Invariants of disordered semimetals via the spectral localizer

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Topological invariants in solid state

Here: focus on tight-binding models in one-particle electronic systems

This covers topological insulators and semimetals

Complex theory: no real symmetries (TRS, BdG, but chiral/sublattice)

• odd invariants: (higher) winding numbers (also odd Chern numbers)

• Even invariants: (higher) Chern numbers

• Strong invariants: involve all *d* space directions, $\mathbb{Z}$-valued

• Weak invariants: involve less than *d* space directions, $\mathbb{R}$-valued

• Other invariants: number of Weyl or Dirac points in semimetals

Real invariants: requires real symmetries (TRS, BdG)

• often $\mathbb{Z}_2$-valued

Aim: spectral localizer as numerical technique for computation

Formulas: bulk invariants and index pairings

$P = \chi(H < 0)$ Fermi projection of Hamiltonian H on $\ell^2(\mathbb{Z}^d, \mathbb{C}^L)$

$X = (X_1, \dots, X_d)$ position and $D = \sum_{j=1}^{k} X_{i_j} \Gamma_{i_j}$ partial (dual) Dirac

$dP = i[D, P]$ bounded or at least Besov (localization or pseudogap)

$$\mathrm{Ch}_k(P) \;=\; c_k\, \mathcal{T}\big(P(dP)^k\big) \qquad , \qquad \text{even Chern for } k \text{ even}$$

If chiral symmetry $JPJ = \mathbf{1} - P$ for $J = J^* = J^{-1}$

$$\mathrm{Ch}_k(P) \;=\; c_k\, \mathcal{T}\big(JP(dP)^k\big) \qquad , \qquad \text{odd Chern for } k \text{ odd}$$

Strong invariant for $k = d$. By index theorems (many references):

$$\mathrm{Ch}_k(P) \;=\; \mathcal{T}\text{-Ind}(T) \qquad , \qquad T = PFP + \mathbf{1} - P\,,\; k \text{ even}$$
$$\mathrm{Ch}_k(P) \;=\; \mathcal{T}\text{-Ind}(T) \qquad , \qquad T = \Pi U \Pi + \mathbf{1} - \Pi\,,\; k \text{ odd}$$

$\Pi = \chi(D > 0)$ Hardy, F Dirac phase, $U = A|A|^{-1}$ Fermi unitary $H = \begin{pmatrix} 0 & A \\ A* & 0 \end{pmatrix}$

General framework: strong 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 = Hamiltonian in Dirac trap

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

$$L^{\rm od}_{\kappa} = \begin{pmatrix} \kappa\, D & A \\ A^* & -\kappa\, D \end{pmatrix} \quad , \qquad H = \begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}$$

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

$$L^{\rm od}_{\kappa,\rho} = \begin{pmatrix} \kappa\, D_\rho & A_\rho \\ A^*_\rho & -\kappa\, D_\rho \end{pmatrix}$$

Clearly selfadjoint matrix:

$$(L^{\rm od}_{\kappa,\rho})^* = L^{\rm od}_{\kappa,\rho}$$

Fact 1: $L^{\rm od}_{\kappa,\rho}$ is gapped, namely $0 \notin L^{\rm od}_{\kappa,\rho}$ (A is like a mass)

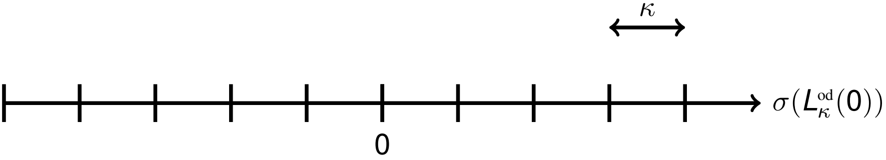
Fact 2: $L^{\rm od}_{\kappa,\rho}$ has spectral asymmetry measured by signature

