Computational K-theory via the spectral localizer

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Plan of the talk

- Reminder on index pairings (just functional analysis perspective)
- Construction of and intuition for associated spectral localizer (index pairing as a semiclassical KK-product)
- Main result: pairing as half-signature of spectral localizer
- Proof via spectral flow
- Even dimensional case (Chern numbers)
- Numerical illustration for a topological insulator
- $\mathbb{Z}_2$-invariants via spectral localizer (pairings with real symmetries)
- Spectral localizer for semifinite index pairings
- Semiclassical perspective and Callias-type index theorem
- Numerical illustration of Weyl point count for a topological semimetal

General framework: odd index pairings

A bounded invertible operator on Hilbert space $\mathcal{H}$ (K_1-class)

D selfadjoint Dirac operator on $\mathcal{H}$ with compact resolvent (K^1-class)

A differentiable w.r.t. D, namely commutator $[D, A]$ bounded

D then called odd Fredholm module for A (Atiyah, Kasparov)

Hardy projection $\Pi = \chi(D > 0)$ Set: $T = \Pi A \Pi + (\mathbf{1} - \Pi)$

Fact: T Fredholm operator and $\mathrm{Ind}(T)$ called index pairing

Index theorems (Atiyah-Singer, Connes, ...):
local formula for $\mathrm{Ind}(T)$

Best-known example: Noether index theorem for winding number

Aim here: numerical technique for calculation of $\mathrm{Ind}(T)$

Spectral localizer

For (semiclassical) parameter $\kappa > 0$ introduce spectral localizer:

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

A_ρ restriction of A (Dirichlet) to finite-dimensional range of $\chi(|D| \leqslant \rho)$

$$L_{\kappa,\rho} \;=\; \begin{pmatrix} \kappa\, D_\rho & A_\rho \\ A_\rho^* & -\kappa\, D_\rho \end{pmatrix}$$

Clearly selfadjoint matrix:

$$(L_{\kappa,\rho})^* \;=\; L_{\kappa,\rho}$$

Fact 1: $L_{\kappa,\rho}$ is gapped, namely $0 \notin L_{\kappa,\rho}$ (A is like a mass)

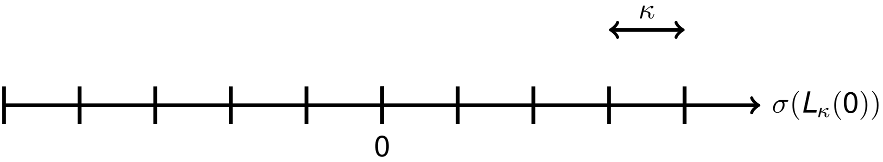
Fact 2: $L_{\kappa,\rho}$ has spectral asymmetry measured by signature

Fact 3: signature linked to topological invariant

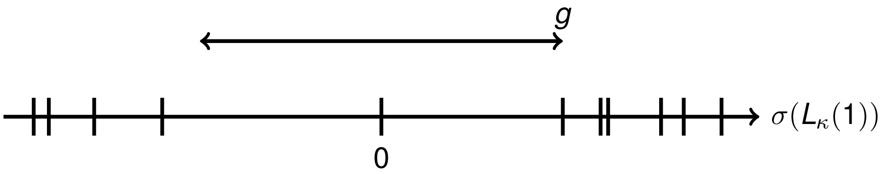
Schematic representation

$$L_\kappa(\lambda) \;=\; \begin{pmatrix} \kappa\, D & \lambda\, A \\ \lambda\, A^* & -\kappa\, D \end{pmatrix} \qquad , \qquad \lambda \geqslant 0$$

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!)

Theorem (with Loring 2017)

Given $D = D^*$ with compact resolvent and invertible A with invertibility gap $g = \|A^{-1}\|^{-1}$. Provided that

$$\|[D, A]\| \leqslant \frac{g^3}{12\,\|A\|\,\kappa} \qquad (*)$$

and

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

the matrix $L_{\kappa,\rho}$ is invertible and with $\Pi = \chi(D \geqslant 0)$

$$\frac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho}) = \mathrm{Ind}\big(\Pi A \Pi + (\mathbf{1} - \Pi)\big)$$

How to use: form (*) infer κ, then ρ from (**)

If A unitary, $g = \|A\| = 1$ and $\kappa = (12\|[D, A]\|)^{-1}$ then $\rho = \frac{2}{\kappa}$

Hence **small** matrix with $\rho \leqslant 100$ sufficient! Great for numerics!

