An Introduction to the Theory of Topological Insulators

At the Intersection of Analysis and Topology

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Quick Dictionary between Physics and Mathematics

Hermitian = Selfadjoint

Non-Hermitian = Non-Selfadjoint

$$H^\dagger = H^*$$

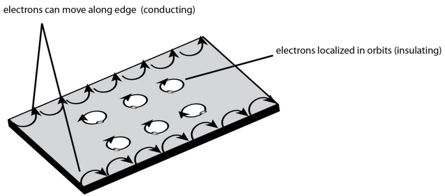
$$H^* = \overline{H}$$

1 Overview of Topological Phenomena in Physics

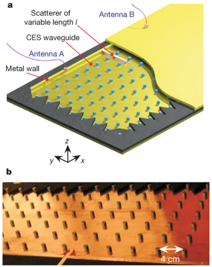
2 Homotopy Definition of Topological Phases

3 Discrete Symmetries

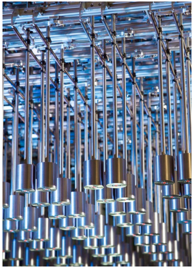
What Are Topological Phenomena?



Quantum Hall Effect



Electromagnetic waves



Coupled Oscillators

What makes a physical effect topological?

Find a *mathematical object* (e. g. projection or vector bundle) *whose topology* manifests itself on the level of physics.

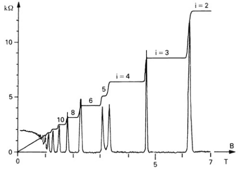
Bulk-Boundary Correspondence

$$O_{\text{bdy}}(t) \approx T_{\text{bdy}} = f(T_{\text{bulk}})$$

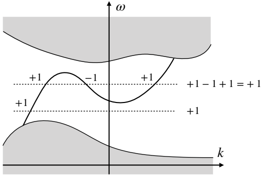
Step 1: Bulk Classification

- **Classify systems with certain symmetries**
- Identify all topological invariants

Bulk-Boundary Correspondences



Transverse conductivity (von Klitzing et. al)



Spectral flow

$$\sigma^{\perp}_{\text{edge}} \approx \frac{e^2}{h}\,\mathrm{Sf} = \frac{e^2}{h}\left(\mathrm{Ch}_{\mathrm{L}} - \mathrm{Ch}_{\mathrm{R}}\right)$$

Quantum Hall Effect

- Transverse edge conductivity
- Spectral flow
- Chern number

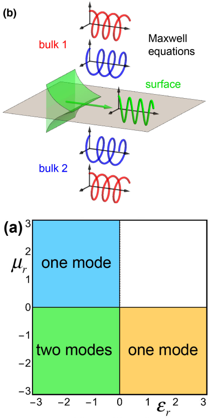
Bulk-Boundary Correspondences

$$O_{\text{bdy}}(t) \approx T_{\text{bdy}} = f(T_{\text{bulk}})$$

Generic case

- Physical observable on the boundary
- Topological **boundary** invariant
- Topological **bulk** invariant

Bulk-Boundary Correspondences



Bliokh, Leykam, L. & Nori, Nature Communications **10**, issue 1, article 580, 2019

Conjecture (Bulk-Boundary Conjecture (Bliokh, Leykam, L. & Nori 2019))

$$N^{\Sigma}_{\text{surf}} = N^{\text{TE}}_{\text{surf}} + N^{\text{TM}}_{\text{surf}}$$
$$N^{\text{TE}}_{\text{surf}} = \tfrac{1}{2}\big(1 - \operatorname{sgn}\varepsilon_{\text{r}}\big) = \tfrac{1}{2}\big(1 - \operatorname{sgn}(\varepsilon_1)\operatorname{sgn}(\varepsilon_2)\big)$$
$$N^{\text{TM}}_{\text{surf}} = \tfrac{1}{2}\big(1 - \operatorname{sgn}\mu_{\text{r}}\big) = \tfrac{1}{2}\big(1 - \operatorname{sgn}(\mu_1)\operatorname{sgn}(\mu_2)\big)$$

Electromagnetic interface modes

- Number of boundary modes
- Topological **boundary** invariant
- Topological **bulk** invariant

Bare Basics of Topological **Bulk** Classifications

- $\left.\begin{array}{c}\text{Symmetries of } H \\ \text{Spectral gap}\end{array}\right\} \longleftrightarrow$ Topological class of H
- Topological class $= \bigcup\{$Topological phases$\}$
- Topological phase = Operators connected by symmetry- and gap-preserving continuous deformations
- Homotopy definition of topological phase