Fact 3: signature linked to topological invariant

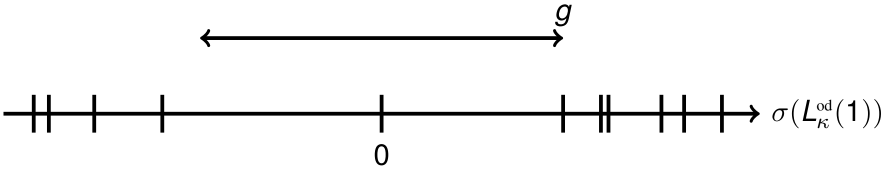
Schematic representation of intuition

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

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 $L^{\mathrm{od}}_{\kappa,\rho}$ is invertible and with $\Pi = \chi(D \geqslant 0)$

$$\tfrac{1}{2}\,\mathrm{Sig}(L^{\mathrm{od}}_{\kappa,\rho}) = \mathrm{Ind}\big(\Pi A \Pi + (\mathbf{1} - \Pi)\big)$$

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 (**)

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

$$\mathrm{Ch}_3(A) = \mathrm{Wind}_3(A) = \frac{1}{24\pi^2} \int_{\mathbb{T}^3} \mathrm{Tr}\big(A^{-1}\, dA\, dA^{-1}\, dA\big)$$

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

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

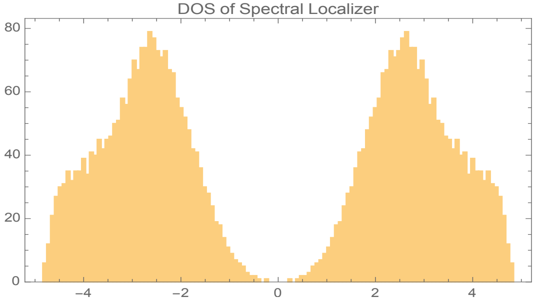
Spectrum and signature of localizer

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

Spectral localizer:

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

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 strong 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 $\Gamma = \Gamma_{d+1} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$

Thus $D = -\Gamma D \Gamma = \begin{pmatrix} 0 & D_0^* \\ D_0 & 0 \end{pmatrix}$ and Dirac phase $F = D_0 |D_0|^{-1}$

$[H, D_0]$ bounded $\implies T = PFP + (\mathbf{1} - P)$ Fredholm (index = Chern #)

Spectral localizer = Hamiltonian in Dirac trap

$$L_\kappa^{\text{ev}} = \begin{pmatrix} -H & \kappa D_0^* \\ \kappa D_0 & H \end{pmatrix}$$

Theorem (with Loring 2018)

Suppose $\|[H, D_0]\| < \infty$ *and* κ, ρ *with* (*) *and* (**)

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

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

$$L^{\mathrm{sk}}_{\kappa} \;=\; \begin{pmatrix} 0 & \kappa D - iH \\ \kappa D + iH & 0 \end{pmatrix}$$

Theorem (with Doll 2021)

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

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

Semifinite (here odd) index pairings (weak invar.)

$(\mathcal{N}, \mathcal{T})$ 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 weak invariant via index theorem (with Prodan, Bourne, Stoiber)

Semifinite (weak) odd spectral localizer

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

$$L^{\rm od}_\kappa \;=\; \begin{pmatrix} \kappa D & A \\ A^* & -\kappa D \end{pmatrix}$$

and restrictions

$$L^{\rm od}_{\kappa,\rho} \;=\; \Pi_\rho L^{\rm we}_\kappa \Pi_\rho \qquad , \qquad \Pi_\rho \;=\; \chi(D^2 < \rho^2)$$

Theorem (with Stoiber 2021)

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

$$\langle [U], [D] \rangle \;=\; \tfrac{1}{2}\, \mathcal{T}\text{-Sig}(L^{\rm od}_{\kappa,\rho})$$

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.

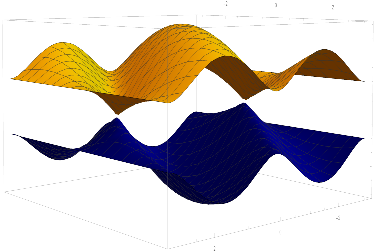
$2d$ topological semimetal: graphene

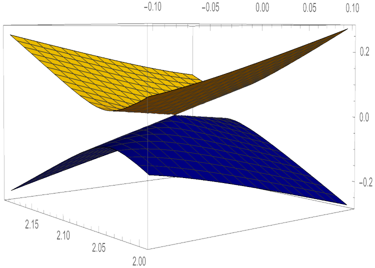
On honeycomb lattice = decorated triangular lattice, so on $\ell^2(\mathbb{Z}^2)\otimes\mathbb{C}^2$

$$H \;=\; \begin{pmatrix} 0 & S_1 + S_1^* S_2 + 1 \\ S_1^* + S_2^* S_1 + 1 & 0 \end{pmatrix}$$

where S_1, S_2 shifts on $\ell^2(\mathbb{Z}^2)$. Clearly chiral $\sigma_3 H \sigma_3 = -H$. Fourier:

