Toeplitz operators with Besov symbols

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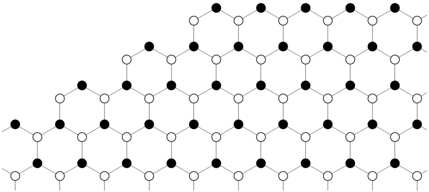
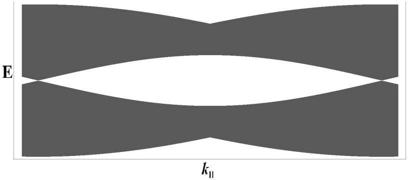
Edge states on the honeycomb lattice

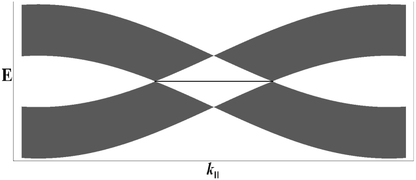
Hamiltonian with nearest-neighbor couplings on the Honeycomb lattice:



$$h = \begin{pmatrix} h_{AA} & h_{AB} \\ h_{BA} & h_{BB} \end{pmatrix} = \begin{pmatrix} 0 & a \\ a^* & 0 \end{pmatrix}$$

with the off-diagonal part a sum of three shift operators on $\ell^2(\mathbb{Z}^2)$



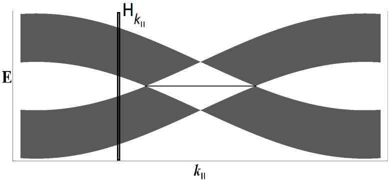


Surface band structure: Flat band at zero-energy for zigzag-, but not for armchair edges (see e.g. Nakada et al. (1996), Delplace et al. (2011)).

Edge states on the honeycomb lattice

Topological Zak-phase argument:

- Fourier transform for directions parallel to boundary: Slices $H_{k_{||}}$ with fixed momentum are 1D chiral systems
- Bulk Winding number for fixed $k_{||}$



$$\mathrm{Wind}(k_{||}) = 2\pi i \int \mathrm{d}k_{\perp} \frac{\det a_k}{|\det a_k|} \in \mathbb{Z}$$

- Bulk-Boundary Correspondence: At least $\left|\mathrm{Wind}(k_{||})\right|$ zero-energy bound states at edge
- $\mathrm{Wind}(k_{||})$ constant between gap-closing points: Either Flat band or no topological eigenstates

Edge states on the honeycomb lattice

Can show flat band for many edges, but

- Dimensional reduction only possible for periodic systems (no bulk disorder)
- boundary conditions must not break translational symmetry (no rough edges, only certain angles possible)
- chiral symmetry must be preserved by the boundary

We address the first two points for chiral semimetals.

Setting: Bulk

Bulk Hamiltonian h on $\mathbb{C}^N \otimes \ell^2(\mathbb{Z}^d)$ element of the von Neumann-algebra $\mathcal{M}$ of the disordered non-commutative torus.

- h finite sum

$$h = \sum_{x \in \mathbb{Z}^d} \phi_x S^x$$

  v_x ergodic random variables (hopping amplitudes)
  S^x (magnetic) shifts

- h chirally symmetric

$$JhJ = -h, \qquad J = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}.$$

  i.e. h and its phase $\mathrm{sgn}(h) = h|h|^{-1}$ are of the form

$$h = \begin{pmatrix} 0 & a^* \\ a & 0 \end{pmatrix} \qquad \mathrm{sgn}(h) = \begin{pmatrix} 0 & u^* \\ u & 0 \end{pmatrix}$$

- 0 not an eigenvalue: u unitary.

Setting: Boundary

Let $\xi \in \mathbb{S}^{d-1}$ be the normal vector of the boundary hyperplane

- Half-space Hamiltonian $\hat{h}$: restrict h to the half-space of points $x \in \mathbb{Z}^d$ with $\xi \cdot x > 0$,
  chiral, semi-infinite system, Dirichlet boundary conditions
- 0 can be infinitely degenerate eigenvalue,
  Eigenvectors localized at boundary
  $\longrightarrow$ This is the titular flat band!
- Eigenspace decomposes $\mathrm{Proj}_{\mathrm{Ker}(\hat{h})} = \hat{\pi}_+ \oplus \hat{\pi}_-$ in the grading of J

