The spectral localizer as numerical tool for topological materials

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Short history on Chern numbers in integer QHE

TKN_2 for periodic 1-particle Hamiltonian H in $d = 2$ on $\ell^2(\mathbb{Z}^2, \mathbb{C}^L)$

Parital diagonalization $H \cong \int_{\mathbb{T}^2}^{\oplus} dk\, H_k$ by Bloch-Floquet

$P = \chi(H \leqslant \mu) \cong \int_{\mathbb{T}^2}^{\oplus} dk\, P_k$ smooth Fermi projection below gap μ

$$\mathrm{Ch}(P) \;=\; 2\pi i \int_{\mathbb{T}^2} \frac{dk}{(2\pi)^2}\, \mathrm{Tr}\big(P_k[\partial_{k_1} P_k, \partial_{k_2} P_k]\big) \;\in\; \mathbb{Z}$$

Disordered analog for random family $H = (H_\omega)_{\omega \in \Omega}$

$$\mathrm{Ch}(P) \;=\; 2\pi i\, \mathbb{E}\, \mathrm{Tr}\big(\langle 0| P\, \big[[X_1, P], [X_2, P]\big] |0\rangle\big)$$

Index theorem (Connes, Bellissard, Avron.., 1980's): Almost surely

$$\mathrm{Ch}(P) \;=\; \mathrm{Ind}(PFP) \;\in\; \mathbb{Z} \qquad , \qquad F \;=\; \frac{X_1 + iX_2}{|X_1 + iX_2|}$$

If $\Delta \subset \mathbb{R}$ Anderson localized, then $\mu \in \Delta \mapsto \mathrm{Ch}(P)$ constant

Numerical computation of Chern number

Periodic system: implementation of k-integral, twisted BC

disordered system: compute P from H (costly), then above, or Kitaev

Topological photonic crystals: 100's of bands, not feasible

Spectral localizer on $\ell^2(\mathbb{Z}^2,\mathbb{C}^{2L})$ is Hamiltonian in a (dual) Dirac trap

$$L_\kappa \;=\; \begin{pmatrix} -(H-\mu) & \kappa(X_1-iX_2) \\ \kappa(X_1+iX_2) & H-\mu \end{pmatrix}$$

Selfadjoint $L_\kappa=(L_\kappa)^*$ with compact resolvent. **Fact:** gap at 0

$L_{\kappa,\rho}$ finite volume restriction to $[-\rho,\rho]^2$. For κ small and ρ large:

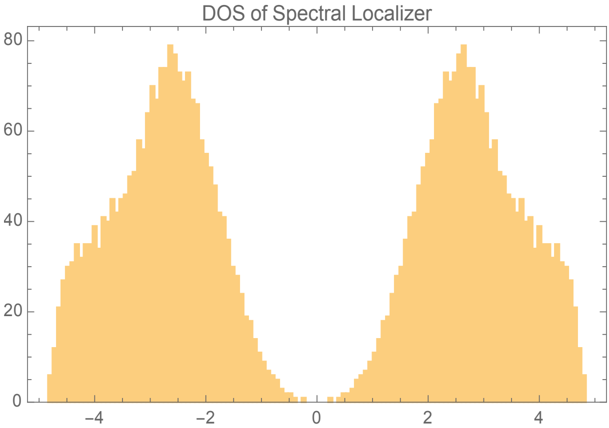
$$\boxed{\mathrm{Ch}(P) \;=\; \frac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho})}$$

Computation: only LDL necessary for Sig! **No spectral calculus!**

Implementation for dirty $p + ip$ superconductor

Standard toy model (like disordered Harper or Haldane)

DOS of the localizer for $\kappa = 0.1$ and $\rho = 20$



Looks harmless, however, note gap at 0

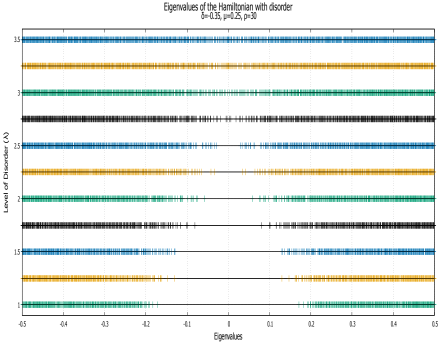
Spectral asymmetry: count number of positve/negative eigenvalues