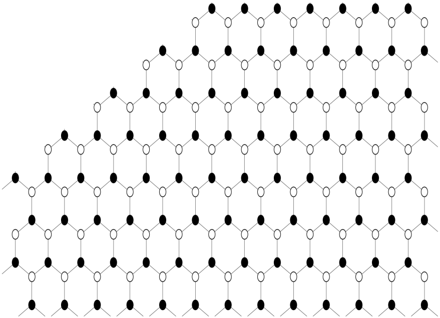
$$H \;\cong\; \int_{\mathbb{T}^2}^{\oplus} dk \;\begin{pmatrix} 0 & e^{ik_1} + e^{i(k_2-k_1)} + 1 \\ e^{-ik_1} + e^{-i(k_2-k_1)} + 1 & 0 \end{pmatrix}$$

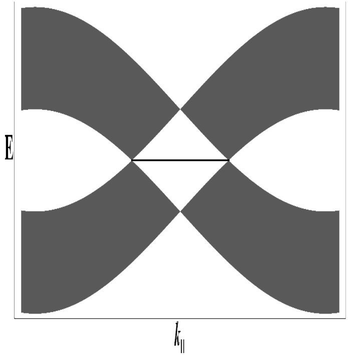




Dirac points $k_\pm = (\frac{(3\pm1)\pi}{3}, 0)$ DOS vanishes at $E = 0$ (pseudogap)

Edges of graphene





Zigzag boundary $\cong$ replace S_1 by unilateral shift $\widehat{S}_1$

Armchair boundary $\cong$ replace S_2 by unilateral shift $\widehat{S}_2$

Fact (Saito, Dresselhaus *et al.* **1988):** edge states only for Zigzag

Edge states and BBC for surface DOS

$\xi = \binom{\xi_1}{\xi_2} \in \mathbb{S}^1$ direction perpendicular to boundary (possibly irrational)

$\widehat{H} = \Pi_\xi \, H \, \Pi_\xi$ half-space restriction of graphene Hamiltonian

Kernel projection $\widehat{P} = \widehat{P}_+ + \widehat{P}_-$ on flat band of surface states

$\widehat{\mathcal{T}}$ trace per unit volume along the boundary

bulk Fermi unitary $U = (S_1 + S_1^* S_2 + 1)|S_1 + S_1^* S_2 + 1|^{-1}$ (singular!)

Theorem (Semimetal BBC - with Stoiber)

$$i\,\mathcal{T}(U^{-1}\nabla_\xi U) \;=\; \widehat{\mathcal{T}}(\widehat{P}_+) - \widehat{\mathcal{T}}(\widehat{P}_-)$$

where $\mathcal{T}(B) = \mathbf{E}\,\mathrm{Tr}(\langle 0|B|0\rangle)$ *and* $\nabla_\xi = \xi \cdot \nabla$ *with* $\nabla_j B = i[X_j, B]$

Moreover, result stable under chiral surface disorder

Flat band in clean graphene as weak invariants $i\,\mathcal{T}(U^{-1}\nabla_j U) = \frac{1}{3}\,\delta_{j,1}$

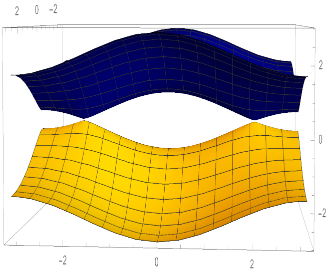
Other chiral $2d$ toy model: Stacked SSH

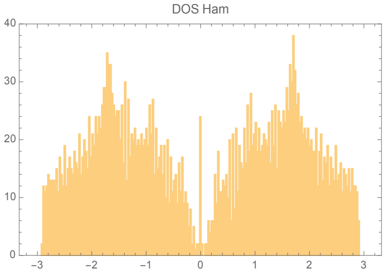
SSH in direction 1 with coupling in direction 2 and chiral randomness

$$H = \begin{pmatrix} 0 & S_1 - \mu \\ S_1^* - \mu & 0 \end{pmatrix} - \delta \begin{pmatrix} 0 & S_2 + S_2^* \\ S_2 + S_2^* & 0 \end{pmatrix} + \lambda \sum_{n \in \mathbb{Z}^2} v_n \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

where v_n i.i.d. random variables with uniform distribution in $[-\frac{1}{2}, \frac{1}{2}]$