  $\rightsquigarrow$ Usually first-principles starting point
- Phases labeled by a finite set of topological invariants

  $\rightsquigarrow$ Typically take values in $\mathbb{Z}$ or $\mathbb{Z}_2$
- Number and nature of topological invariants depends on topological class and dimension

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Electromagnetic Interface Modes at Metal-Dielectric Interfaces

Maxwell's equations for homogeneous media

$$\begin{pmatrix} \varepsilon & 0 \\ 0 & \mu \end{pmatrix} \frac{\partial}{\partial t} \begin{pmatrix} \mathbf{E}(t) \\ \mathbf{H}(t) \end{pmatrix} = \begin{pmatrix} +\nabla \times \mathbf{E}(t) \\ -\nabla \times \mathbf{H}(t) \end{pmatrix}$$

$$\begin{pmatrix} \nabla \cdot \varepsilon \mathbf{E}(t) \\ \nabla \cdot \mu \mathbf{H}(t) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

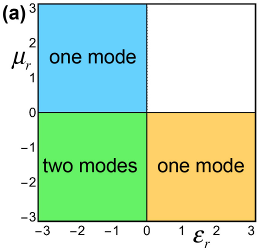
Physical parameters

- Electric permittivity ε
- Magnetic permeability μ

- Parameter space $(\varepsilon, \mu) \in X := (\mathbb{R} \setminus \{0\})^2$
- Topological bulk phases
  - ⇝ Set of connected components $\pi_0(X)$
  - ⇝ Homotopy definition
- $[(\varepsilon, \mu)] \in \pi_0(X) = \{++, +-, -+, --\}$
  - ⇝ **Not** a group

Bliokh, Leykam, L. & Nori, Nature Comm. **10**, 2019

Electromagnetic Interface Modes at Metal-Dielectric Interfaces



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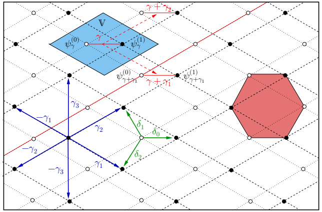
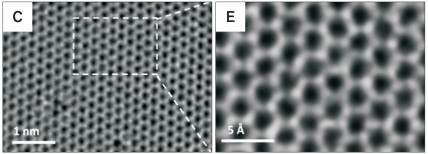
$$[(\varepsilon, \mu)] := \Big\{ (\varepsilon', \mu') \in X \;\Big|\; \exists \text{ continuous path } \gamma : [0,1] \longrightarrow X,\ \gamma(0) = (\varepsilon, \mu),\ \gamma(1) = (\varepsilon', \mu') \Big\}$$

Bliokh, Leykam, L. & Nori, Nature Comm. **10**, 2019

Quantization of Piezocurrents in Graphene-Like Materials





Single layer of boron nitride: honeycomb

$$\mathrm{i}\varepsilon\partial_t\Psi(t) = H(t)\Psi(t)$$
$$H(t+T) = H(t) = H(t)^* \in \mathcal{B}(\ell^2(\mathbb{Z}^2, \mathbb{C}^2))$$

- ε adiabatic parameter
- Adiabatic approximation for time evolution
  $\rightsquigarrow$ Simpler approximate time evolution

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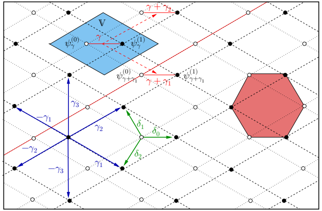
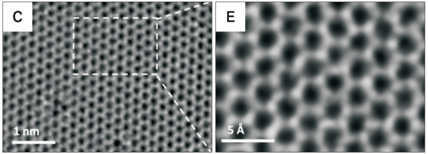




Single layer of boron nitride: honeycomb

Charge accumulated over one cycle in direction j approximately given by

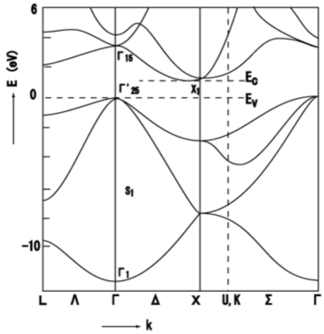
$$\Delta \mathcal{P}_j \approx \mathrm{i} \int_0^T \mathrm{d}t \, \mathcal{T}\Big(P(t) \, \big[\partial_t P(t) \, , \, \partial_{k_j} P(t) \big] \Big) \in \mathbb{Z}$$

$\rightsquigarrow$ Formula for Chern number of a vector bundle over $\mathbb{T}^3$

$\Longrightarrow \Delta \mathcal{P}_j \in \mathbb{Z}$, robust under continuous, gap-preserving transformations