N.B.: scaling $A \mapsto \lambda A$ in (*) forces $\kappa \mapsto \lambda\kappa$, so same ρ due to (**)

Why it can work:

Proposition

If (*) and (**) hold,

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

Proof:

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

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 (Phillips' basic approach)

Using $\mathrm{SF} = \mathrm{Ind}$ for phase $U = A|A|^{-1}$ and properties of SF:

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

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

Sketch on how to use this in a concrete situation

Solid state system in $d = 3$ in one-particle tight-binding approximation

$H : \ell^2(\mathbb{Z}^3, \mathbb{C}^{2L}) \to \ell^2(\mathbb{Z}^3, \mathbb{C}^{2L})$ with $2L$ orbitals per unit cell

H is local, namely only matrix elements between neighboring sites

Matrix elements from quantum chemistry (tunneling, exchange)

H gapped (insulator!) and has a chiral (or sublattice) symmetry

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

If H periodic, in Fourier space $k \in \mathbb{T}^3 \mapsto A(k) \in \mathbb{C}^{L \times L}$ smooth invertible

$$\mathrm{Wind}_3(A) = \int_{\mathbb{T}^3} \frac{dk}{24\pi^2} \sum_{\eta \in S_3} \mathrm{sgn}(\eta)\, \mathrm{Tr}\Big(\prod_{i=1,2,3} A(k)^{-1} \partial_{k_{\eta(i)}} A(k) \Big)$$

Index theorem $\Pi = \chi(\sum_{i=1}^3 \sigma_i \partial_{k_i} > 0)$ spectral projection of Dirac

$$\mathrm{Wind}_3(A) = -\,\mathrm{Ind}\big(\Pi A \Pi + (\mathbf{1} - \Pi)\big)$$

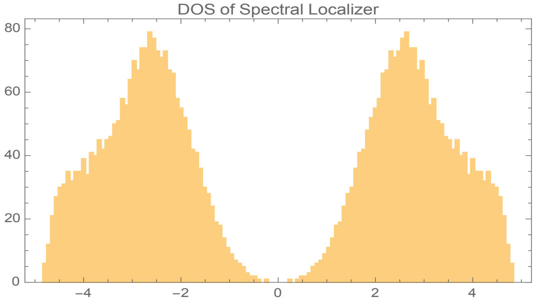
Spectrum and signature of localizer

(Dual) Dirac $D = \sum_{i=1}^{3} \sigma_i X_i$ on $\ell^2(\mathbb{Z}^3, \mathbb{C}^2)$ locality: $\|[D, H]\| < \infty$

Spectral localizer (placing Hamiltonian in a Dirac trap):

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

No functional calculus, just place H and D in 2×2: Typical result:



$\rho = 6$, $\kappa = 0.1$, etc. half-signature easy to compute

Even index pairings (in even dimension d)

Consider gapped Hamiltonian $H = H^*$ on $\mathcal{H}$ and $P = \chi(H < 0)$

Dirac operator D on $\mathcal{H} \oplus \mathcal{H}$ is odd w.r.t. grading $\Gamma = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$

Thus $D = -\Gamma D \Gamma = \begin{pmatrix} 0 & D' \\ (D')^* & 0 \end{pmatrix}$ and Dirac phase $F = D'|D'|^{-1}$

$[H, D']$ bounded $\Longrightarrow$ $PFP + (\mathbf{1} - P)$ Fredholm (index = Chern #)

Spectral localizer

$$L_\kappa = \begin{pmatrix} -H & \kappa D' \\ \kappa (D')^* & H \end{pmatrix} = -H \otimes \Gamma + \kappa D$$

Theorem (with Loring 2018)

Suppose $\|[H, D']\| < \infty$ *and* D' *normal, and* κ, ρ *with* (*) *and* (**)

$$\mathrm{Ind}\big(PFP + (\mathbf{1} - P)\big) = \tfrac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho})$$

Proof: K-theoretic via fuzzy spheres or again by spectral flow

Numerics: $p + ip$ dirty superconductor

$p + ip$ Hamiltonian on $\ell^2(\mathbb{Z}^2, \mathbb{C}^2)$ depending on μ and δ

$$H = \begin{pmatrix} S_1 + S_1^* + S_2 + S_2^* - \mu & \delta\big(S_1 - S_1^* + \imath(S_2 - S_2^*)\big) \\ \delta\big(S_1 - S_1^* + \imath(S_2 - S_2^*)\big)^* & -(S_1 + S_1^* + S_2 + S_2^* - \mu) \end{pmatrix} + \lambda\, V_{\text{dis}}$$