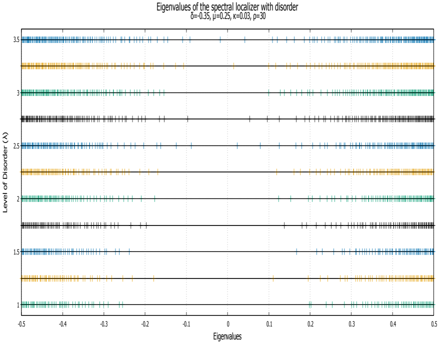
More numerics for dirty $p + ip$ superconductor

Disorder strength λ is increased

Low lying spectra of H_ρ and $L_{\kappa,\rho}$

For each realization: $\frac{1}{2}\,\mathrm{Sig} = 1$





Remarkable: even when H has only mobility gap, half-signature works!

Not covered by theorem stated next:

Main theorem on spectral localizer

Theorem (with Terry Loring)

Let $g = \|(H-\mu)^{-1}\|^{-1}$ *be gap of insulator Hamiltonian* H

Suppose

$$\kappa < \frac{12\, g^3}{\|H\|\,\|[X_1 + iX_2, H]\|} \qquad (*)$$

and

$$\rho > \frac{2\, g}{\kappa} \qquad (**)$$

Then $L_{\kappa,\rho}$ *has gap* $\frac{g}{2}$ *at* 0 *and*

$$\mathrm{Ch}(P) = \mathrm{Ind}(PFP) = \frac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho})$$

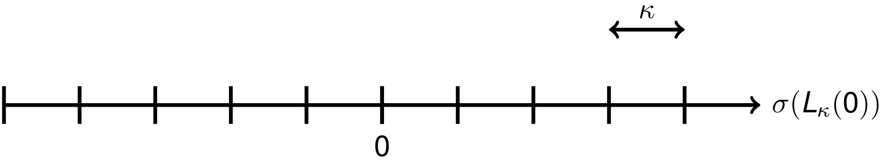
Constants not optimal   Numerics: typically $\kappa \approx 0.1$, $\rho \approx 20$ sufficient

Proof: *K*-theory of fuzzy spheres or spectral flow (discussions...)

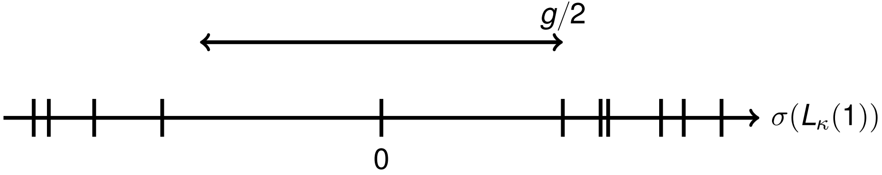
Intuition: H topological mass term

$$L_\kappa(\lambda) \;=\; \begin{pmatrix} -\lambda\, H & \kappa\,(X_1 - iX_2) \\ \kappa\,(X_1 + iX_2) & \lambda\, H \end{pmatrix} \qquad , \qquad \lambda \geqslant 0$$

Spectrum for $\lambda = 0$ symmetric and with space quanta κ



Spectrum for $\lambda = 1$: less regular, central gap open and asymmetry



Spectral asymmetry determined by low-lying spectrum (finite volume!)

First generalization: higher even dimension d

$$\mathrm{Ch}_{\{1,\dots,d\}}(P) \;=\; \frac{(2i\pi)^{\frac{d}{2}}}{\frac{d}{2}!} \sum_{\sigma\in S_d} (-1)^\sigma \,\mathrm{Tr}\Big(\langle 0|P\prod_{j=1}^{d}\nabla_{\sigma_j}P|0\rangle\Big)$$

For $d=4$ and $X_d =$ time, $\mathrm{Ch}_{\{1,\dots,4\}}(P)$ magneto-electric response

(Dual) Dirac opeator from $\{\gamma_j,\gamma_i\} \;=\; 2\delta_{i,j}$

$$D \;=\; \sum_{j=1}^{d} X_j\otimes\gamma_j \;=\; \begin{pmatrix} 0 & D_0^* \\ D_0 & 0 \end{pmatrix}$$

