Topological invariants and corner states for Hamiltonians on a three dimensional lattice

Shin HAYASHI
AIST/TohokuU MathAM-OIL

Topology and Computer 2018
Nara Women’s University

October 13, 2018

Reference: Shin HAYASHI, Comm. Math. Phys., 2018
Table of contents

1. Topological invariants and the bulk-edge correspondence

2. (Secondary) topological invariants and the “bulk-edge and corner correspondence”

3. Numerical calculations and concave corners
Section 1: Topological invariants and the bulk-edge correspondence
Setting

\( V \) : a finite rank Hermitian vector space.
\( \mathbb{T} \) : unit circle in the complex plane.
\( \mu \) : a real number.

We consider a self-adjoint operator of the following form.

\[ H := H_{\text{Bulk}} : l^2(\mathbb{Z} \times \mathbb{Z}; V) \rightarrow l^2(\mathbb{Z} \times \mathbb{Z}; V), \]

\[ (H_{\text{Bulk}} \varphi)_{x,y} = \sum_{\text{finite}} A_{p,q} \varphi_{x-p,y-q}, \quad (A_{p,q} \in \text{End}_\mathbb{C}(V)) \]

\( (A_{p,q} = 0, \text{ except for finitely many } (p, q) \in \mathbb{Z} \times \mathbb{Z}). \)

We call \( H_{\text{Bulk}} \) the bulk Hamiltonian.

**Assumption** : \( \mu \notin \text{sp}(H_{\text{Bulk}}) \) (spectral gap condition\(^2\))

In this talk, we take \( \mu = 0 \), for simplicity.

---

\(^1\) An element \( \varphi \) in \( l^2(\mathbb{Z} \times \mathbb{Z}; V) \) is a sequence \( \varphi = \{\varphi_{x,y}\}_{(x,y)\in\mathbb{Z} \times \mathbb{Z}} \) of elements \( \varphi_{x,y} \in V \) which satisfies \( \sum_{x,y} ||\varphi_{x,y}||^2 < \infty \).

\(^2\) This condition says that the bulk is an insulator.
By the Fourier transform, we have a continuous map,

\[ \mathbb{T} \times \mathbb{T} \to \text{End}_\mathbb{C}(\mathcal{V}), \quad (s, t) \mapsto H_{\text{Bulk}}(s, t) \]

For each \((s, t) \in \mathbb{T} \times \mathbb{T}\), we gather together eigenvectors of \(H_{\text{Bulk}}(s, t)\) whose eigenvalues are less than \(\mu = 0\) and obtain a finite rank complex vector bundle,

\[ E_B \to \mathbb{T} \times \mathbb{T} \quad \text{(Bloch bundle)}. \]

The following is a topological invariant for our bulk system, which is called the TKNN number (Thouless, et al. 1982).

**Definition 1 (Bulk invariant)**

\[ \mathcal{I}_{\text{Bulk}}(H) := \langle c_1(E_B), [\mathbb{T} \times \mathbb{T}] \rangle \in \mathbb{Z} \]

We fix a counter clock-wise orientation on \(\mathbb{T}\) and take a product orientation on \(\mathbb{T} \times \mathbb{T}\).
By partial Fourier transform, we have a family,

\[ H_{\text{Bulk}} \stackrel{\text{Fourier}}{\sim} \{ H_{\text{Bulk}}(t) : l^2(\mathbb{Z}; V) \rightarrow l^2(\mathbb{Z}; V) \}_{t \in \mathbb{T}}. \]

Let \( P_{\geq 0} \) be the orthogonal projection of \( l^2(\mathbb{Z}; V) \) onto \( l^2(\mathbb{Z}_{\geq 0}; V) \). We consider the following family of self-adjoint operators:

\[ \{ H_{\text{Edge}}(t) := P_{\geq 0} H_{\text{Bulk}}(t) P_{\geq 0} : l^2(\mathbb{Z}_{\geq 0}; V) \rightarrow l^2(\mathbb{Z}_{\geq 0}; V) \}_{t \in \mathbb{T}}, \]

and call the edge Hamiltonian. (called Toeplitz operators.)

\[
\begin{array}{cccccc}
\vdots & -1 & 0 & 1 & 2 & \cdots \\
\mathbb{Z}_{\geq 0}, & l^2(\mathbb{Z}_{\geq 0}; V)
\end{array}
\]
The edge topological invariant is defined by using the spectral flow.