where S_1, S_2 shifts and disorder strength λ and i.i.d. entries in

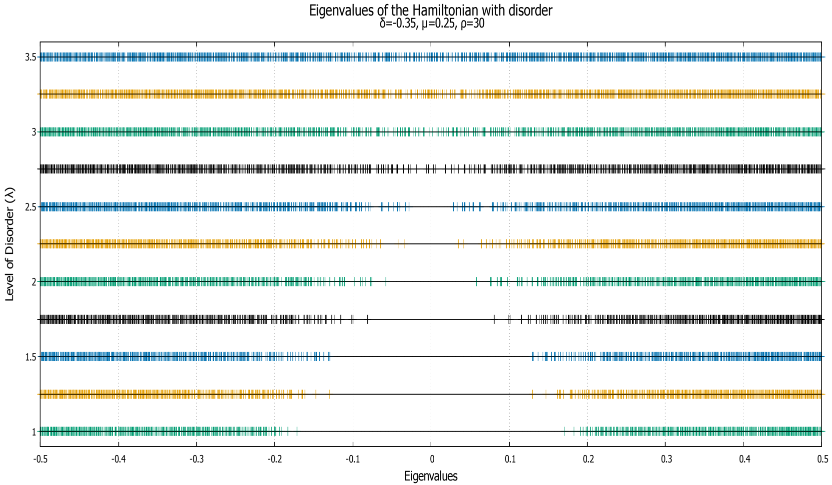
$$V_{\text{dis}} = \sum_{n \in \mathbb{Z}^2} \begin{pmatrix} v_{n,0} & 0 \\ 0 & v_{n,1} \end{pmatrix} |n\rangle\langle n|$$

Build even spectral localizer from $D = X_1\sigma_1 + X_2\sigma_2 = -\sigma_3 D \sigma_3$:

$$L_{\kappa,\rho} = \begin{pmatrix} -H_\rho & \kappa\,(X_1 + iX_2)_\rho \\ \kappa\,(X_1 - iX_2)_\rho & H_\rho \end{pmatrix}$$

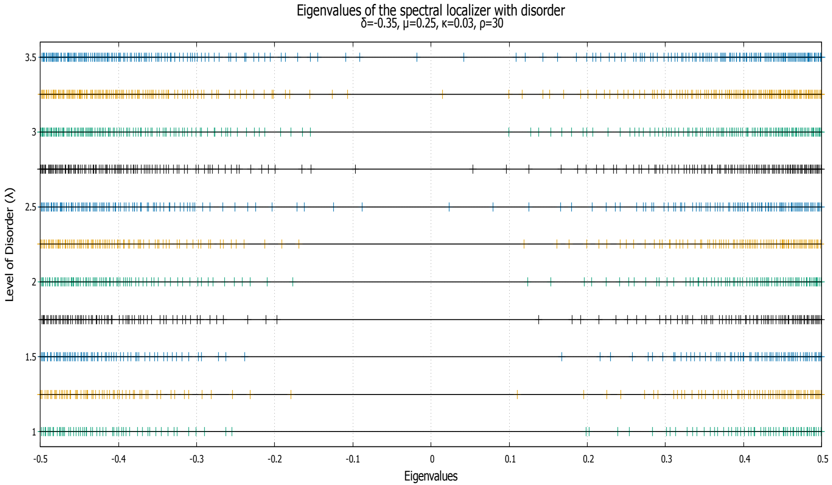
Calculation of signature by block Chualesky algorithm

Low-lying spectrum of one random Hamiltonian



Nota bene: beyond $\lambda \approx 2.7$ no spectral gap, but Anderson localization

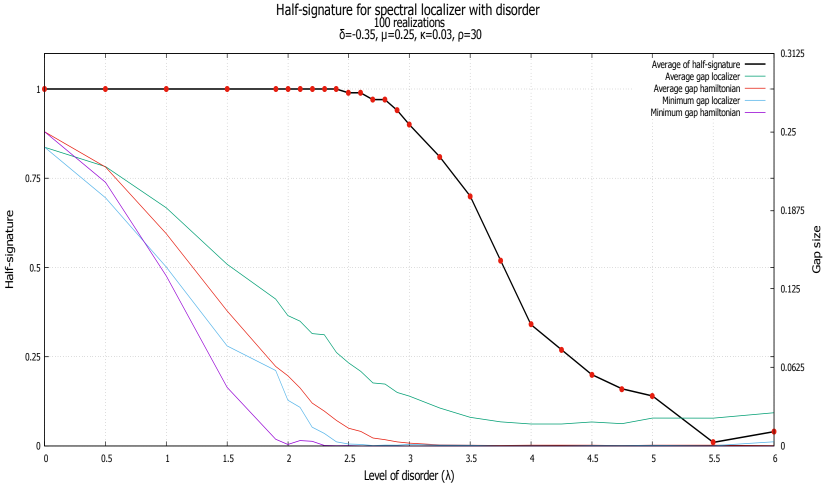
Low-lying spectrum of spectral localizer