Spectral localizer:

$$L_\kappa \;=\; \begin{pmatrix} -(H-\mu)\otimes\mathbf{1} & \kappa\, D_0^* \\ \kappa\, D_0 & (H-\mu)\otimes\mathbf{1} \end{pmatrix}$$

Finite volume restriction $L_{\kappa,\rho}$ on $\mathrm{Ran}(|D|\leqslant\rho)$

Under same condition (*) and (**) with bounded $[D_0,H]$,

$$\mathrm{Ch}_{\{1,\dots,d\}}(P) \;=\; \frac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho})$$

Modification: odd dimension d

Chiral Hamiltonian with (mobility) gap at 0

$$H \;=\; -JHJ \;=\; \begin{pmatrix} 0 & A^* \\ A & 0 \end{pmatrix} \qquad , \qquad J \;=\; \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$$

Also approximate chirality $\|H + JHJ\| < 2g$ is actually sufficient

Odd Chern numbers (higher winding numbers)

$$\mathrm{Ch}_{\{1,\ldots,d\}}(A) \;=\; \frac{i(i\pi)^{\frac{d-1}{2}}}{d!!} \sum_{\sigma\in S_d} (-1)^{\sigma}\; \mathrm{Tr}\Big(\langle 0| \prod_{j=1}^{d} (A^{-1}\nabla_{\sigma_j} A)|0\rangle\Big)$$

Build odd spectral localizer from Dirac (not chiral for odd d)

$$L_\kappa \;=\; \begin{pmatrix} \kappa D & A^* \\ A & -\kappa D \end{pmatrix}$$

Under same condition (*) and (**) with bounded $[A, D]$

$$\mathrm{Ch}_{\{1,\ldots,d\}}(A) \;=\; \frac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho})$$

Weak invariants (here winding numbers)

For chiral Hamiltonian (possibly d even), $I \subset \{1, \ldots, d\}$ with $|I|$ odd

$$\mathrm{Ch}_I(A) \;=\; \frac{i(i\pi)^{\frac{|I|-1}{2}}}{|I|!!} \sum_{\sigma \in S_I} (-1)^\sigma \, \mathrm{Tr}\Big(\langle 0| \prod_{j=1}^{|I|} (A^{-1} \nabla_{\sigma_j} A) |0\rangle\Big)$$

Example: weak winding numbers $\mathrm{Ch}_{\{1\}}(A)$ and $\mathrm{Ch}_{\{2\}}(A)$ of graphene

(well-defined and topologlical even though only pseudogap)

Localizer from $D_I = \sum_{j \in I} X_j \otimes \gamma_j$ and H periodized in directions $j \notin I$

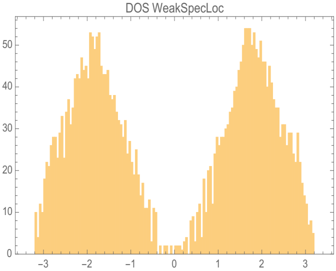
$$L_\kappa \;=\; \begin{pmatrix} \kappa\, D_I & A_{\mathrm{per}}^* \\ A_{\mathrm{per}} & -\kappa\, D_I \end{pmatrix} \qquad\qquad H_{\mathrm{per}} \;=\; \begin{pmatrix} 0 & A_{\mathrm{per}}^* \\ A_{\mathrm{per}} & 0 \end{pmatrix}$$

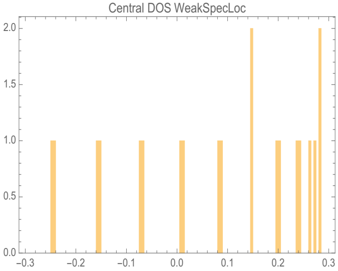
Weak invariants given by half-signature density:

$$\mathrm{Ch}_I(A) \;=\; \frac{1}{2} \lim_{\rho \to \infty} \frac{1}{\rho^{d-|I|}} \mathrm{Sig}(L_{\kappa,\rho}) \;\in\; \mathbb{R}$$

Numerical example of $\mathrm{Ch}_{\{1\}}(A)$ in graphene

Graphene with $\kappa = 0.1$ and volume $[-\rho, \rho]^2$ with $\rho = 20$





Half-signature density of $L_{\kappa,\rho} \approx \frac{14}{41} \approx \frac{1}{3} = \mathrm{Ch}_{\{1\}}(A)$ Why care?

