New Directions in Materials Science Guided by Research in Operator Algebras

Emil Prodan

Yeshiva University, New York, USA

Operator Algebras in the Twenty-First Century

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My Talk's Goals:

- Identify and communicate the main principle that drives the research in topological materials and meta-materials.
- Convince you that there is already a program in place: high throughput materials design enabled by operator algebras
- Enumerate the tools from operator algebras that are needed
- Convince you that these ideas can be implemented in laboratory, no matter how abstract/complicated the algebras are

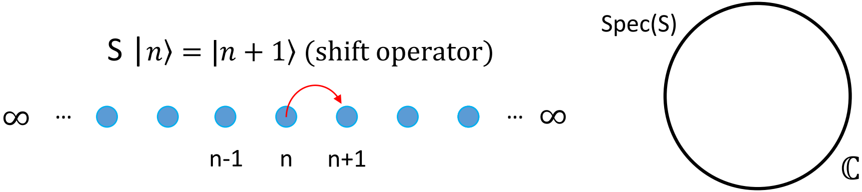

Figure: Shift operator on $\ell^2(\mathbb{Z})$

And about how this topology gets changed when edges and interfaces are created

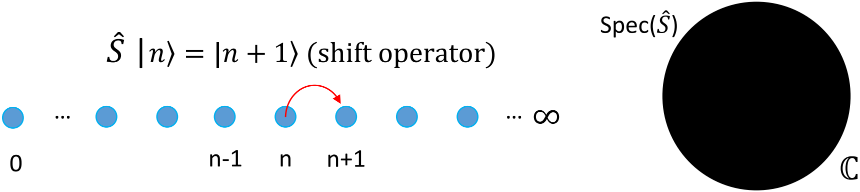

Figure: Shift operator on $\ell^2(\mathbb{N})$

Generically one finds:

$$N = S + 0.5\, S^{-1} + 1.5\, S^{2} + 2\, S^{-2}$$

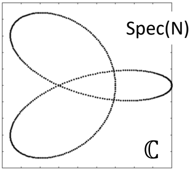

Figure: A normal operator on $\ell^2(\mathbb{Z})$

In this case, one finds:

$$\widehat{N} = \hat{S} + 0.5\,\hat{S}^{-1} + 1.5\,\hat{S}^{2} + 2\hat{S}^{-2}$$

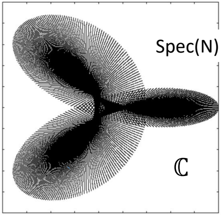

Figure: Same operator on $\ell^2(\mathbb{N})$

But this is not all of it

Browsing through "Analytic K-Homology" (by Higson & Roe), one learns about:

- essentially normal operators (ENO) and their essentially unitary equivalence
- the group $\mathrm{Ext}(X)$ of classes of ENO with $X \subset \mathbb{C}^2$ as essential spectrum

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A conjecture ...

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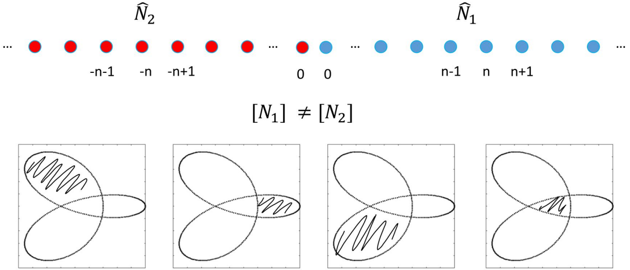
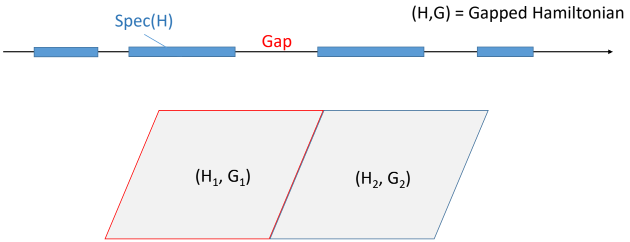


Figure: The conjecture is that we can selectively fill in the bubbles.



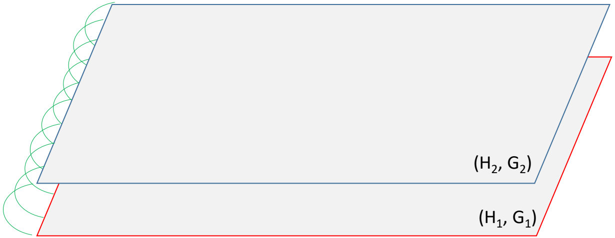
In a first stage, the program consists in:

1. Classifying the gapped Hamiltonians (under stable homotopy + possible symmetry constraints)
2. Understanding when the topology of the essential bulk spectrum is modified when two representatives are interfaced.

The main challenge:

Produce statements that are independent of the boundary condition!!!

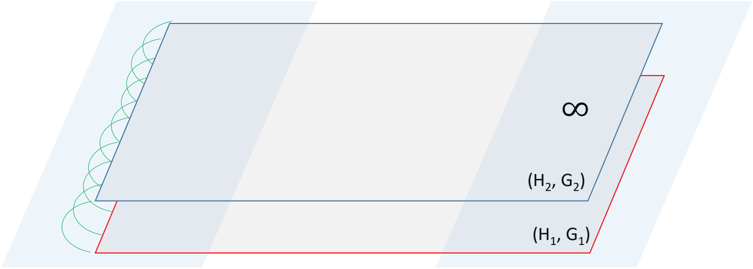
How can we approach such a problem?



