Invariants of disordered semimetals via the spectral localizer

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paper with same title in
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details in `arXiv:2203.15014`

Plan of the talk

- What is a semimetal?
- What are the invariants in a semimetal?
- What is the spectral localizer?
- Semiclassical Weyl/Dirac point count
- Numerical illustration
- Normal form: spectral localizer for a Weyl/Dirac Hamiltonian
- Topological charges and Fermion doubling theorem
- Generalized Callias index theorem

⋆ Weak invariants via weak spectral localizer

⋆ Application: weak winding numbers imply flat band of edge states

Ideal semimetals

periodic tight-binding H on $\ell^2(\mathbb{Z}^d,\mathbb{C}^N)$ with pseudogap at $E_F = 0$

After discrete Fourier transform $k \in \mathbb{T}^d \mapsto H_k = (H_k)^* \in \mathbb{C}^{N\times N}$

Fermi surface $\mathcal{Z}(H) = \{k \in \mathbb{T}^d \,:\, \dim(\mathrm{Ker}(H_k)) \geqslant 1\} = \{k_1^*, \ldots, k_I^*\}$

For each $k^* \in \mathcal{Z}(H)$ locally $k \in B_\delta(k^*) \mapsto W_k \in \mathrm{U}(N)$ such that

$$W_k H_k W_k^* = \begin{pmatrix} H_k^0 & 0 \\ 0 & H_k^Q + H_k^R \end{pmatrix}$$

with invertible H_k^0, remainder $\|H_k^R\| \leqslant C|k - k^*|^2$, and

linear term H_k^Q given by a direct sum of q^* summands of the form

$$H_k^{W/D} = \sum_{j=1}^{d} s_j (k - k^*)_j \Gamma_j$$

with slopes $s_1, \ldots, s_d \in \mathbb{R}\backslash\{0\}$ and $\Gamma_1, \ldots, \Gamma_d$ irrep of Clifford alg. $\mathbb{C}_d$

Terminology for d odd/even: Weyl/Dirac point of multiplicity q^*

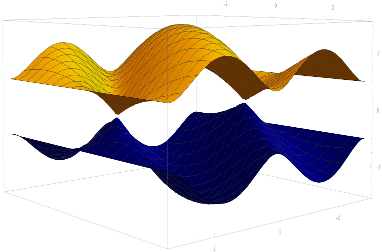
Example of $2d$ semimetal: graphene

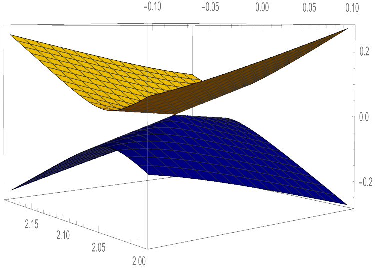
On honeycomb lattice = decorated triangular lattice, so on $\ell^2(\mathbb{Z}^2)\otimes\mathbb{C}^2$

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

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)

Instability of semimetals

In $d = 2$, Dirac points are stable only if chiral symmetry preserved

In $d = 3$, Weyl points are stable and generic (Wigner-von Neumann)

But move energetically, unless some symmetry fixes them at $E_F = 0$

Points of ”topological phase transitions” are often semimetals

There are variants: *e.g.* line node semimetals

Disordered semimetal: random (potential) perturbation of the above

Open: in $d = 2$ pseudogap stable for chiral random perturbation?

Invariants (that will be addressed here):

- number of Weyl/Dirac points, possibly weighted by topological charge
- weak invariants in direction $j = 1, \ldots, d$ (like winding $\#$ in $d > 1$)

$$\mathrm{Ch}_{\{j\}}(A) \;=\; \imath\,\mathbb{E}\,\mathrm{Tr}\,\langle 0|A^{-1}\imath[A, X_j]|0\rangle \qquad , \qquad H = \begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}$$

Spectral localizer (strong even pairings in even d)

Hamiltonian $H = H^*$ on $\mathcal{H}$ and $P = \chi(H < 0)$ with gap $g = \|H^{-1}\|^{-1}$

Dirac operator $D = \sum_{j=1}^{d} \gamma_j X_j$ on $\mathcal{H} \oplus \mathcal{H}$ is odd w.r.t. $\Gamma = \gamma_{d+1} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$

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

$[H, D']$ bounded $\Longrightarrow \mathrm{Ch}_d(P) = \mathrm{Ind}(PFP + \mathbf{1} - P)$ index theorem

$$L_\kappa = \begin{pmatrix} -H & \kappa D' \\ \kappa (D')^* & H \end{pmatrix} = -H \otimes \Gamma + \kappa D \qquad , \qquad \kappa > 0$$

Theorem (with Loring 2018)