Non-commutative analysis

- Winding number from Zak phase argument:

$$\mathrm{Wind}_\xi(u) := i\tau(u^*\nabla_\xi u) = \left[\int \mathrm{d}k_\parallel \mathrm{Wind}(k_\parallel)\right]$$

- τ the trace per unit volume

$$\tau(a) = \lim_{L\to\infty} \frac{1}{(2L)^d} \sum_{\|x\|_\infty < L} \mathrm{Tr}_N \langle x|a|x\rangle = \int_{\mathbb{T}^d} \mathrm{Tr}(a_k)\mathrm{d}^d k$$

- ∇_ξ the derivation in the direction ξ

$$\nabla_\xi\left(\sum_{x\in\mathbb{Z}^d} \phi_x S^x\right) := -i\sum_{x\in\mathbb{Z}^d} (\xi\cdot x)\phi_x S^x = (\xi\cdot\nabla_k)a_k$$

- trace per unit surface area

$$\hat{\tau}(a) = \lim_{L\to\infty} \frac{1}{(2L)^{d-1}} \sum_{\|x\|_\infty < L} \mathrm{Tr}_N \langle x|a|x\rangle = \int_{\mathbb{T}^{d-1}} \mathrm{Tr}_{\ell^2(\mathbb{N})}(a_{k_\parallel})\mathrm{d}^{d-1}k_\parallel$$

Main result

Theorem

For the set-up as above, if the integrated density of states of h vanishes at $E = 0$ *in the sense that*

$$\tau(\chi_{[-E,E]}(h)) \leq CE^{1+s}$$

for some $C, s > 0$. *Then*

$$\hat{\tau}(\hat{\pi}_+ - \hat{\pi}_-) = \imath\,\tau(u^*\nabla_\xi u) = \imath \sum_{j=1,..,d} \xi_j \tau(u^*\nabla_{e_j} u)\,,$$

- Same as for weak topological insulators, but no gap required! Example: h periodic and linear dispersion at zero energy, e.g. chiral semimetal with Dirac points or nodal lines at the Fermi energy.
- works for arbitrary boundary hyperplane and also rough edges

Weak Chern numbers

Weak Chern numbers for $n \leq d$ independent directions $\zeta_1, \ldots, \zeta_n \in S^{d-1}$

- if n even for projections $p \in \mathcal{M}$

$$\mathrm{Ch}_n(p) = \sum_{\sigma \in \mathrm{Perm}(1,\ldots,n)} \mathrm{sgn}(\sigma)\tau\left(p\nabla_{\zeta_{\sigma(1)}} p \ldots \nabla_{\zeta_{\sigma(n)}} p\right).$$

- if n odd for unitaries $u \in \mathcal{M}$

$$\mathrm{Ch}_n(u) = \sum_{\sigma \in \mathrm{Perm}(1,\ldots,n)} \mathrm{sgn}(\sigma)\tau\left(u\nabla_{\zeta_{\sigma(1)}} u^* \ldots \nabla_{\zeta_{\sigma(n)}} u\right).$$

Well-defined if u respectively p in the non-commutative Sobolev-space $W_n^1(\mathcal{M})$, i.e. right-hand-side is τ-trace-class.
When do these expressions admit semifinite index formulas?

Non-commutative L^p-spaces

For a von Neumann-Algebra $\mathcal{N}$ with semifinite trace $\hat{\tau}$ define

- L^p-spaces $L^p(\mathcal{N}, \hat{\tau})$ as the completion of $\mathrm{Dom}(\hat{\tau})$ under

$$\|x\|_p = \left(\hat{\tau}(|x|^p)\right)^{1/p}.$$

- $\hat{\tau}$-compact operators $\mathcal{K}$ as C^*-completion of $\mathrm{Dom}(\hat{\tau})$.

$T \in \mathcal{N}$ is called $\hat{\tau}$-Fredholm if it is invertible modulo $\mathcal{K}$ and therefore has a semifinite index

$$\hat{\tau}\text{-Ind}(T) = \hat{\tau}(\mathrm{Ker}\, T) - \hat{\tau}(\mathrm{Ker}\, T^*) \in \mathbb{R}$$

Invariant under continuous deformations and $\hat{\tau}$-compact perturbations.

