

Noncommutative topological approach to topological phases

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(Partial) Overview on the theory of topological phases in the C^* -algebraic approach to solid state physics proposed by [J. Bellissard in 1984](#).

- 1 Topological phases in the 1-particle approximation
- 2 K-theoretic formulation of topological phases
- 3 Symmetry protection
- 4 Boundary invariants and KK-classes
- 5 Bulk boundary correspondence
- 6 Numerical invariants (outlook)

A theory of topological phases for interacting fermions in a solid is an active area of research, but not discussed here (second quantization, study of the topology of the ground state separated from the rest by a gap, captured by (higher) category theory).

What is a topological insulator?

Deep inside the material (bulk): configuration space \mathbb{R}^d or \mathbb{Z}^d .

Electron-electron interaction gives rise to an effective potential V for a single quasi-particle described by a stationary Schrödinger equation in $\mathcal{H} = L^2(\mathbb{R}^d, \mathbb{C}^N)$ or $\ell^2(\mathbb{Z}^d, \mathbb{C}^N)$ (\mathbb{C}^N internal (spin) degrees of freedom).

$$H\Psi = E\Psi, \quad H = -\Delta + V$$

Examples: Landau Hamiltonian for a free electron in a magnetic field, Hofstadter Hamiltonian (its tight binding analog), but also models without magnetic field (Kane-Mele).

Main assumption: the system is (bulk) insulating: the Fermi energy lies in a gap of the spectrum of H .

Definition

Two models (Hamiltonians H_0, H_1) belong to the same topological phase if they can be deformed into each other preserving the gap:

There is a continuous path $H(t) \in A$ of gapped Hamiltonians in some background topological space A linking the two.

In the following we do not talk about a specific Hamiltonians, but only of their homotopy classes in A . We choose A to be a C^* -algebra. Its form has to be physically motivated.

A describes the physics deep inside the material (the **bulk**).

In the tight binding approx. (configuration space \mathbb{Z}^d) A is generated by

- 1 **bounded potentials** $C_{pot}(\mathbb{Z}^d) \subset \{V : \mathbb{Z}^d \rightarrow \mathbb{C}, bdd\}$
- 2 **translations** (possibly twisted by magnetic field Θ) $T_1, \dots, T_d, T_i \psi(x) = \psi(x + e_i)$

$$T_i^* T_i = 1 = T_i T_i^* \quad T_i T_j = e^{i\Theta_{ij}} T_j T_i \quad (1)$$

$$T_i V T_i^*(x) = V(x + e_i) \quad (2)$$

- 3 (finitely many) **internal degrees of freedom** (spin), internal Hilbert space \mathbb{C}^N :
 A acts on $\ell^2(\mathbb{Z}^d) \otimes \mathbb{C}^N$

$$A = A' \otimes M_N(\mathbb{C})$$

A' is a twisted crossed product algebra

$$A' = C_{pot}(\mathbb{Z}^d) \rtimes_{\alpha, \Theta} \mathbb{Z}^d$$

Continuous version: $A = C_{pot}(\mathbb{R}^d) \rtimes_{\alpha, \Theta} \mathbb{R}^d \otimes M_N(\mathbb{C})$

Examples (tight binding)

$$A = C_{pot}(\mathbb{Z}^d) \rtimes_{\alpha, \Theta} \mathbb{Z}^d \otimes M_N(\mathbb{C})$$

- 1 **All bounded potentials** are allowed (no symmetry constraint) $C_{pot}(\mathbb{Z}^d) = C_b(\mathbb{Z}^d)$:
 A is the algebra of all **local** tight binding operators with at most N internal degrees of freedom.
 A is non-separable so has relatively poor K -theory.
- 2 **Crystals**: potentials are periodic, internal Hilbert space contains elementary cell:
 $C_{pot}(\mathbb{Z}^d) = \mathbb{C}$. If no magnetic field:

$$A = M_N(\mathbb{C}) \rtimes_{\alpha} \mathbb{Z}^d \cong C(\mathbb{T}^d, M_N(\mathbb{C}))$$

Most often used in solid state physics (N Bloch bands).