$L_{\kappa,\rho}$ restriction (Dirichlet) to finite-dimensional range of $\chi(|D| \leqslant \rho)$ with

$$\|[H, D']\| \leqslant \frac{g^3}{12\,\|H\|\,\kappa} \qquad , \qquad \frac{2\,g}{\kappa} \leqslant \rho$$

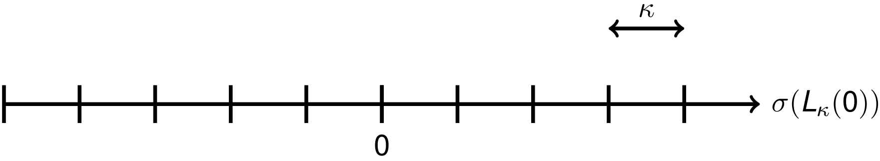
Then $L_{\kappa,\rho}$ has gap $\frac{g}{2}$ and

$$\mathrm{Ch}_d(P) = \frac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho}) \in \mathbb{Z}$$

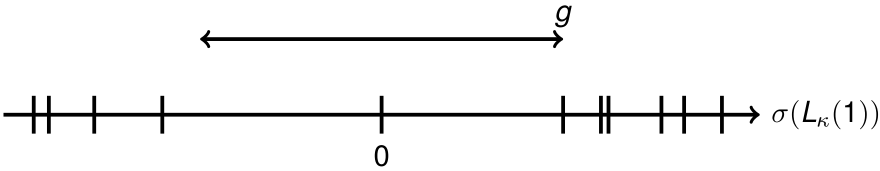
Schematic representation

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

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!)

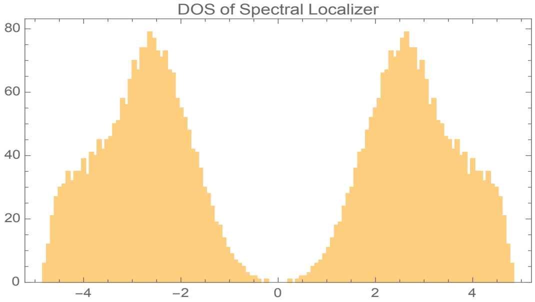
Spectrum and signature of localizer

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

Spectral localizer (placing Hamiltonian in a Dirac trap):

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

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



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

Spectral localizer (strong odd pairings in odd d)

For chiral Hamiltonian with gap $g = \|H^{-1}\|^{-1}$

$$H = \begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}$$

Odd Chern # $\mathrm{Ch}_d(P)$ are (higher) winding numbers. Index theorem

$$\mathrm{Ch}_d(P) = \mathrm{Ind}(EUE + \mathbf{1} - E)$$

where $E = \chi(D > 0)$ and $U = A|A|^{-1}$. Odd spectral localizer:

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

Theorem (with Loring 2017)

For κ and ρ as above, $L_{\kappa,\rho}$ is invertible and

$$\mathrm{Ch}_d(P) = \tfrac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho})$$

Motivation for Weyl/Dirac point count

$m \in \mathbb{R} \mapsto H(m)$ path of periodic Hamiltonians on $\ell^2(\mathbb{Z}^d, \mathbb{C}^N)$

Focus on d even (for d odd: chiral symmetry)

Suppose "topological transition" through semimetal at $m = 0$

$H(m)$ gapped at $E_F = 0$ for $|m| \in (0, m_0)$, but no gap for $m = 0$

$$\mathrm{Ch}_d(P(m)) \;=\; \tfrac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho}(m))$$

Transfer of topological charge given by

$$\begin{aligned}\mathrm{Ch}_d(P(m)) - \mathrm{Ch}_d(P(-m)) \;&=\; \tfrac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho}(m)) - \tfrac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho}(-m))\\ &=\; \tfrac{1}{2}\,\mathrm{SF}\big(m' \in [-m, m] \mapsto L_\kappa(m')\big)\end{aligned}$$

Guess: eigenvalue crossings precisely at $m' = 0$

Not covered by earlier results (which require gaps)!

Semiclassical Weyl/Dirac point count

Theorem

H ideal semimetal with I singular points at Fermi level

Multiplicities are $q_1^*, \dots, q_I^*$

Use even localizer $L_\kappa = \begin{pmatrix} -H & \kappa D \\ \kappa D & H \end{pmatrix}$ *for odd d, and odd one for even d*