Nota bene: up to $\lambda \approx 3.3$ localizer has gap (not covered by Theorem)

Spectral asymmetry difficult to see, but easy to compute

Half-signature and gaps for $p + ip$ superconductor



Up to $\lambda \approx 3.2$ almost no configurations with ”wrong signature”

16 Real $\mathbb{Z}_2$-valued index pairings (Real K-theory)

Real structure $\mathcal{C}$ = complex conjugation on $\mathcal{H}$, then $\overline{A} = \mathcal{C}A\mathcal{C}$

Possible: $P = \overline{P}$ real, P quaternionic, $P = \mathbf{1} - \overline{P}$ Lagrangian , odd Lag.

Depending on d: $D = \overline{D}$ real, $D = -\overline{D}$ imaginary, D (odd) quaternionic

Focus on BdG, $d = 1$: $H = -\overline{H}$ with $P = \chi(H < 0) = \mathbf{1} - \overline{P}$ and $D = \overline{D}$

With $\Pi = \chi(D > 0)$ again $T = \Pi(\mathbf{1} - 2P)\Pi + \mathbf{1} - \Pi$ Fredholm and

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

Real skew spectral localizer

$$L_\kappa \;=\; \begin{pmatrix} 0 & \kappa D - iH \\ \kappa D + iH & 0 \end{pmatrix}$$

Theorem (with Doll 2020)

Suppose $\|[H, D]\| < \infty$ *and* κ, ρ *with* (*) *and* (**)

$$\mathrm{Ind}_2\big(PFP + (\mathbf{1} - P)\big) \;=\; \mathrm{sgn}(\mathrm{Pf}(L_{\kappa,\rho})) \;=\; \mathrm{sgn}(\det(\kappa D_\rho + \imath H_\rho))$$

Semifinite index pairings (here only odd case)

$(\mathcal{N}, \mathcal{T})$ semifinite von Neumann with $\mathcal{T}$ normal, faithful

$\mathcal{K}$ norm-closure of span of $\mathcal{T}$-finite projections. Then Calkin sequence:

$$0 \;\to\; \mathcal{K} \;\to\; \mathcal{N} \;\overset{\pi}{\to}\; \mathcal{N}/\mathcal{K} \;\to\; 0$$

$T \in \mathcal{N}$ Fredholm if $\pi(T)$ invertible

Definition

Breuer-Fredholm index of $T \in \mathcal{N}$ w.r.t. projections $P, Q \in \mathcal{N}$

$$\mathcal{T}\text{-Ind}_{(P.Q)}(T) \;=\; \mathcal{T}\big(\mathrm{Ker}(T) \cap Q\big) \;-\; \mathcal{T}\big(\mathrm{Ker}(T^*) \cap P\big)$$

provided $\mathrm{Ker}(T) \cap Q$ and $\mathrm{Ker}(T^*) \cap P$ are $\mathcal{T}$-finite

For $\Pi = \chi(D > 0)$, $U \in \mathcal{N}$ and $[D, U](1 + D^2)^{-\frac{1}{2}} \in \mathcal{K}$, index pairing

$$\langle [U], [D] \rangle \;=\; \mathcal{T}\text{-Ind}_{(\Pi.\Pi)}(\Pi U \Pi) \;\in\; \mathbb{R}$$

Link to spectral flow: Carey, Gayrel, Phillips, Rennie 2015

Semifinite spectral localizer

for $U = A|A|^{-1}$

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

and restrictions

$$L_{\kappa,\rho} = \Pi_\rho L_\kappa \Pi_\rho \qquad , \qquad \Pi_\rho = \chi(D^2 < \rho^2)$$

Theorem (with Stoiber 2021)

For κ, ρ satisfying (*) and (**), and $U = A|A|^{-1}$ as above,

$$\langle [U], [D] \rangle = \tfrac{1}{2}\, \mathcal{T}\text{-Sig}(L_{\kappa,\rho})$$

where $\mathcal{T}\text{-Sig}(L) = \mathcal{T}(\chi(L > 0)) - \mathcal{T}(\chi(L < 0))$

Application: numerical method for weak invariants of topo. insul.