- 3 **Long range order / quasicrystals**: atomic positions described by point set $\mathcal{L} \subset \mathbb{R}^d$, restrict $C_b(\mathcal{L})$ to functions respecting long range order.

This has been introduced by [Bellissard 1986]: $C_b(\mathcal{L}) \cong C(\Omega)$ where Ω is the hull of the configuration \mathcal{L} .

Towards K -theoretic formulation of a topological phase

[K. 2017; Kubota 2017]

Fix the Fermi energy to be 0 (shift the spectral gap to 0).

- H has gap at 0 $\Leftrightarrow H$ is invertible

Bands below energy 0 are filled, those above unfilled.

Example: $H = 1$ is a Hamiltonian whose bands are completely unfilled. $H = -1$ is a Hamiltonian whose bands are completely filled. Both are topologically trivial.

Definition (same definition)

A topological phase of an **insulator in A** is a path connected component of the open set

$$GL(A)^{s.a.} = \{H \in A : H^* = H, H^{-1} \in A\}$$

Spectral flattening: every element of $GL(A)^{s.a.}$ is homotopic to a self-adjoint unitary $H^* = H = H^{-1}$.

Definition (rough)

Let A be a C^* -algebra with a unit. $K_0(A)$ is $GL(A)^{s.a.} / \sim_{homotopy}$ turned into an abelian group.

$K_0(A)$ is $GL(A)^{s.a.} / \sim_{homotopy}$ turned into an abelian group means the following:

- 1 **Stabilise:** $GL(M_n(A))^{s.a.} \ni x \mapsto x \oplus 1 \in GL(M_{n+1}(A))^{s.a.}$ (adding unfilled bands).
 $V(A) = \bigcup_{n \geq 1} GL(M_n(A))^{s.a.} / \sim_{homotopy}$ is an abelian semigroup

$$[x] + [y] = [x \oplus y] = [y \oplus x]$$

- 2 **Turn into a group:** $K_0(A) = V(A) \times V(A) / \sim_{Grothendieck}$ (adding filled bands).

Definition (slightly weaker definition)

A topological phase of an insulator (slightly weaker sense) in A is an element of $K_0(A)$.

We have allowed adding of unfilled bands and of filled bands (stacking):

Two Hamiltonians are in the same topological phase (in a slightly weaker sense) if, after adding unfilled and filled bands they can be deformed into each other inside $M_n(A)$ without closing the gap.

The Hamiltonian H may be subject to symmetry conditions:

- Ordinary symmetries given by a group G representation ρ : \mathbb{C} -linear $\rho_g \in \text{Aut}_{\mathbb{R}}(A)$ such that $\rho_g(H) = H$.
Restrict A to G -invariant elements.
- Quasiperiodicity (long range order): restrict $C_{pot}(\mathbb{Z}^d)$ to quasiperiodic functions.

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Restrict A to G -invariant elements.
- Quasiperiodicity (long range order): restrict $C_{pot}(\mathbb{Z}^d)$ to quasiperiodic functions.

Extra ordinary symmetries \mathcal{E} :

- Time reversal symmetry TRS
anti-linear $t \in \text{Aut}_{\mathbb{R}}(A)$ of order 2 and $t(H) = H$ (real structure)
- Charge conjugation (particle hole symmetry) PHS
anti-linear $c \in \text{Aut}_{\mathbb{R}}(A)$ of order 2 and $c(H) = -H$ (real structure)
- Chiral symmetry CS
 \mathbb{C} -linear $\gamma \in \text{Aut}_{\mathbb{C}}(A)$ of order 2 and $\gamma(H) = -H$ (balanced grading)

Definition

A topological phase of an insulator in A with protecting symmetry \mathcal{E} is a path connected component of the open set

$$GL(A, \mathcal{E})^{s.a.} = \{H \in A : H^* = H, H^{-1} \in A, H \text{ satisfies } \mathcal{E}\}$$

or, slightly weaker, an element of $K(A, \mathcal{E})$, obtained as above by turning $GL(A, \mathcal{E})^{s.a.}$ into a group.