Standard approach

- Define Dirac operator

$$D = \sum_{j=1}^{n} \gamma_j \otimes D_j$$

where
$\gamma_1, ..., \gamma_n$ generators of a complex Clifford algebra
$D_j = \zeta_j \cdot X$ with X position operator on $\ell^2(\mathbb{Z}^d)$.

- Let $\mathcal{N}$ be von Neumann-algebra generated by $\mathcal{M}$ and bounded Borel functions of $D_1, ..., D_n$
- $P_+ = \chi_{\mathbb{R}^+}(D), \quad P_- = 1 - P_+, \quad \mathrm{sgn}(D) = P_+ - P_- \in \mathcal{N}$
- $\mathcal{N} \simeq \mathcal{M} \rtimes \mathbb{T}^k \rtimes \mathbb{R}^{n-k} \to \tau$ induces semifinite trace $\hat{\tau}$ on $\mathcal{N}$.
- When do we have $[\mathrm{sgn}(D), a] \in L^{n+1}(\mathcal{N}, \hat{\tau})$ in terms of $a \in \mathcal{M}$?

Besov spaces

- Fourier multipliers $\hat{f} : \widehat{\mathbb{R}}^d \to \mathbb{C}$ act on $\mathcal{M}$

$$\hat{f} * \left(\sum_{x \in \mathbb{Z}^d} \phi_x S^x \right) = \sum_{x \in \mathbb{Z}^d} \hat{f}(x) \phi_x S^x.$$

- Choose partition of $(\widehat{W_k})_{k \in \mathbb{N}}$ of $\mathbb{R}^d$ such that

$$\operatorname{supp} \widehat{W_k} \subset B_{2^{k+1}}(0) \setminus B_{2^{k-1}}(0), k > 0$$

- For $s > 0, p, q \geq 1$ define Besov space $B^s_{pq}(\mathcal{M})$ as subspace of $L^p(\mathcal{M}, \tau)$ with

$$\|a\|_{B^s_{pq}} := \left(\sum_{k \in \mathbb{N}} \left(2^{sk} \left\| \widehat{W_k} * a \right\|_p \right)^q \right)^{1/q} = \left\| 2^{s\cdot} \left\| \widehat{W_\cdot} * a \right\|_p \right\|_{\ell^q} < \infty.$$

Besov spaces: Basic properties

- Fourier multipliers are well-behaved with L^p-norms:

$$\left\|\hat{f} * a\right\|_p \leq \|f\|_{L^1} \|a\|_p$$

- $a = \sum_{k\in\mathbb{N}} \widehat{W_k} * a$ converges in L^p-norm for any $a \in L^p(\mathcal{M})$, for $a \in B^s_{pq}(\mathcal{M})$ absolute convergence
- $B^s_{pq}(\mathcal{M})$ embeds into weighted sequence space $\ell^s_q(L^p(\mathcal{M}))$ $\rightarrow$ compatible with interpolation.
- s measures smoothness, $B^s_{pp}(\mathcal{M}) \sim$ fractional Sobolev spaces
- If $a \in B^s_{pq}(\mathcal{M})$ then $\left\|\widehat{W_k} * a\right\|_p \leq C2^{-sk}$

Non-commutative Peller criterion

Peller (1980): Schatten-von Neumann-class of a Hankel operator
$\longleftrightarrow$ Besov-regularity of its symbol.

Here: $[\mathrm{sgn}(D), a] \sim P_- \, a \, P_+ \sim$ noncommutative Hankel operator.

Theorem

For $p > n$ and $a \in B^{\frac{n}{p}}_{p,p}(\mathcal{M})$ we have

$$[\mathrm{sgn}(D), a] \in L^p(\mathcal{N}, \hat{\tau}).$$

If $n = 1$, then the result also holds for $p = n = 1$.

Proof: Interpolation of analytic families with endpoint estimates for the L^2- and L^∞-cases and weighted versions of the commutator.