Theorem (Semimetal BBC with Tom Stoiber)

$\mathrm{Ch}_{\{1\}}(A)$ *equal to surface density of flat band of edge states of half-space graphene Hamiltonian cut on 2-axis*

Numerical verification: works like a charm

$\mathbb{Z}_2$-invariants via skew localizer

Works for all 16 AZ-classes with strong $\mathbb{Z}_2$ index

Focus: $d = 2$ and odd TRS $I^*\overline{H}I = H$ with $I = i\sigma_2$ (Kane-Mele, QSHE)

Fredholm $T = PFP$ satisfies $I^* T^t I = T$ and thus well-defined

$$\mathrm{Ind}_2(T) \;=\; \dim(\mathrm{Ker}(T)) \bmod 2 \;\in\; \mathbb{Z}_2$$

Real skew localizer from $\Re(H) = \frac{1}{2}(H + \overline{H})$ and $\Im(H) = \frac{1}{2i}(H - \overline{H})$

$$L_\kappa \;=\; \begin{pmatrix} \Im(H) + \kappa X_1 I & \Re(H) I + \kappa X_2 \\ I\,\Re(H) - \kappa X_2 & \Im(H) - \kappa X_1 I \end{pmatrix} \;=\; \overline{L_\kappa} \;=\; -\,(L_\kappa)^*$$

Theorem (with Doll)

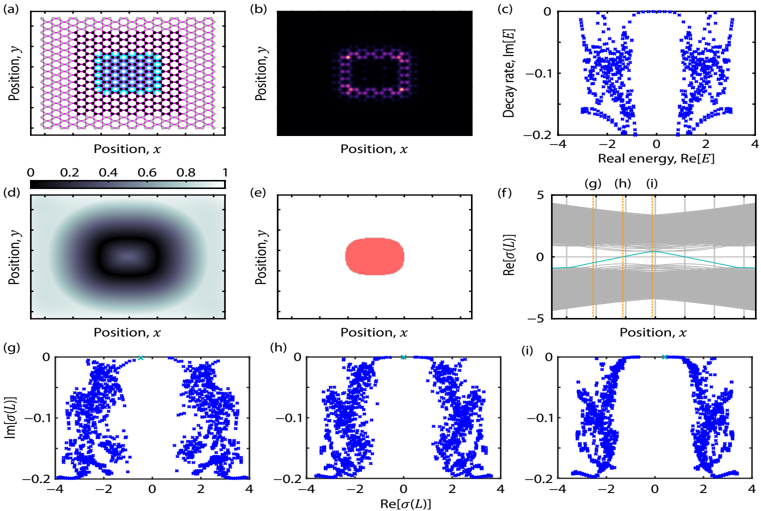
If (*) and (**),

$$\mathrm{Ind}_2\big(PFP\big) \;=\; \mathrm{sgn}(\mathrm{Pf}(L_{\kappa,\rho}))$$

For 8 of 16 cases, skew localizer is off-diagonal & only det needed

Non-hermitian, line-gapped $2d$ heterostructure

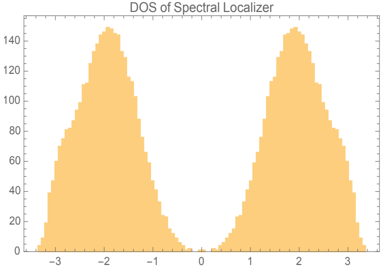
$$L_\kappa(x) = \begin{pmatrix} -H & \kappa D_0(x)^* \\ \kappa D_0(x) & H^* \end{pmatrix}$$ also line-gapped, so $\mathrm{Sig}(L_\kappa)$ defined