(2 or 4) Dirac points for periodic model if $k_1 = 0, \pi$, $2\delta \cos(k_2) + \mu = \pm 1$

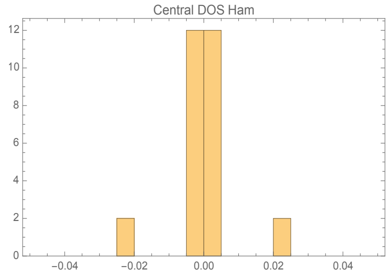




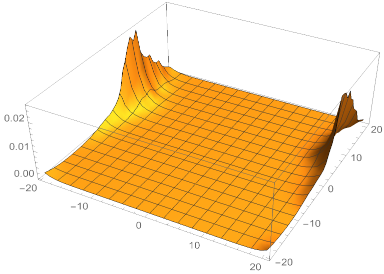
$\lambda = 0.2$, $\mu = 1.3$, $\delta = 0.3$ and volume $[-\rho, \rho]^2$ with $\rho = 20$

Central DOS and edge states

Zoom into the central DOS



Same parameters as above



There are $28 = 2 \cdot 14$ (approximate) zero modes of H

Corresponding eigenstates only on two opposite edges

(edges weakly coupled, edge states vanish on other edges!)

Edge state dens. $= \frac{14}{41} \approx i\mathcal{T}(U^{-1}\nabla_1 U) = \int \frac{dk_2}{2\pi}\,\chi(\mu + 2\delta\cos(k_2) < 1) \approx \frac{1}{3}$

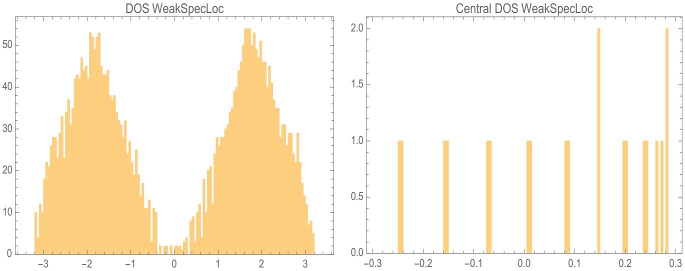
Here first $\approx$ is precisely the equality in the theorem (1 chiral sector)

Weak spectral localizer for weak winding numbers

$$L_\kappa^{\text{od}} = \begin{pmatrix} \kappa X_1 & A_{\text{per}}^* \\ A_{\text{per}} & -\kappa X_1 \end{pmatrix} \qquad H_{\text{per}} = \begin{pmatrix} 0 & A_{\text{per}}^* \\ A_{\text{per}} & 0 \end{pmatrix}$$

H_{per} stacked SSH H periodized in 2-direction $\quad \kappa = 0.1$

As above $\lambda = 0.2$, $\mu = 1.3$, $\delta = 0.3$ and volume $[-\rho, \rho]^2$ with $\rho = 20$



Half-signature of $L_{\kappa,\rho}^{\text{od}} \approx 14$

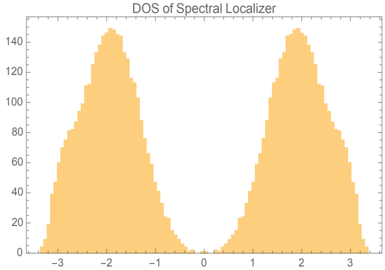
weak winding number $i\mathcal{T}(U^{-1}\nabla_1 U) =$ half-signature density $\approx \frac{14}{41} \approx \frac{1}{3}$

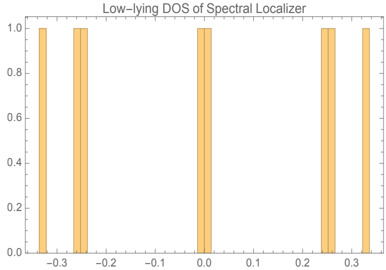
Approximate zero modes of spectral localizer

$$L_\kappa^{\text{ev}} = \begin{pmatrix} -H & \kappa\,\mathbf{1}_2 \otimes (X_1 + \imath X_2) \\ \kappa\,\mathbf{1}_2 \otimes (X_1 - \imath X_2) & H \end{pmatrix} = -\sigma_1 \otimes \mathbf{1}\, L_\kappa^{\text{ev}}\, \sigma_1 \otimes \mathbf{1}$$