**Definition 2 (Edge Invariant)**

\[ \mathcal{I}_{\text{Edge}}(H) := \text{sf}\{H_{\text{Edge}}(t)\}_{t \in \mathbb{T}} \in \mathbb{Z} \]

(Roughly speaking) The spectral flow counts the net number of crossing points (edge states) of the spectrum of the edge Hamiltonian (red line) and 0 (green line). In the case of this figure, \( \text{sf}\{H_{\text{Edge}}(t)\}_{t \in \mathbb{T}} = +1 \).

**Theorem 3 (Bulk-edge correspondence (Hatsugai, 1993))**

\[ \mathcal{I}_{\text{Bulk}}(H) = \mathcal{I}_{\text{Edge}}(H). \]
Section 2: Topological invariants and the “bulk-edge and corner correspondence”
Let \( H_{\text{Bulk}} \) be a self-adjoint operator on the Hilbert space \( l^2(\mathbb{Z} \times \mathbb{Z} \times \mathbb{Z}; V) \) of the following form,

\[
(H_{\text{Bulk}} \varphi)(x,y,z) = \sum_{\text{finite}} A_{p,q,r} \varphi_{x-p,y-q,z-r}. \quad (A_{p,q,r} \in \text{End}_\mathbb{C}(V))
\]

We call \( H := H_{\text{Bulk}} \) the bulk Hamiltonian.

**Given**: \( \alpha < \beta \), real numbers.
(We can take \( \alpha = -\infty \) or \( \beta = +\infty \), but not both.)

**Consider**: By the partial Fourier transform in the \( z \)-direction (parallel to the corner), we obtain

\[
H_{\text{Bulk}} \xrightarrow{\text{Fourier}} \{ H_{\text{Bulk}}(t) : l^2(\mathbb{Z} \times \mathbb{Z}; V) \to l^2(\mathbb{Z} \times \mathbb{Z}; V) \}_{t \in \mathbb{T}}
\]
Edge Hamiltonians

Let $\mathcal{H}^\alpha$ and $\mathcal{H}^\beta$ be closed subspaces of $l^2(\mathbb{Z}^2)$ corresponding to following yellow and blue area, respectively. Let $P^\alpha$ and $P^\beta$ be orthogonal projections of $l^2(\mathbb{Z}^2)$ onto $\mathcal{H}^\alpha$ and $\mathcal{H}^\beta$, respectively.

Consider a compression of $H_{\text{Bulk}}(t)$ onto half planes $\mathcal{H}^\alpha$ and $\mathcal{H}^\beta$.

\[
H_{\text{Edge}}^\alpha(t) := P^\alpha H_{\text{Bulk}}(t) P^\alpha : \mathcal{H}^\alpha \to \mathcal{H}^\alpha,
\]

\[
H_{\text{Edge}}^\beta(t) := P^\beta H_{\text{Bulk}}(t) P^\beta : \mathcal{H}^\beta \to \mathcal{H}^\beta.
\]

and call edge Hamiltonians (half-plane Toeplitz operators).
Corner Hamiltonian

Let \( \hat{\mathcal{H}}^{\alpha,\beta} = \mathcal{H}^\alpha \cap \mathcal{H}^\beta \) (corresponding to the green area).
\( \hat{P}^{\alpha,\beta} = P^\alpha P^\beta = P^\beta P^\alpha \) is the orthogonal projection of \( l^2(\mathbb{Z}^2) \) onto \( \hat{\mathcal{H}}^{\alpha,\beta} \).

Consider : Compression of \( H_{\text{Bulk}}(t) \) onto \( \hat{\mathcal{H}}^{\alpha,\beta} \).

\[
\hat{H}_{\text{Corner}}^{\alpha,\beta}(t) := \hat{P}^{\alpha,\beta} H_{\text{Bulk}}(t) \hat{P}^{\alpha,\beta} : \hat{\mathcal{H}}^{\alpha,\beta} \to \hat{\mathcal{H}}^{\alpha,\beta}.
\]

and call the corner Hamiltonian. (quarter-plane Toeplitz operator).

Assumption : \( 0 \notin \text{sp}(H_{\text{Edge}}^\alpha(t)) \) and \( 0 \notin \text{sp}(H_{\text{Edge}}^\beta(t)) \) for any \( t \in \mathbb{T} \), i.e., \( H_{\text{Edge}}^\alpha(t) \) and \( H_{\text{Edge}}^\beta(t) \) has a common spectral gap at \( \mu = 0 \in \mathbb{R} \).
(Under this assumption, \( 0 \notin \text{sp}(H_{\text{Bulk}}(t)) \) holds.)
Key result

Let $\hat{T}^{\alpha,\beta}$ be the $C^*$-algebra generated by quarter-plane Toeplitz operators (called the quarter-plane Toeplitz $C^*$-algebra).

