Bulk-edge duality for topological insulators

Gian Michele Graf ETH Zurich

Journes de Physique Mathmathique Lyon Topological Insulators September 11-13, 2013

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> joint work with Marcello Porta thanks to Yosi Avron

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Introduction

Rueda de casino

Hamiltonians

Indices

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Insulator in the Bulk: Excitation gap
 For independent electrons: band gap at Fermi energy

Insulator in the Bulk: Excitation gap
 For independent electrons: band gap at Fermi energy

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Time-reversal invariant fermionic system

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 For independent electrons: band gap at Fermi energy
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Topology: In the space of Hamiltonians, a topological insulator can not be deformed in an ordinary one, while keeping the gap open and time-reversal invariance.

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 For independent electrons: band gap at Fermi energy
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► Topology: In the space of Hamiltonians, a topological insulator can not be deformed in an ordinary one, while keeping the gap open and time-reversal invariance. Analogy: torus ≠ sphere (differ by genus).

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Contributors to the field: Kane, Mele, Zhang, Moore; Fröhlich



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Θ time-reversal

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• On the two edges (net): parallel charge currents, anti-parallel spin currents



• On the two edges (net): parallel charge currents, anti-parallel spin currents

 \bullet Stable against backscattering, $|\psi\rangle \to \Theta |\psi\rangle,$ induced by disorder

$$\langle \Theta \psi | V | \psi
angle = 0$$

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if V is time-reversal invariant.



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if *V* is time-reversal invariant. Indeed:

$$\langle \Theta \psi, V \psi \rangle =$$



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$$\langle \Theta \psi, V \psi \rangle = \langle \Theta V \psi, \Theta^2 \psi \rangle =$$



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$$\langle \Theta \psi, \mathbf{V} \psi \rangle = \langle \Theta \mathbf{V} \psi, \Theta^2 \psi \rangle = - \langle \mathbf{V} \Theta \psi, \psi \rangle = - \langle \Theta \psi, \mathbf{V} \psi \rangle$$



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- if V is time-reversal invariant.
- Backscattering to other edge suppressed by separation



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- if V is time-reversal invariant.
- Backscattering to other edge suppressed by separation
- Autobahn principle (Zhang); U.S. patent 20120138887

Deformation as interpolation in physical space:



 Gap must close somewhere in between. Hence: Interface states at Fermi energy.

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Deformation as interpolation in physical space:



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Ordinary insulator ~ void: Edge states

Deformation as interpolation in physical space:



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- Ordinary insulator ~ void: Edge states
- Bulk-edge correspondence: Termination of bulk of a topological insulator implies edge states.

Deformation as interpolation in physical space:



- Gap must close somewhere in between. Hence: Interface states at Fermi energy.
- Ordinary insulator ~ void: Edge states
- Bulk-edge correspondence: Termination of bulk of a topological insulator implies edge states. (But not conversely!)



In a nutshell: Termination of bulk of a topological insulator implies edge states

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In a nutshell: Termination of bulk of a topological insulator implies edge states

 State the (intrinsic) topological property distinguishing different classes of insulators.

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In a nutshell: Termination of bulk of a topological insulator implies edge states

 State the (intrinsic) topological property distinguishing different classes of insulators.

More precisely:

 Express that property as an Index relating to the Bulk, resp. to the Edge.

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In a nutshell: Termination of bulk of a topological insulator implies edge states

 State the (intrinsic) topological property distinguishing different classes of insulators.

- Express that property as an Index relating to the Bulk, resp. to the Edge.
- Bulk-edge duality: Can it be shown that the two indices agree?

Bulk-edge correspondence. Done?



In a nutshell: Termination of bulk of a topological insulator implies edge states

 State the (intrinsic) topological property distinguishing different classes of insulators.

- Express that property as an Index relating to the Bulk, resp. to the Edge. Yes, e.g. Kane and Mele.
- Bulk-edge duality: Can it be shown that the two indices agree? Schulz-Baldes et al.; Essin & Gurarie

Bulk-edge correspondence. Today



In a nutshell: Termination of bulk of a topological insulator implies edge states

 State the (intrinsic) topological property distinguishing different classes of insulators.

- Express that property as an Index relating to the Bulk, resp. to the Edge. Done differently.
- Bulk-edge duality: Can it be shown that the two indices agree? Done differently.

Introduction

Rueda de casino

Hamiltonians

Indices

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Rueda de casino. Time 0'15"



Rueda de casino. Time 0'44"



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Rueda de casino. Time 0'44.25"



(日)

Rueda de casino. Time 0'44.50"



(日)

Rueda de casino. Time 0'44.75"



Rueda de casino. Time 0'45"


Rueda de casino. Time 0'45.25"



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Rueda de casino. Time 0'45.50"



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Rueda de casino. Time 3'23"



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Rules of the dance

Dancers

- start in pairs, anywhere
- end in pairs, anywhere (possibly elseways & elsewhere)

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- are free in between
- must never step on center of the floor

Rules of the dance

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Rules of the dance

Dancers

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There are dances which can not be deformed into one another.