Panati, Sparber & Teufel, Arch. Rational Mech. Anal. **191**, 2009, L., diploma thesis, 2005, De Nittis & L., J. Phys. A **46**, 2013

Periodic Operators, Their Band Spectrum and the Bloch Bundle



Band spectrum of silicon along special directions

Exploit periodicity

- Discrete Fourier transform decomposes

$$H \cong \mathcal{F}\, H\, \mathcal{F}^{-1} = \int_{\mathbb{T}^d}^{\oplus} \mathrm{d}k\, H(k)$$

- $k \mapsto H(k)$ analytic
- $\sigma\big(H(k)\big) = \sigma_{\mathrm{disc}}\big(H(k)\big)$

$$H(k)\varphi_n(k) = E_n(k)\,\varphi_n(k)$$

Kuchment, *Floquet Theory for Partial Differential Equations*, 1993

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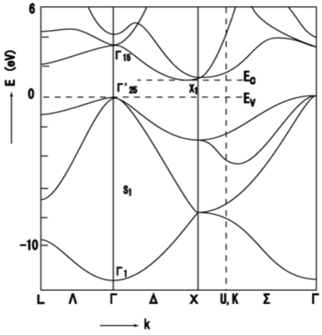

Band spectrum of silicon along special directions

Analyticity of $k \mapsto H(k)$ implies

$$H(k)\varphi_n(k) = E_n(k)\,\varphi_n(k)$$

- Band functions $k \mapsto E_n(k)$ continuous, **locally analytic** away from band crossings
- Bloch functions (eigenfunctions) $k \mapsto \varphi_n(k)$ **locally analytic** away from band crossings (suitable choice of phase)
- For family of bands **separated by a gap**: associated projection

$$P(k) = \sum_{n \in \mathcal{I}} |\varphi_n(k)\rangle\langle\varphi_n(k)|$$

is **analytic on all of $\mathbb{T}^d$**

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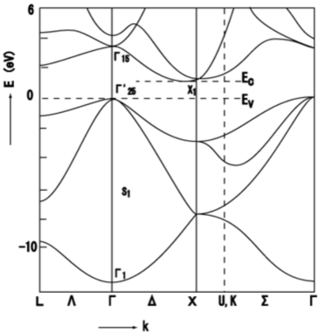


Band spectrum of silicon along special directions

The Bloch bundle

$$\mathcal{E}(P) : \bigsqcup_{k \in \mathbb{T}^d} \mathrm{ran}\, P(k) \longrightarrow \mathbb{T}^d$$

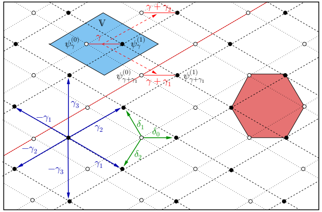
- Analytic vector bundle
- **Oka principle** applies: analytic triviality = topological triviality
- Topology of vector bundle (up to equivalence) characterized by Chern numbers ($d \leq 4$)
- $d = 2 + 1$: 2 of 3 Chern numbers are

$$\Delta \mathcal{P}_j := \mathrm{i} \int_0^T \mathrm{d}t \, \mathcal{T} \Big(P(t) \left[\partial_t P(t) \, , \, \partial_{k_j} P(t) \right] \Big) \in \mathbb{Z}$$

Hatcher, *Vector Bundles and K-Theory*, 2009

A Simple Model for Graphene-Like Materials and Its Parameter Space

$$H(q_1, q_2, q_3) = \begin{pmatrix} 0 & \mathbb{1} + q_1\, S_1 + q_2\, S_2 \\ \mathbb{1} + q_1\, S_1 + q_2\, S_2 & 0 \end{pmatrix} + \begin{pmatrix} +q_3 & 0 \\ 0 & -q_3 \end{pmatrix}$$



- Nearest-neighbor hopping parameters $q_1, q_2 \in \mathbb{R}$
- Stagger $q_3 \in \mathbb{R}$
- S_j shift operators in the $j = 1, 2$ direction

De Nittis & L., J. Phys. A **46**, 2013

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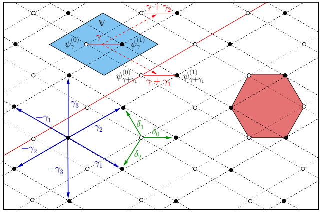

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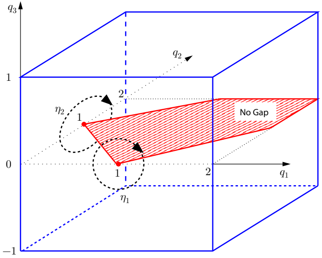

- Relevant energy gap at $E = 0$
- $0 \in \sigma(H(q))$?

