Mathematics for topological materials

Hermann Schulz-Baldes, FAU

.

Trends in Mathematical Sciences, Erlangen, June 2024

Abstract: This talk will provide an overview of topological materials and the mathematical challenges linked to them. In particular, topological invariants are introduced as index pairings in noncommutative geometry, then it is shown how to compute them numerically by means of the spectral localizer and finally the bulk-boundary correspondence is described as a robust mathematical concept based on suitable exact sequences.

Why am a speaker in this conference?

True reason: office of Erlangen organizer is above mine

Current scientific collaborations with Latin America:

- Villegas (Cuernavaca)
- Ballesteros & Franco & Naumkin (UNAM)
- Sadel (Catolica, Santiago di Chile)

Earlier collaborations

- de Nittis (Catolica, Santiago di Chile)
- J. C. Avila (Guadalajara)
- del Rio (UNAM)
- Lozano Viesca (Cuernavaca)

Outsider to: control, optimization, non-linear PDEs, networks

Trend (rather in physics than in math): topological materials

What is a topological material?

- Historically first example: quantum Hall effect (QHE, 1980)
  two-dimensional electron gas with non-vanishing Chern number
  (topological invariant measuring global twist in wave functions)
- bulk-boundary correspondence (BBC) $\Longrightarrow \exists$ boundary modes
- Since 2005: topological insulators of electrons in all dimensions
- In particular: anomalous QHE and topological superconductors
- Since 2010: topological meta materials, photonic crystals, *etc.*

Common feature of topological materials:

periodic wave-type equation with spectral gaps

non-trivial topology in Bloch bands & stability to disorder

Nobel prizes:

1985 (Klitzing), 1998 (Laughlin *et al*), 2016 (Thouless, Haldane)

Example: topological mechanics

Coupled pendula in Huber group, ETH Zürich, 2015

coupling only with springs, but in a complex manner

(inspired by quantum spin Hall systems)

coupling mechanism

Boundary modes at frequencies in gap of bulk

Potential applications of topological materials

Numerous, but unpredictable

- topological high-temperature superconductor
- topological Majorana modes for quantum computers
- topological light-wires and logical elements (light computer)
- evacuation of vibrations on rockets
- dissipationless spintronics
- data transmission with topological photonic crystals
- ...
- ...
- ???

From K-theory to physics and back

(sub-title from my 2016 book with Prodan)

Beautiful deep math related to topological materials:

- K-theory (of vector bundles and C^*-algebras)
- cyclic cohomology and noncommutative geometry
- exact sequences of C^*-algebras connecting bulk and boundary
- spectral flow for Fredholm operators (first book on subject)
- applied index theory
- new field of numerical K-theory for engineering of top. materials
- analysis of random operators and random matrices

Fields medals related to these topics:

1966 (Atiyah), 1982 (Connes), 1990 (Witten)

Topological invariants and index theorem in $1d$

$1d$ chiral periodic Hamiltonian H on $\ell^2(\mathbb{Z},\mathbb{C}^{2L})$

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

with A short-range discrete differential operator on $\ell^2(\mathbb{Z},\mathbb{C}^{2L})$

Partial diagonalization by Fourier transform $\mathcal{F}A\mathcal{F}^* = \int_{\mathbb{T}^1}^{\oplus} dk\, A_k$

Here the bulk topological invariant is: $\mathrm{Wind}(A) = i\int \mathrm{Tr}(A^{-1}dA)$

Fritz Noether's index theorem from 1921

Π Hardy projection onto $\ell^2(\mathbb{N}) \subset \ell^2(\mathbb{Z}) \Longrightarrow \Pi A\Pi$ Fredholm and

$$\mathrm{Wind}(A) = -\mathrm{Ind}(\Pi A\Pi)$$

BBC: zero-energy boundary states of half-space Hamilt. $\widehat{H} = \Pi H\Pi$

$$\mathrm{Wind}(A) = \dim\left(\mathrm{Ker}(\widehat{H})\cap\mathrm{Ker}(J+\mathbf{1})\right) - \dim\left(\mathrm{Ker}(\widehat{H})\cap\mathrm{Ker}(J-\mathbf{1})\right)$$

Chern numbers in $2d$ (QHE and AQHE)

Periodic short-range 1-particle Hamiltonian H on $\ell^2(\mathbb{Z}^2, \mathbb{C}^L)$

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

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

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

Noncommutative analog for random $H = (H_\omega)_{\omega\in\Omega}$ using positions