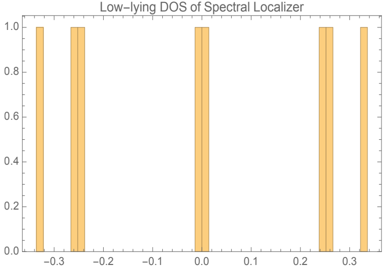


Approximate zero modes of localizer for graphene

$$L_\kappa = \begin{pmatrix} -H & \kappa\,(X_1 - iX_2) \\ \kappa\,(X_1 + iX_2) & H \end{pmatrix} = -J\,L_\kappa\,J \qquad , \qquad JHJ = -H$$

Vanishing signature (Chern number vanishes due to chiral symmetry)





Approximate kernel of multiplicity 2 = number of Dirac points

Splitting between two levels $\approx e^{-1/\kappa}$ (phase space tunnelling)

Very large gap to first excited $\approx \sqrt{\kappa}$ (as for double Dirac Hamiltonian)

Measures points on Fermi surface – stable under disordered perturb.

Why it works so well (for general dimension d):

H periodic ideal semimetal (only Dirac/Weyl points at Fermi surface)

$$\mathcal{F} L_\kappa^2 \mathcal{F}^* \;=\; -\kappa^2 \sum_{j=1}^{d} \partial_{k_j}^2 \;+\; \begin{pmatrix} (H_k)^2 & \kappa \sum_{j=1}^d \gamma_j (\partial_{k_j} H_k) \\ \kappa \sum_{j=1}^d \gamma_j (\partial_{k_j} H_k) & (H_k)^2 \end{pmatrix}$$

Second oder differential operator on $L^2(\mathbb{T}^d, \mathbb{C}^{2L})$

As in semi-classical analysis with $\hbar = \kappa$

IMS localization isolates Dirac/Weyl points

At each such point, explicitly solvable double Dirac Hamiltonians

Each double Dirac has simple zero mode and a gap of order κ

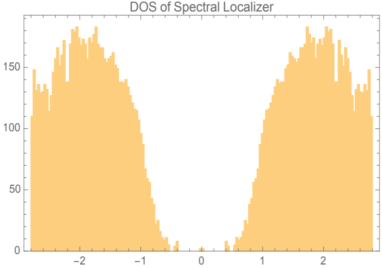
Theorem (with Stoiber)

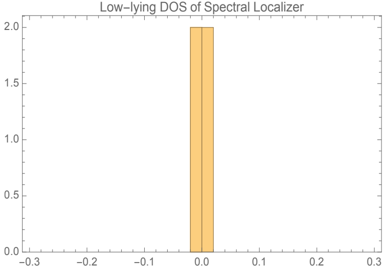
L_κ has as many eigenvalues $\leqslant \kappa$ as H has Dirac/Weyl points

Next excited level is $\mathcal{O}(\sqrt{\kappa})$

Weyl points of $3d$ systems (same strategy)

$$H = H_{p+ip} + \delta \begin{pmatrix} 0 & S_3 + S_3^* \\ S_3 + S_3^* & 0 \end{pmatrix} + \lambda H_{\text{dis}}$$





$\rho = 7$, so cube of size 15, $\delta = 0.6$, $\mu = 1.2$, $\lambda = 0.5$, $\kappa = 0.1$

Approximate kernel dimension counts number of Weyl points

Left out:

Franca/Grushin (2023): length of Fermi surface in metals via localizer

with Doll (2021): Spin Chern numbers and alike (approximate sym.)

just add ”spin twist” to position

with Cerjan, Loring (to come): localizer for corner states

based on spatial symmetries (C_2, inversion, reflection, ...)

other ”twists” with the operators implementing spatial sym.

In the future? extensions to certain interacting systems

?

Proofs (case of odd chiral dimension):

Proposition (Why the technique it works)

If (*) and (**) hold,

$$L^2_{\kappa,\rho} \geqslant \frac{g^2}{2}$$

Proof:

$$L^2_{\kappa,\rho} = \begin{pmatrix} A_\rho A_\rho^* & 0 \\ 0 & A_\rho^* A_\rho \end{pmatrix} + \kappa^2 \begin{pmatrix} D_\rho^2 & 0 \\ 0 & D_\rho^2 \end{pmatrix} + \kappa \begin{pmatrix} 0 & [D_\rho, A_\rho] \\ [D_\rho, A_\rho]^* & 0 \end{pmatrix}$$

Last term is a perturbation controlled by (*)

First two terms positive (indeed: close to origin and away from it)

Now $A^*A \geqslant g^2$, but $(A^*A)_\rho \neq A_\rho^* A_\rho$

This issue can be dealt with by tapering argument!