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Which is the index that makes the difference?

A snapshot of the dance





A snapshot of the dance



Dance D as a whole



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A snapshot of the dance



Dance D as a whole



A snapshot of the dance



Dance D as a whole



A snapshot of the dance



Dance D as a whole



 $\mathcal{I}(D)$ = parity of number of crossings of fiducial line

Introduction

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Hamiltonian on the lattice $\mathbb{Z} \times \mathbb{Z}$ (plane)



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Hamiltonian on the lattice $\mathbb{Z} \times \mathbb{Z}$ (plane)



Hamiltonian on the lattice $\mathbb{Z} \times \mathbb{Z}$ (plane)

translation invariant in the vertical direction

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period may be assumed to be 1:

Hamiltonian on the lattice $\mathbb{Z} \times \mathbb{Z}$ (plane)

- translation invariant in the vertical direction
- period may be assumed to be 1: sites within a period as labels of internal d.o.f.

Hamiltonian on the lattice $\mathbb{Z} \times \mathbb{Z}$ (plane)

- translation invariant in the vertical direction
- period may be assumed to be 1: sites within a period as labels of internal d.o.f., along with others (spin, ...)

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Hamiltonian on the lattice $\mathbb{Z} \times \mathbb{Z}$ (plane)

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- ▶ Bloch reduction by quasi-momentum $k \in S^1 := \mathbb{R}/2\pi\mathbb{Z}$

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End up with wave-functions $\psi = (\psi_n)_{n \in \mathbb{Z}} \in \ell^2(\mathbb{Z}; \mathbb{C}^N)$ and Bulk Hamiltonian

$$\left(\boldsymbol{H}(\boldsymbol{k})\boldsymbol{\psi}\right)_{n} = \boldsymbol{A}(\boldsymbol{k})\boldsymbol{\psi}_{n-1} + \boldsymbol{A}(\boldsymbol{k})^{*}\boldsymbol{\psi}_{n+1} + \boldsymbol{V}_{n}(\boldsymbol{k})\boldsymbol{\psi}_{n}$$

with

 $V_n(k) = V_n(k)^* \in M_N(\mathbb{C})$ (potential) $A(k) \in GL(N)$ (hopping)

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with

 $V_n(k) = V_n(k)^* \in M_N(\mathbb{C})$ (potential) $A(k) \in GL(N)$ (hopping): Schrödinger eq. is the 2nd order difference equation

Hamiltonian on the lattice $\mathbb{N} \times \mathbb{Z}$ (half-plane) with $\mathbb{N} = \{1, 2, \ldots\}$



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Hamiltonian on the lattice $\mathbb{N} \times \mathbb{Z}$ (half-plane) with $\mathbb{N} = \{1, 2, \ldots\}$

► translation invariant as before (hence Bloch reduction) Wave-functions $\psi \in \ell^2(\mathbb{N}; \mathbb{C}^N)$ and Edge Hamiltonian

$$\left(\boldsymbol{H}^{\sharp}(k)\boldsymbol{\psi}\right)_{n} = \boldsymbol{A}(k)\boldsymbol{\psi}_{n-1} + \boldsymbol{A}(k)^{*}\boldsymbol{\psi}_{n+1} + \boldsymbol{V}_{n}^{\sharp}(k)\boldsymbol{\psi}_{n}$$

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which

 agrees with Bulk Hamiltonian outside of collar near edge (width n₀)

$$V_n^{\sharp}(k) = V_n(k) , \qquad (n > n_0)$$

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$$V_n^{\sharp}(k) = V_n(k) , \qquad (n > n_0)$$

▶ has Dirichlet boundary conditions: for n = 1 set $\psi_0 = 0$ Note: $\sigma_{\text{ess}}(H^{\sharp}(k)) \subset \sigma_{\text{ess}}(H(k))$, but typically $\sigma_{\text{disc}}(H^{\sharp}(k)) \not\subset \sigma_{\text{disc}}(H(k))$

Graphene as an example

Hamiltonian is nearest neighbor hopping on honeycomb lattice



(a) zigzag, resp. (b) armchair boundaries

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Dimers (N = 2).