Let $\mathcal{T}^\alpha$ and $\mathcal{T}^\beta$ be half-plane Toeplitz algebras and $S^{\alpha,\beta} \subset \mathcal{T}^\alpha \oplus \mathcal{T}^\beta$ be some $C^*$-subalgebra.

**Theorem 4 (Douglas-Howe ’71, Park ’90)**

There is the following short exact sequence,

$$0 \to \mathcal{K}(\hat{\mathcal{H}}^{\alpha,\beta}) \to \hat{T}^{\alpha,\beta} \xrightarrow{\hat{\gamma}} S^{\alpha,\beta} \to 0.$$ 

Note that, for any $t \in \mathbb{T}$,

$$\hat{\gamma}(\hat{\mathcal{H}}_{\text{Corner}}^{\alpha,\beta}(t)) = (H^{\alpha}_{\text{Edge}}(t), H^{\beta}_{\text{Edge}}(t)).$$
Let \( h: \mathbb{R} \setminus \{0\} \rightarrow \mathbb{R} \) where \( h = 1 \) on \((-\infty, 0)\) and \( h = 0 \) on \((0, +\infty)\). We consider a projective element,

\[
p := h(H_{\text{Edge}}^\alpha(t), H_{\text{Edge}}^\beta(t)) \in M_{\text{rank } \nu} (\mathbb{S}^{\alpha, \beta} \otimes C(\mathbb{T})).
\]

**Definition 5 (H. Topological invariants)**

Under our assumption, gapped/gapless topological invariants \( I_{\text{Bulk–Edge}}(H) \) and \( I_{\text{Corner}}(H) \) for our system are defined:

\[
I_{\text{Bulk–Edge}}(H) := [p]_0 \in K_0(\mathbb{S}^{\alpha, \beta} \otimes C(\mathbb{T})), \quad I_{\text{Corner}}(H) := sf\{\hat{H}_{\text{Corner}}^{\alpha, \beta}(t)\}_{t \in \mathbb{T}}
\]

Our corner invariant counts the net number of crossing points of the spectrum of the corner Hamiltonian (red) and 0 (green). In the case of this figure, \( I_{\text{Corner}}(H) = +1 \), and there is a topologically protected corner state.
Main theorem

Associated to the short exact sequence,

\[ 0 \to K(\hat{\mathcal{H}}^{\alpha,\beta}) \to \hat{\mathcal{F}}^{\alpha,\beta} \to S^{\alpha,\beta} \to 0, \]

we have the following maps.

\[ K_0(S^{\alpha,\beta} \otimes C(\mathbb{T})) \xrightarrow{\delta_0} K_1(K(\hat{\mathcal{H}}^{\alpha,\beta}) \otimes C(\mathbb{T})) \xrightarrow{sf} \mathbb{Z} \]

\[ \mathcal{I}^{3D,A}_{\text{Bulk-Edge}}(H) \xrightarrow{\psi} \mathcal{I}^{3D,A}_{\text{Corner}}(H) \]

**Theorem 6 (H. “Bulk-edge and corner correspondence”)**

\[ \text{sf} \circ \hat{\delta}_0(\mathcal{I}_{\text{Bulk-Edge}}(H)) = \hat{\mathcal{I}}_{\text{Corner}}(H). \]

Thus, if (the bulk and) two edges are gapped, there is a topological invariant which is related to gapless corner states.

**Remark:** Actually, for our edges gapped systems, bulk topological invariants are zero. In this sense, topological invariants considered in this section are secondary invariant.
Example

Let $H_1$ be the following self-adjoint operator on $\mathbb{C}^2 \otimes l^2(\mathbb{Z} \times \mathbb{Z})$.

$$H_1 = \frac{1}{2\sqrt{-1}} \sum_{j=x,y} \sigma_j \otimes (S_j - S_j^*) + \sigma_z \otimes (-1 + \frac{1}{2} \sum_{j=x,y} (S_j + S_j^*)).$$