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More precisely: Call A balanced graded if it contains an odd self-adjoint unitary e (OSU). e plays the role of a basepoint, or trivial insulator.

Definition (van Daele '84)

Let (A, γ) be a balanced graded real or complex C^* -algebra. Choose e . Van Daele K -group $DK_e(A, \gamma)$ is obtained from $GL(A, \{\gamma\})^{s.a.}$ as above except $GL(M_n(A), \{\gamma\})^{s.a.} \ni x \mapsto x \oplus e \in GL(M_{n+1}(A), \{\gamma\})^{s.a.}$

$$K(A, \mathcal{E}) = DK_e(A, \gamma) \text{ or } DK_e(A_{\mathbb{R}}, \gamma) \text{ if } \mathcal{E} \text{ contains a chiral symmetry } \gamma$$

up to isom. $DK_e(A, \gamma)$ does not depend on the choice of e

Classification into 10 symmetry types via Clifford algebras $Cl_{r,s}$

Odd case (chiral symmetry)

Recall $A = C_{pot}(\mathbb{Z}^d) \rtimes_{\alpha} \mathbb{Z}^d \otimes M_N(\mathbb{C})$

Suppose \mathcal{E} acts on internal degrees of freedom, i.e. on $M_N(\mathbb{C})$.

If \mathcal{E} contains chiral sym. γ then $(M_N(\mathbb{C}), \gamma) \cong (M_n(\mathbb{C}) \otimes Cl_2, Ad_{\sigma_3})$, $N = 2n$.

Up to equivalence, there are 4 real structures τ on $M_N(\mathbb{C})$ commuting with γ .

even TRS: $M_N(\mathbb{C})^{\tau} = M_N(\mathbb{R}) \cong M_n(\mathbb{R}) \otimes Cl_{1,1}$ (σ_3 is real)

even PHS: $M_N(\mathbb{C})^{\tau} \cong M_n(\mathbb{R}) \otimes Cl_{2,0}$ (σ_3 is imag.)

odd TRS: $M_N(\mathbb{C})^{\tau} \cong M_k(\mathbb{R}) \otimes \mathbb{H} \otimes Cl_{1,1} \cong M_k(\mathbb{R}) \otimes Cl_{0,4}$ (σ_3 real), $N = 4k$

odd PHS: $M_N(\mathbb{C})^{\tau} \cong M_n(\mathbb{R}) \otimes Cl_{0,2}$ (σ_3 is imag.)

All Clifford algebras with even number of generators appear up to Morita equiv..

Definition (higher K -groups)

(A, γ) a real or complex balanced graded algebra.

$K_{1+s-r}(A, \gamma) := DK_e(A \otimes Cl_{r,s}, \gamma \otimes st)$.

- $K(A, \mathcal{E}) \cong KU_1(A)$ if no real symetries (complex K -theorie, Bott 2-periodic)
- $K(A, \mathcal{E}) \cong KO_{1+s-r}(A_{\mathbb{R}})$ with real symmetries (real K -theorie, Bott 8-periodic)

Classification into 10 symmetry types via Clifford algebras

Even case, no chiral symmetry

\mathcal{E} does not contain a chiral sym. Trick: add an outer one.

Replace A by $A \otimes \mathbb{C}l_1$, with outer grading γ . Replace \mathcal{E} by $\mathcal{E} \cup \{\gamma\}$.

Up to equivalence, there are 4 real structures τ on $M_N(\mathbb{C}) \otimes \mathbb{C}l_1$ commuting with γ .

$$\text{even TRS: } (M_N(\mathbb{C}) \otimes \mathbb{C}l_1)^\tau \cong M_N(\mathbb{R}) \otimes Cl_{1,0}$$

$$\text{even PHS: } (M_N(\mathbb{C}) \otimes \mathbb{C}l_1)^\tau \cong M_N(\mathbb{R}) \otimes Cl_{0,1}$$

$$\text{odd TRS: } (M_N(\mathbb{C}) \otimes \mathbb{C}l_1)^\tau \cong M_n(\mathbb{R}) \otimes \mathbb{H} \otimes Cl_{1,0} \cong M_n(\mathbb{R}) \otimes Cl_{0,3}$$

$$\text{odd PHS: } (M_N(\mathbb{C}) \otimes \mathbb{C}l_1)^\tau \cong M_n(\mathbb{R}) \otimes \mathbb{H} \otimes Cl_{0,1} \cong M_n(\mathbb{R}) \otimes Cl_{3,0}$$

All Clifford algebras with odd number of gen. appear up to Morita equiv..