Graphene as an example

Hamiltonian is nearest neighbor hopping on honeycomb lattice



(a) zigzag, resp. (b) armchair boundaries

Dimers (N = 2). For (b):

$$\psi_n = \begin{pmatrix} \psi_n^A \\ \psi_n^B \end{pmatrix} \in \mathbb{C}^{N=2} , \quad A(k) = -t \begin{pmatrix} 0 & 1 \\ e^{ik} & 0 \end{pmatrix} , \quad V_n(k) = -t \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

For (a): too, but $A(k) \notin GL(N)$ Also: Extensions with spin, spin orbit coupling leading to topological insulators (Kane & Mele)

General assumptions

• Gap assumption: Fermi energy μ lies in a gap for all $k \in S^1$:

 $\mu\notin\sigma(H(k))$

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General assumptions

• Gap assumption: Fermi energy μ lies in a gap for all $k \in S^1$:

$$\mu \notin \sigma(H(k))$$

- Fermionic time-reversal symmetry: $\Theta : \mathbb{C}^N \to \mathbb{C}^N$
 - Θ is anti-unitary and $\Theta^2 = -1$;
 - For all $k \in S^1$,

$$H(-k) = \Theta H(k) \Theta^{-1}$$

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where Θ also denotes the map induced on $\ell^2(\mathbb{Z}; \mathbb{C}^N)$. Likewise for $H^{\sharp}(k)$ Elementary consequences of $H(-k) = \Theta H(k) \Theta^{-1}$ • $\sigma(H(k)) = \sigma(H(-k))$. Same for $H^{\sharp}(k)$.

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• $\sigma(H(k)) = \sigma(H(-k))$. Same for $H^{\sharp}(k)$.

• Time-reversal invariant points, k = -k,

- $\sigma(H(k)) = \sigma(H(-k))$. Same for $H^{\sharp}(k)$.
- Time-reversal invariant points, k = -k, at $k = 0, \pi$.

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- $\sigma(H(k)) = \sigma(H(-k))$. Same for $H^{\sharp}(k)$.
- ► Time-reversal invariant points, k = -k, at $k = 0, \pi$. There

$$H = \Theta H \Theta^{-1}$$
 $(H = H(k) \text{ or } H^{\sharp}(k))$

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Hence any eigenvalue is even degenerate (Kramers).

- $\sigma(H(k)) = \sigma(H(-k))$. Same for $H^{\sharp}(k)$.
- ► Time-reversal invariant points, k = -k, at $k = 0, \pi$. There

$$H = \Theta H \Theta^{-1}$$
 $(H = H(k) \text{ or } H^{\sharp}(k))$

Hence any eigenvalue is even degenerate (Kramers). Indeed

$$H\psi = E\psi \implies H(\Theta\psi) = E(\Theta\psi)$$

and $\Theta \psi = \lambda \psi$, ($\lambda \in \mathbb{C}$) is impossible:

$$-\psi = \Theta^2 \psi = \bar{\lambda} \Theta \psi = \bar{\lambda} \lambda \psi \qquad (\Rightarrow \Leftarrow)$$

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Elementary consequences of $H(-k) = \Theta H(k) \Theta^{-1}$

- $\sigma(H(k)) = \sigma(H(-k))$. Same for $H^{\sharp}(k)$.
- Time-reversal invariant points, k = -k, at $k = 0, \pi$. There

$$H = \Theta H \Theta^{-1}$$
 $(H = H(k) \text{ or } H^{\sharp}(k))$

Hence any eigenvalue is even degenerate (Kramers).



Bands, Fermi line (one half fat), edge states

Introduction

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The edge index

The spectrum of $H^{\sharp}(k)$

symmetric on $-\pi \leq k \leq 0$



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Bands, Fermi line, edge states

Definition: Edge Index

 $\mathcal{I}^{\sharp} =$ parity of number of eigenvalue crossings

The edge index

The spectrum of $H^{\sharp}(k)$

symmetric on $-\pi \leq k \leq 0$



Bands, Fermi line, edge states

Definition: Edge Index

 \mathcal{I}^{\sharp} = parity of number of eigenvalue crossings

At fixed *k*, map gap to $S^1 \setminus \{1\}$ and bands to $1 \in S^1$: Edge Index is index of a rueda.

Towards the bulk index

Let $z \in \mathbb{C}$. The Schrödinger equation

$$(H(k)-z)\psi=0$$

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(as a 2nd order difference equation) has 2*N* solutions $\psi = (\psi_n)_{n \in \mathbb{Z}}, \ \psi_n \in \mathbb{C}^N$.

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Let $z \notin \sigma(H(k))$. Then

$$E_{z,k} = \{ \psi \mid \psi \text{ solution, } \psi_n \to 0, \ (n \to +\infty) \}$$

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 $Loop \gamma$ and torus $\mathbb{I} = \gamma \times S$

Vector bundle *E* with base $\mathbb{T} \ni (z, k)$, fibers $E_{z,k}$, and involution Θ .

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Loop γ and torus $\mathbb{T} = \gamma \times S^1$

Vector bundle *E* with base $\mathbb{T} \ni (z, k)$, fibers $E_{z,k}$, and involution Θ .