Let $H_2$ and $\Pi$ be following self-adjoint operators on the Hilbert space $\mathbb{C}^2 \otimes l^2(\mathbb{Z})$,

$$H_2 = \frac{1}{2}(\sigma_x + \sqrt{-1}\sigma_y) \otimes S + \frac{1}{2}(\sigma_x - \sqrt{-1}\sigma_y) \otimes S^*, \ \Pi = \sigma_z \otimes 1.$$

We consider the following self-adjoint operator $H_{\text{Bulk}}$ on $l^2(\mathbb{Z}^3, \mathbb{C}^4)$, (and take $\alpha = 0, \beta = \infty, \mu = 0$).

$$\tilde{H} = \tilde{H}_{\text{Bulk}} = H_1 \otimes \Pi + 1 \otimes H_2.$$

Then, this Hamiltonian satisfies our spectral gap condition and we can calculate that,

$$\mathcal{I}_{\text{Corner}}(\tilde{H}) = 1.$$

where,

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \ \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
Section 3 : Numerical calculations and concave corners

Remark : In this section, we consider the following “concave” corner.

Quarter-plane (convex corner)    Concave corner

We have an example ⇒ Numerical calculations!.
Consider $\tilde{H} \overset{\text{Fourier}}{\mapsto} \{\tilde{H}(k_z)\}_{k_z \in \mathbb{T}}$.

Restrict $\tilde{H}(k_z)$ onto the green region under the Dirichlet boundary condition and compute its spectrum and eigen-function.

Numerical calculation by T. Nakanishi.
Numerical Calculation

![Graph showing bulk-edge correspondence and corner correspondence.]

- **Bulk-edge correspondence**
  - $m_1 = -1.1$
  - $m_2 = 0.1$

- **Bulk-edge and corner correspondence**

**Numerical calculations**
Numerical Calculation

\[ m_1 = -1.1 \]
\[ m_2 = 0.1 \]
Numerical Calculation

$m_1 = -1.1$
$m_2 = 0.1$
Originally, our theory is just for convex corners.

By the result of numerical calculations, there seems to be (topologically protected) corner states also on a concave corner.

⇒ There should be some mathematical theory behind it!

Mathematical Problem

Consider a “concave corner” Toeplitz algebra and show a short exact sequence as in Douglas–Howe and Park.
“Concave corner” Toeplitz algebra

Let $\mathcal{H}^{\alpha,\beta}$ be the closed subspace of $l^2(\mathbb{Z}^2)$ corresponding to the following dashed area. Let $\mathcal{P}^{\alpha,\beta}$ be the orthogonal projection of $l^2(\mathbb{Z}^2)$ onto $\mathcal{H}^{\alpha,\beta}$. We define the concave corner Toeplitz algebra $\mathcal{T}^{\alpha,\beta}$ to be the $C^*$-algebra generated by $\{\mathcal{P}^{\alpha,\beta}M_{m,n}\mathcal{P}^{\alpha,\beta} | (m, n) \in \mathbb{Z}^2\}$.

**Theorem 7 (H.)**

There is the following short exact sequence of $C^*$-algebras:

$$0 \to K(\mathcal{H}^{\alpha,\beta}) \to \mathcal{T}^{\alpha,\beta} \stackrel{\tilde{\gamma}}{\to} S^{\alpha,\beta} \to 0.$$  

$\tilde{\gamma}$ maps $\mathcal{P}^{\alpha,\beta}M_{m,n}\mathcal{P}^{\alpha,\beta}$ to the pair $(P^{\alpha}M_{m,n}P^{\alpha}, P^{\beta}M_{m,n}P^{\beta})$.

By using this, similar results as in Sect. 2 holds for concave corners.

In order to distinguish these two cases, we put hat "∧" for objects associated with convex corners and put check "∨" for that with concave corners (e.g. $\mathcal{H}^{\alpha,\beta}$ and $\tilde{\mathcal{H}}^{\alpha,\beta}$).
We consider a 3D system with codimension two corner. We assume that the bulk and two edges are gapped.

We defined two topological invariants; $\mathcal{I}_{\text{Bulk-Edge}}(H)$ and $\hat{\mathcal{I}}_{\text{Corner}}(H)$ and showed their relation. $\hat{\mathcal{I}}_{\text{Corner}}(H)$ is related to corner states.

We constructed a specific example and carried out a numerical calculation.

By its results, we predicted a short exact sequence associated with concave corners and proved it.

Recently, such (bulk and) edge-gapped systems and corner states take interest in condensed matter physics under the name of “higher-order topological insulators” (Benalcazar–Bernevig–Hughes. Science 2017).