Then exist constants c and C such that

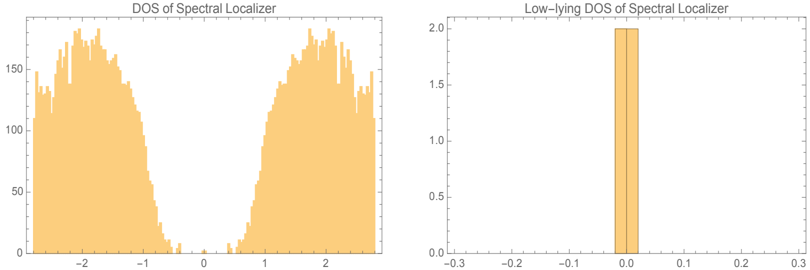
$$\sum_{i=1}^{I} q_i^* \;=\; \mathrm{Tr}\big(\chi(|L_\kappa| \leqslant c\kappa^{\frac{2}{3}})\big) \;=\; \mathrm{Tr}\big(\chi(|L_\kappa| \leqslant C\kappa^{\frac{1}{2}})\big)$$

Two facts:

- spectrum in $[-c\kappa^{\frac{2}{3}}, c\kappa^{\frac{2}{3}}]$ consists of $\sum_{i=1}^{I} q_i^*$ eigenvalues
- no further spectrum in $[-C\kappa^{\frac{1}{2}}, C\kappa^{\frac{1}{2}}]$

Numerical example: Weyl points of $d = 3$ system

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



$\rho = 7$, 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

Also: eigenvalues in $[-e^{-c'/\kappa}, -e^{-c'/\kappa}]$ (tunnel effect in k-space)

N.B.: Weyl point count stable under small disordered perturbation

Semiclassical perspective on spectral localizer

Consider Cayley transform of even spectral localizer for d odd:

$$\widetilde{L}_\kappa \;=\; C^* \, L_\kappa \, C \;=\; \begin{pmatrix} 0 & \kappa D - \imath H \\ \kappa D + \imath H & 0 \end{pmatrix}$$

As $\mathrm{Ker}(L_\kappa) = \mathrm{Ker}(L_\kappa^2) = C\,\mathrm{Ker}(\widetilde{L}_\kappa^2)$, approximate kernel is linked

to semiclassical Schrödinger-like operators on $L^2(\mathbb{T}^d, \mathbb{C}^{2N})$:

$$\mathcal{F}\,(\widetilde{L}_\kappa)^2\,\mathcal{F}^* \;=\; \begin{pmatrix} \kappa^2 D^2 + H^2 - \kappa\imath[D,H] & 0 \\ 0 & \kappa^2 D^2 + H^2 + \kappa\imath[D,H] \end{pmatrix}$$

Weyl points of H lead to quadratic wells of potential H^2

However $\pm\kappa i[D,H]$ shift eigenvalues by $\mathcal{O}(\kappa)$

Low-lying spectrum accessible by rough semiclassics

Technique: IMS localization à la Simon with improvements by Shubin

Local normal form: localizer of Weyl Hamiltonian

Weyl Hamiltonian $H^W = \sum_{j=1}^d s_j \Gamma_j X_j$ on $L^2(\mathbb{R}^d, \mathbb{C}^{d'})$ where $d' = 2^{\lfloor \frac{d}{2} \rfloor}$

$$L_\kappa^W = \begin{pmatrix} -H^W & \kappa D \\ \kappa D & H^W \end{pmatrix} = \begin{pmatrix} -\sum_{j=1}^d s_j \Gamma_j X_j & \kappa \sum_{j=1}^d \gamma_j \partial_j \\ \kappa \sum_{j=1}^d \gamma_j \partial_j & \sum_{j=1}^d s_j \Gamma_j X_j \end{pmatrix}$$

Here γ_j and Γ_j commute and act on $\mathbb{C}^{d'} \otimes \mathbb{C}^{d'}$. Hence

$$(L_\kappa^W)^2 = \begin{pmatrix} \sum_{j=1}^d (-\kappa^2 \partial_j^2 + s_j^2 X_j^2) + \kappa M & 0 \\ 0 & \sum_{j=1}^d (-\kappa^2 \partial_j^2 + s_j^2 X_j^2) - \kappa M \end{pmatrix}$$

with selfadjoint matrix $M = \sum_{j=1}^d s_j \gamma_j \Gamma_j$

Harmonic oscillator spectrum with representation theoretic methods:

Lemma

$\mathrm{Ker}(L_\kappa^W)$ *is one-dimensional and first excited state is* $\mathcal{O}(\sqrt{\kappa})$

Together with IMS this implies Theorem for odd d. Even d similar □

Topological charges (chiralities) of Weyl points

For d odd, chirality of singular point k_i^* with small ball $B_\epsilon(k_i^*)$

$$c_i^* \;=\; \mathrm{Ch}_{d-1}(H|H|^{-1}, \partial B_\epsilon(k_i^*))$$

Fact: $c_i^* = (-1)^{\frac{d+1}{2}} \prod_{j=1}^{d} \mathrm{sgn}(s_{i,j})$ determines SF at top. phase trans.