Theorem In general, vector bundles (E, \mathbb{T}, Θ) can be classified by an index $\mathcal{I}(E) = \pm 1$ (besides of $N = \dim E$)

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Time reversal invariant bundles (E, \mathbb{T}, Θ)



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• Time-reversal invariant points, $\varphi = -\varphi$ at $\varphi = (0,0), (\pi,0), (0,\pi), (\pi,\pi)$

•
$$\Theta: E_{\varphi} \to E_{-\varphi}$$
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- $\Theta: E_{\varphi} \to E_{-\varphi}$, Θ antilinear with $\Theta^2 = -1$
- Frame bundle *F*(*E*) has fibers *F*(*E*)_φ ∋ *v* = (*v*₁,... *v*_N) consisting of bases *v* of *E*_φ.

Classification of time reversal invariant bundles Consider the cut torus:





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Lemma On the cut torus the frame bundle admits a section $\varphi \mapsto v(\varphi) \in F(E)_{\varphi}$ which is time-reversal invariant:

$$\mathbf{v}(-\varphi) = (\Theta \mathbf{v}(\varphi))\varepsilon$$

with ε the block diagonal matrix with blocks $\left(\begin{smallmatrix} 0 & -1 \\ 1 & 0 \end{smallmatrix}\right)$

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Idea: At a time reversal invariant point, that means (N = 2)

$$v_2 = \Theta v_1$$
 $v_1 = -\Theta v_2$

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Transition matrix $T(\varphi_2) \in GL(N)$

$$\mathbf{v}_+(\varphi_2) = \mathbf{v}_-(\varphi_2)T(\varphi_2), \qquad (\varphi_2 \in S^1)$$

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with $\Theta_0 = \varepsilon C$, (*C* complex conjugation on \mathbb{C}^N)

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- At time-reversal invariant points, $\varphi_2 = 0, \pi$,

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The statement of the theorem is now complete.

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Side result: $\mathcal{I}(E)$ agrees (in value) with the Pfaffian index of Kane and Mele.

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... aside ends here.

Main result

Theorem Bulk and edge indices agree:

 $\mathcal{I}=\mathcal{I}^{\sharp}$

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Theorem Bulk and edge indices agree:

 $\mathcal{I} = \mathcal{I}^{\sharp}$

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 $\mathcal{I} = +1$: ordinary insulator $\mathcal{I} = -1$: topological insulator

For this slide only: N = 1.

For this slide only: N = 1. Schrödinger (2nd order difference) equation on the half-line

$$(H^{\sharp} - z)\psi^{\sharp} = 0$$
 (no b.c. at $n = 0$)

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Solution is unique up to multiples

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- Solution is unique up to multiples
- $\psi_0^{\sharp} = 1$ picks a unique solution, except if n = 0 is a node
Proof of Theorem (sketch)



Fermi line (one half **fat**) edge states torus

- ▶ ψ , ψ^{\sharp} solutions (bulk, edge) at *z*, *k* decaying at *n* → +∞
- Bijective map $\psi \mapsto \psi^{\sharp}$, so that $\psi_n = \psi_n^{\sharp}$ ($n > n_0$)

$$\exists \psi^{\sharp} \neq \mathbf{0} \mid \psi_{n=0}^{\sharp} = \mathbf{0} \Leftrightarrow z \in \sigma(H^{\sharp}(k))$$

- ► There is a section of the frame bundle F(E), global on T, except at edge eigenvalue crossings
- Cut the torus along the Fermi line; let T(k) be the transition matrix
- There $T(k) = \mathbb{I}_N$, except near eigenvalue crossings
- As k traverses one of them, T(k) has eigenvalues 1 (multiplicity N-1) and $\lambda(k)$ making one turn of S^1

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Proof of Theorem: Dual ruedas



Edge rueda: edge eigenvalues



Bulk rueda: eigenvalues of T(k)

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Proof of Theorem: Dual ruedas



Edge rueda: edge eigenvalues



Bulk rueda: eigenvalues of T(k)

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Ruedas share intersection points.

Proof of Theorem: Dual ruedas



Edge rueda: edge eigenvalues



Bulk rueda: eigenvalues of T(k)

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Ruedas share intersection points. Hence indices are equal \Box

Further results:

In case the Bulk Hamiltonian is doubly periodic:

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In case the Bulk Hamiltonian is doubly periodic: Brillouin zone serves as torus and (*j*-th pair of) Bloch solutions as bundles *E_j*.

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Further results:

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with product over filled pairs

- A direct link between indices of Bloch bundles and the edge index via Levinson's theorem.
- 3d topological insulators (weak and strong indices: 3+1)

Open questions:

No periodicity (disordered case)?

Summary

Bulk = Edge

$$\mathcal{I} = \mathcal{I}^{\sharp}$$



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