Vanishing signature (Chern number vanishes due to chiral symmetry)

$L_{\kappa,\rho}^{\text{ev}}$ restriction to $[-\rho,\rho]^2$ Stacked SSH as above and $\kappa = 0.07$





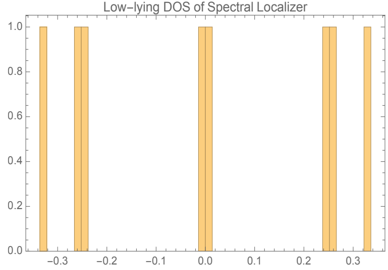
Approximate kernel of multiplicity 2 = number of Dirac points

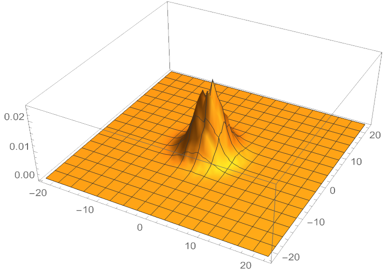
Very large gap to first excited $\approx \sqrt{\kappa} \approx 0.26$ (as for Dirac Ham.)

Gap above groundstate as for Dirac Hamiltonian (explicit computation)

Ground states of spectral localizer

Plot of modulus (over 4-dim fiber) of one of the two ground states:





lowest eigenvalue $\nu \approx C\,\lambda$ with C very small (perturbation theory)

For $\lambda = 0$, one has $\nu \approx e^{-1/\kappa}$ (phase space tunnelling)

Approximate kernel dimension counts number of Dirac points

Conclusion: Concept of number of Dirac points stable under disorder

Moreover: existence of Dirac points $\Longrightarrow$ non-vanishing weak windings

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

In Fourier space:

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

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

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

IMS localization isolates Dirac points

At each Dirac point solvable ”double” Dirac Hamiltonians $\begin{pmatrix} \gamma k & \kappa\Gamma\partial_k \\ \kappa\Gamma\partial_k & -\gamma k \end{pmatrix}$

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

Theorem (with Stoiber)

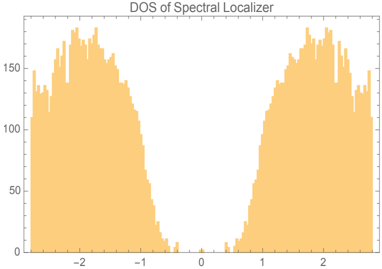
L_κ has as many eigenvalues $\leqslant \kappa$ as H has Dirac points

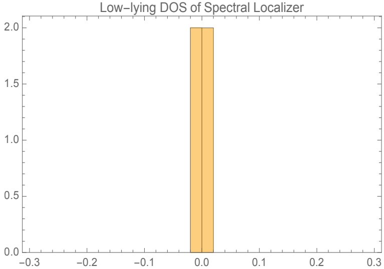
Next excited level is $\mathcal{O}(\sqrt{\kappa})$

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

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

$H_{\text{Weyl shift}}$ shifts Weyl points to different energies (no pseudogap)





$\rho = 7$, 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)

Resumé (four spectral localizers):

$$L_\kappa^{\text{od}} = \begin{pmatrix} \kappa D & A^* \\ A & -\kappa D \end{pmatrix} \quad , \qquad d \text{ odd, chiral class AIII}$$

$$L_\kappa^{\text{ev}} = \begin{pmatrix} -H & \kappa D_0^* \\ \kappa D_0 & H \end{pmatrix} \quad , \qquad d \text{ even, class A}$$

$$L_\kappa^{\text{od}} = \begin{pmatrix} -H & \kappa D \\ \kappa D & H \end{pmatrix} \quad , \qquad d \text{ odd, Weyl point count}$$

$$L_\kappa^{\text{ev}} = \begin{pmatrix} -H & \kappa D_0^* \\ \kappa D_0 & H \end{pmatrix} \quad , \qquad d \text{ even, Dirac point count}$$

spectral localizer is a
fun and versatile new tool

References (all but one on `arXiv`)

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