Semiclassical perspective on spectral localizer

Up to now spectral localizer invertible and with spectral asymmetry

Now situation non-trivial kernel of (Cayley transform of localizer)

$$L_\kappa \;=\; \begin{pmatrix} 0 & \kappa D - iH \\ \kappa D + iH & 0 \end{pmatrix} \;=\; C^* \begin{pmatrix} -H & \kappa D \\ \kappa D & H \end{pmatrix} C$$

with supersymmetric index, provided $\kappa D + iH$ Fredholm,

$$\mathrm{Ind}(\kappa D + iH) \;=\; \mathrm{Sig}(J|_{\mathrm{Ker}(L_\kappa)}) \qquad , \qquad J \;=\; \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$$

Kernel linked to kernel of semiclassical Schrödinger-like operators:

$$(L_\kappa)^2 \;=\; \begin{pmatrix} \kappa^2 D^2 + H^2 - \kappa i[D,H] & 0 \\ 0 & \kappa^2 D^2 + H^2 - \kappa i[D,H] \end{pmatrix}$$

Low-lying spectrum accessible by rough semiclassics (IMS localiza.)

Classical situation: Callias index theorem $x \in \mathbb{R}^d \mapsto H_x = (H_x)^*$

Solid state context: topological semimetals instead of insulators

Callias-type index theorems

C^1-map $x \in \mathbb{R}^d \mapsto H_x = (H_x)^*$ of selfadjoint Fredholm operators

H_x uniformly invertible for $|x| \geqslant R_c$

Hypothesis: zero set $\mathcal{Z}(H) = \{x \in \mathbb{R}^d \,:\, \dim(\mathrm{Ker}(H_x)) \geqslant 1\}$ finite

For each zero $x^* \in \mathcal{Z}(H)$ topological charge $\mathrm{Ch}_{d-1}(H_x|H_x|^{-1}, \partial B_\delta(x^*))$

Theorem (with Stoiber 2021)

d odd and $D = \gamma \cdot \partial$ Dirac operator on $\mathbb{R}^d$. For all $\kappa \leqslant 1$,

$$\mathrm{Ind}(\kappa D + iH) \;=\; \mathrm{Sig}(J|_{\mathrm{Ker}(L_\kappa)}) \;=\; \sum_{x^* \in \mathcal{Z}(H)} \mathrm{Ch}_{d-1}(H_x|H_x|^{-1}, \partial B_\delta(x^*))$$

Even dimensional analogue as Guentner-Higson, but with infinite fiber

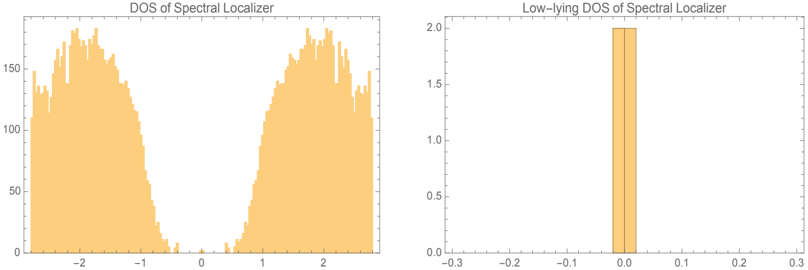
Proof: similar to Witten's semiclassical proof of Morse inequalities

R.h.s.: multiparameter spectral flow counting Weyl points with charge

Topological semimetal: Weyl point count over a Brillouin torus

Weyl points of systems in $d = 3$

$$H = H_{p+ip} + \delta \begin{pmatrix} 0 & S_3 + S_3^* \\ S_3 + S_3^* & 0 \end{pmatrix} + \lambda H_{\text{dis}} \qquad \text{on } \ell^2(\mathbb{Z}^3, \mathbb{C}^2)$$



$\rho = 7$, 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

Existence of Weyl points $\Longrightarrow$ non-vanishing weak Chern numbers

$\Longrightarrow$ surface currents (as in QHE)

References (all on arXiv)

• with Loring, *Finite volume calculations of K-theory invariants*, New York J. Math. (2017)

• with Loring, *The spectral localizer for even index pairings*, J. Noncommutative Geometry (2020)

• with Loring, *Spectral flow argument localizing an odd index pairing*, Cand. Bull. Math. (2019)

• with Doll, *Skew localizer and $\mathbb{Z}_2$-flows for real index pairings*, preprint 2020

• with Stoiber, *The spectral localizer for semifinite spectral triples*, Proc. AMS (2021)

• with Stoiber, *Semiclassical proofs of Callias-type index theorems for multiparameter spectral flow*, draft 2021.