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

Index theorem (Connes, Bellissard, etc. 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 formula

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

Spectral localizer 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:

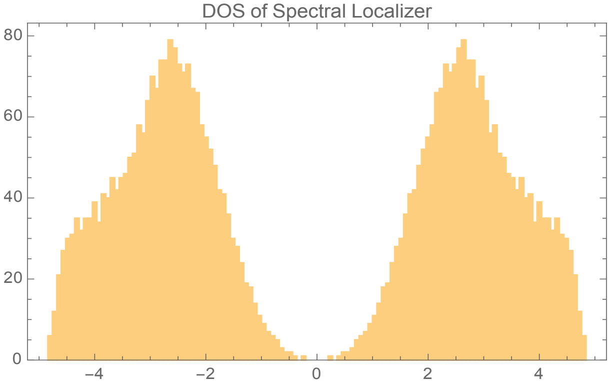
$$\boxed{\mathrm{Ch}(P) = \frac{1}{2}\,\mathrm{Sig}(L_{\kappa,\rho})}$$

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

Implementation for dirty $p + ip$ superconductor

Standard toy model (like disordered Harper or Haldane model)

Density of states (DOS) of the localizer for $\kappa = 0.1$ and $\rho = 20$



Looks harmless, however, note gap at 0

Spectral asymmetry $= \; -2 \;\; = \#$ positive $- \; \#$ negative eigenvalues

Main theorem on spectral localizer

Finite volume computation of K-theory invariants (with Loring)

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

$$\kappa < \frac{12\, g^3}{\|H\|\, \|[X_1 + iX_2, H]\|} \qquad , \qquad \rho > \frac{2\, g}{\kappa}$$

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

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

If H "differentiable", conditions always OK for κ small and ρ large

Numerics: typically $\kappa \approx 0.1$, $\rho \approx 20$ sufficient

Proof: K-theory of fuzzy spheres or spectral flow

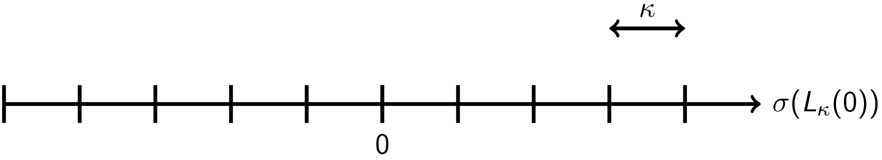
Special case of general statement for KK-theoretic index pairings

Even: $\mathbb{Z}_2$-invariants in Real K-theory or semifinite index pairings

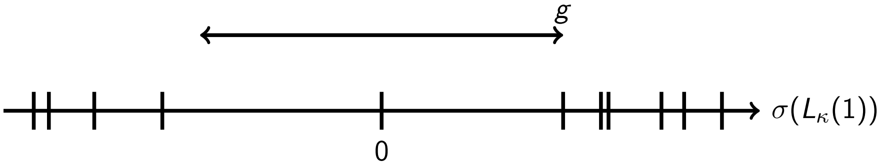
Intuition: H topological mass term added to Dirac

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

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 vol!)

Why care about non-trivial topology?

Bulk-boundary correspondence implies effects at edges or defects

First explain this in $1d$ using Toeplitz extension and its K-theory

S bilateral shift on $\ell^2(\mathbb{Z})$, then $\mathrm{C}^*(S) \cong C(\mathbb{S}^1)$

$\widehat{S}$ unilateral shift on $\ell^2(\mathbb{N})$, only partial isometry with a defect:

$$\widehat{S}^*\widehat{S} = \mathbf{1} \qquad \widehat{S}\,\widehat{S}^* = \mathbf{1} - |0\rangle\langle 0|$$

Then $\mathrm{C}^*(\widehat{S}) = \mathcal{T}$ Toeplitz algebra with short exact sequence:

$$0 \longrightarrow \mathcal{K} \longrightarrow \mathcal{T} \longrightarrow C(\mathbb{S}^1) \longrightarrow 0$$