  ⇝ **Red region** in $q_1 q_2$-plane ($q_3 = 0$)
- Define parameter space

$$X := \left\{ q \in \mathbb{R}^3 \;\middle|\; 0 \notin \sigma(H(q)) \right\}$$

for the **gapped phase**

De Nittis & L., J. Phys. A **46**, 2013

Analyzing the Topology of Parameter Space

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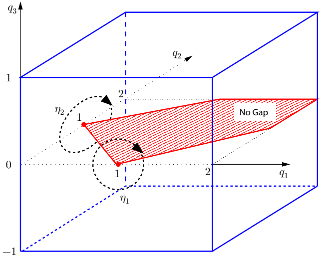

Full Model

- Connected components $\pi_0(X) = \{X\}$
- First homotopy group $\pi_1(X) = \mathbb{Z}^2$

Analyzing the Topology of Parameter Space

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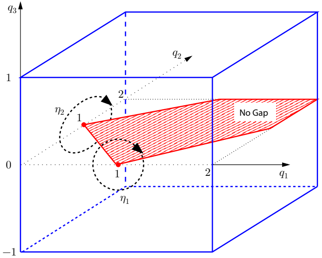

Model with Symmetry

- Impose $U_1\, H\, U_1^{-1} \stackrel{!}{=} H$ where $U_1 = \mathbb{1} \otimes \sigma_1$
- Implies $q_3 = 0$
- Reduced parameter space

$$X_{q_3=0} := \{q \in X \mid q_3 = 0\}$$

where we impose **gap and symmetry**

Analyzing the Topology of Parameter Space

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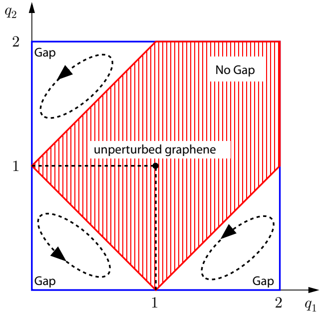

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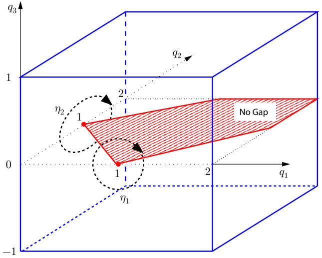
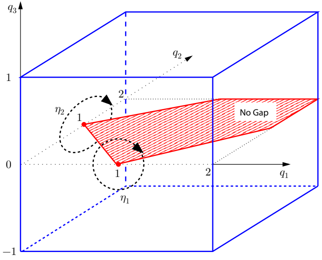


Full Model

- $\pi_0(X) = \{X\}$ vs. $\pi_0(X_{q_3=0}) = \{1, 2, 3\}$
- $\pi_1(X) = \mathbb{Z}^2$ vs. $\pi_1(X_{q_3=0}) = 0$

Periodic Deformations and Loops in Parameter Space



Time-periodic operators

- Assume $H(t) = H(t+T)$ for some $T > 0$
- Assume $H(t)$ of the form from before
- Assume $H(t)$ is gapped for all $t \in \mathbb{R}$

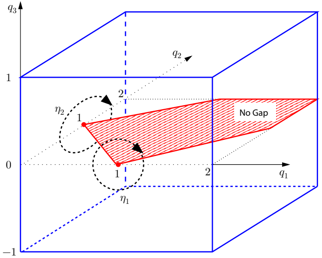
$\Longrightarrow \exists$ loop $\Gamma : [0,T] \longrightarrow X$ with

$$H(t) = H(\Gamma(t)) \quad \Longleftrightarrow \quad \Gamma \leftrightarrow H$$

Topological Charge Only Depends on $[\Gamma] \in \pi_1$

Assuming … is true

a. $\Delta\mathcal{P}_j \in \mathbb{Z}$ topological invariant
b. Invariant under continuous, gap-preserving deformations



A Priori Knowledge

- Value of $\Delta\mathcal{P}_j$ only depends on equivalence class $[\Gamma]$
- Induces maps $\pi_1(X), \pi_1(X_{q_3=0}) \longrightarrow \mathbb{Z}^2$
- $\pi_1(X) = \mathbb{Z}^2$
  $\Longrightarrow$ compute $\Delta\mathcal{P}_j$ for generators of $\pi_1(X)$
- For $[\Gamma] = n_1\,[\nu_1] + n_2\,[\nu_2] \in \pi_1(X)$

$$\Delta\mathcal{P}_j([\Gamma]) = n_1\,\Delta\mathcal{P}_j([\nu_1]) + n_2\,\Delta\mathcal{P}_j([\nu_2])$$