By definition $K(A, \emptyset) := K(A \otimes \mathbb{C}l_1, \{\gamma\}) =: K_0(A)$.

With real symmetry \mathcal{E}

$$K(A, \mathcal{E}) := K(A \otimes \mathbb{C}l_1, \mathcal{E} \cup \{\gamma\}) \cong KO_1(A_{\mathbb{R}} \otimes Cl_{r,s}) =: KO_{1+s-r}(A_{\mathbb{R}})$$

Bulk invariants: First summary and comments

- Physical considerations leads to the choice of the algebra A whose elements describe the physics in the bulk.
- The symmetry protected topological phases can be identified with the elements of $K(A, \mathcal{E})$. These are referred to as the bulk invariants.
- Different extra-ordinary symmetry types correspond to the different higher classical K -groups of A .

Bulk invariants: First summary and comments

- Physical considerations leads to the choice of the algebra A whose elements describe the physics in the bulk.
- The symmetry protected topological phases can be identified with the elements of $K(A, \mathcal{E})$. These are referred to as the bulk invariants.
- Different extra-ordinary symmetry types correspond to the different higher classical K -groups of A .
- If A is commutative then the K -groups can be described by vectorbundles with symmetries (twisted K -theory) [Freed, Moore 2013]
- For $A = \mathbb{C} \rtimes \mathbb{R}^d$ (constant potential, cont. translations) one obtains the famous Kitaev table [Kitaev 2007].

Near the boundary the physics of material is described by operators on halfspace $\mathbb{Z}^{d-1} \times \mathbb{N}$.

Relevant algebra \hat{A} differs from bulk algebra A in one respect: restricting the action of perpendicular translation T_d to $\ell^2(\mathbb{Z}^{d-1} \times \mathbb{N})$ "runs into the wall": T_d^* no longer inject.

\hat{A} is generated by

- 1 bounded potentials $C_{pot}(\mathbb{Z}^d) \subset \{V : \mathbb{Z}^d \rightarrow \mathbb{C}, bdd\}$
- 2 translations (possibly twisted by magnetic field Θ) $\hat{T}_1, \dots, \hat{T}_d, \hat{T}_i \psi(x) = \psi(x + e_i)$

$$\begin{aligned}\hat{T}_i^* \hat{T}_i &= 1 & \hat{T}_i \hat{T}_i^* &= 1 - P_0 & \hat{T}_i \hat{T}_j &= e^{i\Theta_{ij}} \hat{T}_j \hat{T}_i \\ \hat{T}_i V \hat{T}_i^*(x) &= V(x + e_i)\end{aligned}$$

P_0 is a nontrivial projection (projection onto $\ell^2(\mathbb{Z}^{d-1} \otimes \{0\})$)

- 3 internal degrees of freedom (spin, pseudo spin): \hat{A} acts on $\ell^2((\mathbb{Z}^{d-1} \times \mathbb{N}) \otimes \mathbb{C}^N)$

$$\hat{A} = \hat{A}' \otimes M_N(\mathbb{C})$$

$A' = \mathcal{T}(A)$ is the Toeplitz extension of the crossed product algebra A .

As \mathcal{E} acts on the internal degrees of freedom, it also acts on \hat{A} and q intertwines this actions.

Exact sequence underlying the Bulk-Boundary Correspondence

[Richter, Schulz-Baldes +K. 2002]

Shifting the boundary to $+\infty$ corresponds to the surjective algebra homomorphism

$$q: \hat{A} \rightarrow A, \quad q(\hat{T}_i) = T_i$$

Its kernel is generated by P_0

$$J = \ker q = \hat{A}P_0\hat{A}$$

thus **consists of operators localized at the boundary**.