In short: $\mathcal{M} \cap B^{\frac{n}{n+1}}_{n+1,n+1} \sim$ semifinite $(n+1)$-summable Fredholm module

Index theorem

Theorem

If p or $u \in W^1_n(\mathcal{M}) \cap B^{\frac{n}{n+1}}_{n+1,n+1}(\mathcal{M})$ is a projection respectively unitary for n even/odd then

$$\hat{\tau}\text{-Ind}(p\,\mathrm{sgn}(D)\,p) = \Gamma_n\,\hat{\tau}\left([\mathrm{sgn}(D), p]^{n+1}\right) = \widetilde{\Gamma}_n \mathrm{Ch}_n(p)$$

respectively

$$\hat{\tau}\text{-Ind}(P_+ u P_+) = \Gamma_n\,\hat{\tau}\left(J\left([\mathrm{sgn}(D), u][\mathrm{sgn}(D), u^*]\right)^{(n+1)/2}\right) = \widetilde{\Gamma}_n \mathrm{Ch}_n(u)$$

Also sufficient condition: $a \in W^1_{n+\epsilon}(\mathcal{M})$ for some $\epsilon > 0$
No rapid decay of matrix elements necessary.

Bulk-boundary correspondence

- Special case $D = \xi \cdot X$ and $P_+ = \chi_{\mathbb{R}^+}(D)$ half-space projection to points with $x \cdot \xi > 0$.
- $\mathcal{N} \simeq \mathcal{M} \rtimes_\alpha \mathbb{R}$ or $\mathcal{N} \simeq \mathcal{M} \rtimes_\alpha \mathbb{T}$ represented on $\ell(\mathbb{Z}^d)$, $\hat{\tau}$ becomes trace per unit surface area
- h chiral Hamiltonian and $\hat{h} = P_+ h P_+$ with polar decompositions

$$\operatorname{sgn}(h) = \begin{pmatrix} 0 & u^* \\ u & 0 \end{pmatrix}, \qquad \operatorname{sgn}(\hat{h}) = \begin{pmatrix} 0 & \hat{u}^* \\ \hat{u} & 0 \end{pmatrix}.$$

- Idea: If $u \in B^{1/2}_{2,2}$ and $\hat{u} - P_+ u P_+$ $\hat{\tau}$-compact then

$$\hat{\tau}(J\,\mathrm{Ker}(\hat{h})) = \hat{\tau}\text{-Ind}(\hat{u}) = \hat{\tau}\text{-Ind}(P_+ u P_+) = i \sum_{j=1,..,d} \xi_j \tau(u^* \nabla_{e_j} u)$$

- Sufficient conditions for both?

Proposition

If the integrated density of states of h vanishes polynomially in $E = 0$

$$\tau(\chi_{[-E,E]}(h)) \leq C E^{1+s}.$$

Then $u \in B^{1/2}_{2,2}$ and $\hat{u} - P_+ u P_+$ is in $L^{1+\tilde{s}}(\mathcal{N}, \hat{\tau})$ for $\tilde{s} < s$.

Proof idea: DOS condition implies

$$\frac{1}{h} := \lim_{z \to 0} \frac{1}{h+z} \in L^{1+\tilde{s}}(\mathcal{M}), \text{ and } \quad \left\| \frac{1}{h} - \frac{1}{h+z} \right\|_{1+\tilde{s}} \leq C \, |\mathrm{Im} z|^{s/(1+\tilde{s})}.$$

Using $\mathrm{sgn}(h) = \text{s-lim}_{\epsilon \to 0} \tanh(\epsilon^{-1} h)$ this can compensate the discontinuity of sgn.
Decay of $\widehat{W_k} * \mathrm{sgn}(h)$ then carries over from smoothness of h.
Second statement: Use resolvent identities

$$\mathrm{sgn}(\hat{h}) - P_+ \mathrm{sgn}(h) P_+ = \underset{\epsilon \to 0}{\text{s-lim}} \int_{\mathcal{C}_\epsilon} \frac{\mathrm{d}z}{2\pi\imath} \tanh(\tfrac{z}{\epsilon}) \frac{P_+}{P_+ z - \hat{h}} h(\mathbf{1} - P_+) \frac{1}{z - h} P_+$$

Summary

- Extended semifinite index theorems for weak Chern numbers to Besov spaces and thus lower regularity
- Easy proof of bulk-boundary correspondence for 1d weak Chern numbers in chiral pseudo-gapped systems with rough edges

Open problems/future work:

- Persistence of pseudogap for disordered chiral systems (non-rigorous: Fradkin(1986) and others)
  $\rightarrow$ stability of chiral topological semimetals?
- Higher-dimensional odd/even weak Chern numbers,
  e.g. 3D-WSM $\sim$ 1-parameter family of 2D QHE or QSHE-systems
  Stability and persistence of Fermi-arc surface states?