K-groups for any C^*-algebra $\mathcal{A}$ with unitization $\mathcal{A}^+$:

$$\begin{aligned} K_0(\mathcal{A}) &= \{[P] - [s(P)] \ : \ \text{projection in some } M_n(\mathcal{A}^+)\} \\ K_1(\mathcal{A}) &= \{[U] \ : \ \text{unitary in some } M_n(\mathcal{A})\} \end{aligned}$$

with homotopy classes. Abelian group operation: Whitney sum

6-term exact sequence for Toeplitz extension

C*-algebra short exact sequence $\Longrightarrow$ K-theory 6-term sequence

$$\begin{array}{ccccc}
K_0(\mathcal{K}) = \mathbb{Z} & \xrightarrow{i_*} & K_0(\mathcal{T}) = \mathbb{Z} & \xrightarrow{\pi_*} & K_0(C(\mathbb{S}^1)) = \mathbb{Z} \\
\uparrow \mathrm{Ind} & & & & \downarrow \mathrm{Exp} \\
K_1(C(\mathbb{S}^1)) = \mathbb{Z} & \xleftarrow{\pi_*} & K_1(\mathcal{T}) = 0 & \xleftarrow{i_*} & K_1(\mathcal{K}) = 0
\end{array}$$

Here: $[A]_1 \in K_1(C(\mathbb{S}^1))$ and $[\widehat{P}J]_0 = [\widehat{P}_+]_0 - [\widehat{P}_-]_0 \in K_0(\mathcal{K})$

$$\mathrm{Ind}([A]_1) \;=\; [\widehat{P}_+]_0 - [\widehat{P}_-]_0 \qquad \text{(bulk-boundary for } K\text{-theory)}$$

$$\mathrm{Tr}(\mathrm{Ind}(A)) \;=\; \mathrm{Wind}(A) \qquad \text{(bulk-boundary for invariants)}$$

Disordered case: analogous

Higher dimension: analogous

Generalization to dimension d

Random operators $A = (A_\omega)_{\omega\in\Omega}$ on Hilbert space $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^L$

C*-algebra of covariant observables $\mathcal{A}_d = \; C^*(S_1^B, \ldots, S_d^B, V_\omega)$

Here $S_j^B S_i^B = e^{iB_{i,j}} S_i^B S_j^B$ and $(V_\omega)_{\omega\in\Omega}$ covariant matrix potential

Half-space restrictions $\ell^2(\mathbb{Z}^{d-1} \times \mathbb{N}) \otimes \mathbb{C}^L$ form Toeplitz $\mathcal{T}(\mathcal{A}_d)$

Contains boundary operator $\mathcal{E}_d \cong \mathcal{A}_{d-1} \otimes \mathcal{K}(\ell^2(\mathbb{N}))$

$$\begin{array}{ccccccccc} & & \text{edge} & & \text{half-space} & & \text{bulk} & & \\ 0 & \to & \mathcal{E}_d & \to & \mathcal{T}(\mathcal{A}_d) & \to & \mathcal{A}_d & \to & 0 \end{array}$$

Again 6-term exact sequence connecting bulk and edge for d even:

$$\mathrm{Exp} : K_0(\mathcal{A}_d) \to K_1(\mathcal{E}_d) \quad , \quad \mathrm{Exp}(P) \;=\; \exp\big(2\pi i\, \mathrm{Lift}(P)\big)$$

$$\mathrm{Ind} : K_1(\mathcal{A}_{d+1}) \to K_0(\mathcal{E}_{d+1}) \quad , \quad \mathrm{Ind}(A) \;=\; \ldots.$$

Meta Theorem on BBC

Theorem

For d even and $P \in \mathcal{A}_d$ projection

$$\mathrm{Ch}_d(P) = \mathrm{Ch}_{d-1}(\mathrm{Exp}(P))$$

For d even and $A \in \mathcal{A}_{d+1}$ invertible, specifying chiral H,

$$\mathrm{Ch}_{d+1}(A) \; = \; \mathrm{Ch}_d(\mathrm{Ind}(A))$$

Here with $\quad \mathcal{T}(A) = \mathbf{E}_{\mathbb{P}} \, \mathrm{Tr}_L \, \langle 0 | A_\omega | 0 \rangle \quad$ and $\quad \nabla_j A_\omega = i[X_j, A_\omega]$

$$\mathrm{Ch}_{d+1}(A) \; = \; \frac{i(i\pi)^{\frac{d}{2}}}{(d+1)!!} \sum_{\rho \in S_{d+1}} (-1)^\rho \, \mathcal{T}\left(\prod_{j=1}^{d+1} A^{-1} \nabla_{\rho_j} A \right)$$

Concrete situations: boundary invariant has physical interpretation

Current research and open questions

- more exact sequences (bulk to defect)
- respecting symmetries (time-reversal, particle-hole, space groups)
- spectral localizers with symmetries
- spectral localizer in the Anderson localization regime
- topological phase transitions
- topology in non-hermitian physics
- topological scattering theory