K is a homological functor: the exact sequence

$$J \xrightarrow{i} \hat{A} \xrightarrow{q} A$$

induces an isomorphism, the **K -theoretical bulk-boundary correspondence**

$$K_i(A, \mathcal{E}) / \text{im } q_* \xrightarrow{\cong} K_{i-1}(J, \mathcal{E}) \cap \ker i_*$$

Q: How can we understand physically the elements of $K_{i-1}(J)$?

Bulk versus boundary invariants, the rough picture

[Allridge, Max, Zirnbauer 2019; Bourne, Rennie, K. 2020]

There is a linear homomorphism $A \ni T_i \mapsto \hat{T}_i \in \hat{A}$ (not multiplicative!).

Consider a Hamiltonian $H \in GL^{s.a.}(A)$.

- \hat{H} is H with a choice of boundary conditions at the boundary.
 - The class of H in $DK(A, \mathcal{E})$ (van Daele) is the bulk invariant.
 - The class of \hat{H} in $KK(\mathbb{C}, J, \mathcal{E})$ (Kasparov) is the boundary invariant.
 - The Cayley transform induces an isomorphism between van Daele's and Kasparov's picture of K -theory
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- van Daele's picture of K -theory is topological bulk physics
 - Kasparov's picture of K -theory is topological boundary physics

Let B be a (σ -unital) C^* -algebra.

- 1 A (right) B Hilbert- C^* -module X_B is a "Hilbert space" with scalars replaced by B .
 - the scalar product is B -valued
 - $X_B = B$ is a B Hilbert- C^* -module of rank 1 (like \mathbb{C} is a one-dim. Hilbert space)
 - B -compact linear maps $T : X_B \rightarrow X_B$ are defined as closure of finite rank operators
 - the adjoint T^* of a linear map $T : X_B \rightarrow X_B$ is defined with B -valued scalar product

$$\langle x, T y \rangle = \langle T^* x, y \rangle$$

- 2 An endomorphism of X_B is a linear map T which admits an adjoint T^*
- 3 A Kasparov $\mathbb{C} - B$ -cycle (X_B, F) is a B Hilbert- C^* -module together with a self-adjoint endomorphism F such that $F^2 - 1$ is B -compact. They can be added up by direct sum.
- 4 A $KK(\mathbb{C}, B)$ -cycle (X_B, F) is degenerate if $F^2 = 1$.
- 5 The set of equivalence classes of Kasparov $\mathbb{C} - B$ -cycles modulo homotopy, unitary equivalence and addition of degenerate KK -cycles is $KK(\mathbb{C}, B)$. Direct sum induces abelian group structure. $KK(\mathbb{C}, B)$ is isomorphic to $K_{-1}(B)$.

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Extra ordinary symmetries \mathcal{E} can be treated in a similar way as for DK :

- 1 If \mathcal{E} has a chiral symmetry, hence B carries a balanced grading then X_B is required to have a compatible grading and F to be an odd operator.
- 2 If \mathcal{E} has a real symmetry (TRS or PHS / even or odd), hence B carries a real structure then X_B is required to carry a compatible real structure and F to be real or imaginary.

Theorem (Bourne, Rennie, K. 2020)

Let (B, γ) be a balanced graded real or complex C^* -algebra with choice of basepoint e and $H \in B$ and odd self-adjoint unitary. The map (Cayley transform)

$$x \mapsto \left(\overline{(x - e)B}, \frac{1}{2}e(x + e)(x - e)^{-1}|x - e| \right)$$

induces an isomorphism between $DK_e(B, \gamma)$ and $KK(\mathbb{C}, B)$.

Theorem (Alldridge, Max, Zirnbauer 2019; Bourne, Rennie, K. 2020)

Let H be a Hamiltonian $H \in GL^{s.a.}(A)$ with spectral gap Δ at 0. Let $P_\Delta(\hat{H})$ be the spectral projection of \hat{H} to Δ .

$$(J, P_\Delta(\hat{H})\hat{H})$$

is a KK -cycle whose class corresponds to the class of H under the bulk-boundary correspondence:

$$\delta([H]) = [J, P_\Delta(\hat{H})\hat{H}].$$

Recall: H has a spectral gap Δ at the Fermi energy (which we moved to 0).

$$\text{bulk K-group} \ni [H] \xrightarrow{\delta} [J, P_{\Delta}(\hat{H})\hat{H}] \in \text{boundary K-group}$$

and $\ker \delta = \text{im} q_*$.