Lemma

$\exists$ even function $f_\rho : \mathbb{R} \to [0,1]$ with $f_\rho(x) = 0$ for $|x| \geqslant \rho$ and $f_\rho(x) = 1$ for $|x| \leqslant \frac{\rho}{2}$ such that $\|\widehat{f'_\rho}\|_1 = \frac{8}{\rho}$

With this, $f = f_\rho(D) = f_\rho(|D|)$ and $\mathbf{1}_\rho = \chi(|D| \leqslant \rho)$:

$$\begin{aligned} A_\rho^* A_\rho &= \mathbf{1}_\rho A^* \mathbf{1}_\rho A \mathbf{1}_\rho \;\geqslant\; \mathbf{1}_\rho A^* f^2 A \mathbf{1}_\rho \\ &= \mathbf{1}_\rho f A^* A f \mathbf{1}_\rho \;+\; \mathbf{1}_\rho \big([A^*, f] f A + f A^* [f, A] \big) \mathbf{1}_\rho \\ &\geqslant g^2 \, f^2 \;+\; \mathbf{1}_\rho \big([A^*, f] f A + f A^* [f, A] \big) \mathbf{1}_\rho \end{aligned}$$

Due to below, $A_\rho^* A_\rho$ indeed positive close to origin for ρ large ... □

Proposition (Bratelli-Robinson)

For $f : \mathbb{R} \to \mathbb{R}$ with Fourier transform defined without $\sqrt{2\pi}$,

$$\|[f(D), A]\| \;\leqslant\; \|\widehat{f'}\|_1 \, \|[D, A]\|$$

Proof by spectral flow (based on Phillips' results)

Using $\mathrm{SF} = \mathrm{Ind}$ for phase $U = A|A|^{-1}$ and $\Pi = \chi(D > 0)$ Hardy:

$$
\begin{aligned}
\mathrm{Ch}_d(A) &= \mathrm{Ind}(\Pi A \Pi + \mathbf{1} - \Pi) = \mathrm{Ind}(\Pi U \Pi + \mathbf{1} - \Pi) \\
&= \mathrm{SF}(U^* D U, D) = \mathrm{SF}(\kappa\, U^* D U, \kappa\, D) \\
&= \mathrm{SF}\left(\begin{pmatrix} U & 0 \\ 0 & \mathbf{1} \end{pmatrix}^* \begin{pmatrix} \kappa\, D & 0 \\ 0 & -\kappa\, D \end{pmatrix} \begin{pmatrix} U & 0 \\ 0 & \mathbf{1} \end{pmatrix}, \begin{pmatrix} \kappa\, D & 0 \\ 0 & -\kappa\, D \end{pmatrix} \right) \\
&= \mathrm{SF}\left(\begin{pmatrix} U & 0 \\ 0 & \mathbf{1} \end{pmatrix}^* \begin{pmatrix} \kappa\, D & \mathbf{1} \\ \mathbf{1} & -\kappa\, D \end{pmatrix} \begin{pmatrix} U & 0 \\ 0 & \mathbf{1} \end{pmatrix}, \begin{pmatrix} \kappa\, D & 0 \\ 0 & -\kappa\, D \end{pmatrix} \right) \\
&= \mathrm{SF}\left(\begin{pmatrix} \kappa\, U^* D U & U \\ U^* & -\kappa\, D \end{pmatrix}, \begin{pmatrix} \kappa\, D & 0 \\ 0 & -\kappa\, D \end{pmatrix} \right) \\
&= \mathrm{SF}\left(\begin{pmatrix} \kappa\, D & U \\ U^* & -\kappa\, D \end{pmatrix}, \begin{pmatrix} \kappa\, D & 0 \\ 0 & -\kappa\, D \end{pmatrix} \right)
\end{aligned}
$$

Now localize and use $\mathrm{SF} = \frac{1}{2}\,\mathrm{Sig}$-Diff on paths of selfadjoint matrices □