Theorem (Fermion doubling by Nielsen and Ninomiya)

$$\sum_{i=1}^{I} c_i^* \;=\; 0$$

Fact: c_i^* determines whether kernel in upper or lower component of $\widetilde{L}_\kappa$

Supposing kernels are not approximate, with $J = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$,

$$\sum_{i=1}^{I} c_i^* \;\approx\; \mathrm{Sig}(J|_{\mathrm{Ker}(L_\kappa)}) \;=\; \mathrm{Ind}(\kappa D + iH) \;=\; \mathrm{Ind}(\kappa D) \;=\; 0$$

because index on a compact manifold $\mathbb{T}^d$ has vanishing index

Generalized Callias index theorems

Kernel actually empty, but argument gives Callias-type index theorem

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 $x_i^* \in \mathcal{Z}(H)$ topological charge $c_i^* = \mathrm{Ch}_{d-1}(H|H|^{-1}, \partial B_\delta(x_i^*))$

Theorem

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

$$\mathrm{Ind}(\kappa D + iH) \;=\; \mathrm{Sig}(J|_{\mathrm{Ker}(L_\kappa)}) \;=\; \sum_{x_i^* \in \mathcal{Z}(H)} c_i^*$$

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

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

Weak invariants in chiral semimetals

$H = \begin{pmatrix} 0 & A \\ A^* & 0 \end{pmatrix}$ chiral semimetal (such as graphene)

$$\mathrm{Ch}_{\{j\}}(A) \;=\; \imath\,\mathbb{E}\,\mathrm{Tr}\,\langle 0|A^{-1}\imath[A,X_j]|0\rangle \qquad , \qquad j=1,\ldots,d$$

Proposition

$\mathrm{Ch}_{\{j\}}(A)$ *well-defined whenever there is a pseudogap*

Define weak spectral localizer in direction j

$$L^{w,j}_{\kappa,\rho} \;=\; \begin{pmatrix} \kappa\,X_j & A^*_{\rho,j} \\ A_{\rho,j} & -\kappa\,X_j \end{pmatrix} \qquad , \qquad H_{\rho,j} \;=\; \begin{pmatrix} 0 & A^*_{\rho,j} \\ A_{\rho,j} & 0 \end{pmatrix}$$

where $H_{\rho,j}$ on $[-\rho,\rho]^2$ with Dirichlet bc in j and periodic bc in others

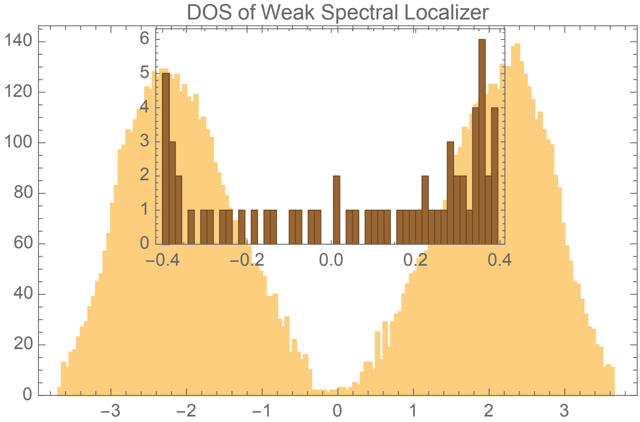
Proposition

$$\mathrm{Ch}_{\{j\}}(A) \;=\; \frac{1}{2\rho+1}\,\mathbb{E}\,\frac{1}{2}\,\mathrm{Sig}(L^{w,j}_{\kappa,\rho}) \;+\; \mathcal{O}(\rho^{-1},\kappa)$$

Numerical example: weak localizer for graphene

Take H graphene Hamiltonian

Histogram of eigenvalues of $L^{w,1}_{\kappa,\rho}$ for $\rho = 34$ and $\kappa = 0.1$



Computed half-signature is 23 so $\mathrm{Ch}_{\{1\}}(A) \approx \frac{23}{69} \approx \frac{1}{3}$ as $2\rho + 1 = 69$

Bulk-boundary correspondence in semimetals

Theorem

Consider an chiral ideal semimetal Hamiltonian $H = -JHJ$

Given $\xi \in \mathbb{S}^{d-1}$, restrict it to a half-space perpendicular to ξ denoted $\widehat{H}$

Random local surface perturbations are allowed. Then

$$\widehat{\mathcal{T}}(J\,\mathrm{Ker}(\widehat{H})) \;=\; \sum_{j=1}^{d} \xi_j\,\mathrm{Ch}_{\{j\}}(A)$$

where $\widehat{\mathcal{T}}$ trace per surface along the boundary

Example for graphene as above, $\xi = e_1$. Flat band $48 \approx 2\,\frac{1}{3}\,69$ states