- 1 If $[H] \notin \text{im} q_*$ then the spectrum of \hat{H} must cover the gap Δ at 0. Therefore **there must be states (resonances) which are localized at the boundary.**
- 2 **These resonances cannot propagate into the bulk.**
- 3 **These resonances cannot be destroyed by bending, denting the boundary or by adding disorder to it.** They are stable against perturbation of the boundary.

Proof:

- 1 If the spectrum of \hat{H} has a gap in Δ then $P_{\Delta}(\hat{H})\hat{H}$ is homotopic to an operator whose square is 1 thus defining a degenerate KK-cycle. This would mean that $[J, P_{\Delta}(\hat{H})\hat{H}] = 0$, a contradiction to $[H] \notin \ker \delta$.
- 2 There is no bulk spectrum in the gap.
- 3 A perturbation which is restricted to the boundary does not affect the bulk invariant. Alternative argument: A perturbation which is restricted to the boundary can change \hat{H} only up to a J -compact operator.

- We have established a correspondence between bulk invariants and boundary invariants for topological insulators.
- Both are derived naturally from the Hamiltonian of the system.
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Questions:

- How can we detect that the bulk invariant is not trivial, $[H] \notin \text{im}q_*$?
- Can one measure the topological invariants?

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- Can one measure the topological invariants?

Answer: Numerical topological invariants

- Any functional $K(A, \mathcal{E}) \rightarrow \mathbb{C}$ or \mathbb{Z}_2 is a numerical invariant for topol. phases.
- A numerical invariant serves to distinguish K -group elements and can detect the topological non-triviality of a material.
- A numerical invariant may be physically measurable (Hall conductivity).

There are two approaches to numerical invariants (partly related through index theory):

Via *KK-theory*: the dual of K -theory $KK(\mathbb{C}, A)$ is K -homology $KK(A, \mathbb{C})$ with \mathbb{R} in place of \mathbb{C} if we have real symmetries.

The duality pairing is the Kasparov product

$$KK_i(\mathbb{C}, A) \times KK_j(A, \mathbb{C}) \rightarrow KK_{i-j}(\mathbb{C}, \mathbb{C})$$

and $KK_{j-i}(\mathbb{C}, \mathbb{C})$ or $KK_{j-i}(\mathbb{R}, \mathbb{R})$ is \mathbb{Z} , \mathbb{Z}_2 or 0. This gives a numerical invariant (an index). [\[Grossmann, Schulz-Baldes 2016\]](#)

For our algebras (crossed product) exists a **fundamental class** $[\lambda_d] \in KK_d(A, \mathbb{C})$ (purely geometric data: Dirac operator in momentum space). The dual boundary map $\delta^* : KK_j(\mathbb{C}, J) \rightarrow KK_{j+1}(\mathbb{C}, A)$ maps $[\lambda_{d-1}]$ to $[\lambda_d]$.

This yields a **numerical bulk-boundary correspondance**:

$$[H] \times [\lambda_d] = [(J, P_\Delta(\hat{H})\hat{H})] \times [\lambda_{d-1}]$$

[\[Bourne,Carey,Rennie,+K 2017\]](#).

Via cyclic cohomology: cyclic cohomology is a generalisation of de Rham cohomology to algebras.

A K -group element may be combined with a cyclic cocycle to obtain a Chern number generalising the integral of a Chern class.

Leads to a numerical bulk-boundary correspondence which is, however, trivial for \mathbb{Z}_2 -invariants [Richter, Schulz-Baldes +K. 2002]

Close to linear response theory [TKNN, Bellissard-Connes] for IQHE

Direct approach fails for \mathbb{Z}_2 -invariants, these need **secondary pairings with cyclic cocycles** [K. 2019].