- **Symmetric model topologically trivial:**
  $\Delta\mathcal{P}_j = 0$ as $\pi_1(X_{q_3=0}) = 0$ and $H(t) \simeq H_0$

De Nittis & L., J. Phys. A **46**, 2013

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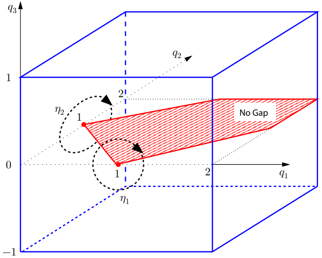

Theorem (De Nittis & L. (2013))

$\Delta \mathcal{P}_j([\nu_k]) = \pm \delta_{jk} \neq 0$, *i. e. model is topologically non-trivial*

$\rightsquigarrow$ Important as $\Delta \mathcal{P}_j([\nu_j]) = 0$ is possible!

$\Rightarrow$ During deformation $\operatorname{sgn} q_3$ needs to change!

De Nittis & L., J. Phys. A **46**, 2013

Take-Away Message

What have we learnt so far?

- **Bulk-boundary correspondences**: physics $\rightarrow$ topology
- Needs to be established on case-by-case basis for classes of operators
- $\pi_0(X)$, $\pi_1(X)$, $\left[\mathbb{T}^d, \mathrm{Gr}_k(\mathbb{R}^j)\right]$ etc. have appeared
- $\mathbb{Z}$- and $\mathbb{Z}_2$-valued topological invariants characterize topological phase

Characterizing Topological Phases

Direct approach

- **Advantage:** *Can* provide exhaustive classification
- Vector bundles with symmetries $\rightsquigarrow$ vector bundles with symmetries (De Nittis & Gomi)
- Topology of non-selfadjoint tight-binding operators $\rightsquigarrow$ braid group

  (Wojcik, Sun, Bzdušek & Fan, Phys. Rev. B **101**, 2020)
- **Downside:** $\pi_0(X)$ and **homotopy groups not algorithmically computable**!
- **Downside:** Typically very hard, limited to specific dimensions and situations

K-theoretic approach

- **Advantage:** K groups are **algorithmically computable**!

  (Prodan & Schulz-Baldes, *Bulk and Boundary Invariants for Complex Topological Insulators*, 2016)
- Can deal with *disorder*
- Symmetries typically require sophisticated versions of K-theory

  (Freed & Moore, Ann. Henri Poincaré **14**, 2013)
- **Downside:** Generally provide a *coarse* classification of topological phases

  $\rightsquigarrow$ May not be enough to distinguish topological phases from one another

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2. Homotopy Definition of Topological Phases
3. Discrete Symmetries

Relevant Symmetries for Selfadjoint Operators

Symmetries for selfadjoint operators

$$U\,H\,U^{-1} = \pm H$$

where U are (anti)unitary maps with $U^2 = \pm\mathbb{1}$

Type	*Condition on* H	$\sigma(H) =$
ordinary	$V\,H\,V^{-1} = +H$	$+\sigma(H)$
chiral	$S\,H\,S^{-1} = -H$	$-\sigma(H)$
$\pm$TR	$T\,H\,T^{-1} = +H$	$+\sigma(H)$
$\pm$PH	$C\,H\,C^{-1} = -H$	$-\sigma(H)$

Reducing out ordinary symmetry V

$$H \cong \begin{pmatrix} H_+ & 0 \\ 0 & H_- \end{pmatrix}$$

⇝ study block operators $H_\pm$ on eigenspaces of V

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Topological Classes

Symmetries of H $\longleftrightarrow$ **Topological Class** of H

- **Relies on** $\mathrm{i}\partial_t \psi = H\psi$ (Schrödinger equation)
- 3 types of (pseudo) symmetries:
  U unitary/antiunitary, $U^2 = \pm\mathbb{1}$,

$U\,H(k)\,U^{-1} = +H(-k)$ time-reversal symmetry ($\pm$TR)
$U\,H(k)\,U^{-1} = -H(-k)$ particle-hole (pseudo) symmetry ($\pm$PH)
$U\,H(k)\,U^{-1} = -H(+k)$ chiral (pseudo) symmetry (χ)

- 1 + 5 + 4 = 10 topological classes
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- Relies on $\mathrm{i}\partial_t \psi = H\psi$ (Schrödinger equation)
- **3 types of (pseudo) symmetries:**
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Thank you!

Q&A