Folding trick:

1. Reduces the problem to that of stacked systems with a boundary.
2. Stacking is naturally dealt with by stabilizing the algebras.

Operator algebras make their entrance



Algebra of boundary conditions $\tilde{A}$

Algebra of bulk observables A

When the algebras enter a short exact sequence:

$$0 \longrightarrow \widetilde{\mathcal{A}} \xrightarrow{\;i\;} \widehat{\mathcal{A}} \xrightarrow{\;\mathrm{ev}\;} \mathcal{A} \longrightarrow 0$$

magic happens.

The six-term exact sequence of complex K-Theory:

$$\begin{array}{ccccc}
K_0(\widetilde{\mathcal{A}}) & \xrightarrow{i_*} & K_0(\widehat{\mathcal{A}}) & \xrightarrow{\text{ev}_*} & K_0(\mathcal{A}) \\
\text{Ind} \uparrow & & & & \downarrow \text{Exp} \\
K_1(\mathcal{A}) & \xleftarrow{\text{ev}_*} & K_1(\widehat{\mathcal{A}}) & \xleftarrow{i_*} & K_1(\widetilde{\mathcal{A}})
\end{array}$$

The connecting maps (Exp and Ind):

1. Enable one to make connection between the bulk and boundary physical observables
2. They involve arbitrary lifts from bulk to half-space $\Rightarrow$ independence of boundary conditions.

This general principle was discovered in:

Kellendonk, Richter, Schulz-Baldes

Edge current channels and Chern numbers in the integer quantum Hall effect

Rev. Math. Phys. **14**, 87-119 (2002)

This work:

- Established the bulk-boundary principle for Integer Quantum Hall Effect.
- The setting is generic: irrational magnetic flux values + disorder
- It continues to serve as a model for all rigorous work on bulk-boundary principle.

Let's see it at work!

Non-commutative Tori + 'Disorder' [encoded in $\tau : \mathbb{Z}^d \to \mathrm{Homeo}(\Omega)$]

Universal algebra $\mathcal{A}_\Phi = C^*(C_N(\Omega), u_1, \ldots, u_d)$:

$$u_i u_j = e^{\imath \phi_{ij}} u_j u_i, \quad \phi_{ij} \in \mathbb{T}^1, \quad f\, u_j = u_j\, (f \circ \tau_j)$$

$$\textit{generic element} -> \sum_{q \in \mathbb{Z}^d} u_q\, a_q, \quad u_q = u_1^{q_1} \ldots u_d^{q_d}, \quad a_q : \Omega \to M_{N\times N}(\mathbb{C}).$$

Conventions:

- For thermally disordered crystals, Ω is a contractible topological space
- For the synthetic crystals, Ω will have the topology of the circle or torus.
- In that case, the generators of $C(\Omega)$ will be counted as part of the u_j's.

In the absence of symmetry constraints:

- Any (h, G) can be continuously deformed into $1 - 2p_G$, with:

$$p_G = \chi_{(-\infty,G]}(h). \quad \text{(gap projector)}$$

- Under stable homotopy, the projectors are classified by the K_0-theory of A_Φ.
- $K_0(\mathcal{A}_\Phi) \simeq \mathbb{Z}^{2^{d-1}}$ with generators $[e_J]_0$, $J \subseteq \{1, \dots d\}$, $|J| = \textit{even}$.

Given (h, G):

$$[p_G]_0 = \bigoplus_J [e_J]_0 \oplus \dots [e_J]_0 = \sum_J C_J [e_J]_0, \quad C_J \in \mathbb{Z}.$$

The class of (h, G) is fully determined by the integer coefficients C_J.

We can be Quantitative

Natural traces:

$$\mathcal{T}_\omega\Big(\sum u_q\, a_q\Big) = \mathrm{tr}\big[a_0(\omega)\big], \quad \omega \in \Omega.$$

$$\mathcal{T}\Big(\sum a_q u_q\Big) = \int_\Omega \mathrm{d}\mathbb{P}(\omega)\ \mathrm{tr}\big[a_0(\omega)\big].$$

The values of traces on the generators is known:

$$\mathcal{T}(e_J) = \mathrm{Pfaff}(\Phi_J)$$

hence:

$$\mathcal{T}(p_G) = \sum_{|J|=\mathrm{even}} C_J\, \mathrm{Pfaff}(\Phi_J), \quad C_J \in \mathbb{Z}.$$

In practice:

$$\mathcal{T}(p_G) = \lim_{Vol\to\infty} \frac{\#\text{ of eigenvalues below G}}{\text{Volume of the sample}} \quad \text{(Integrated Density of States)}$$

Canonical Representation

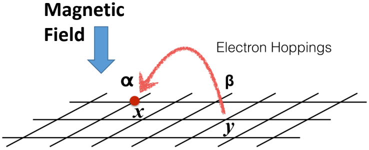
GNS-representations π_ω induced by $\mathcal{T}_\omega$ are:

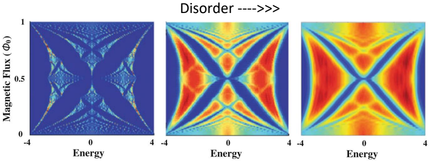
$$u_q \mapsto S_q|x\rangle = e^{\imath\langle q,\Phi x\rangle}|x+q\rangle, \quad f \mapsto \sum_{n\in\mathbb{Z}^d} |n\rangle\langle n| \otimes f(\tau_n\omega)$$

They supply all disordered physical models over $\ell^2(\mathbb{Z}^2)\otimes\mathbb{C}^N$:

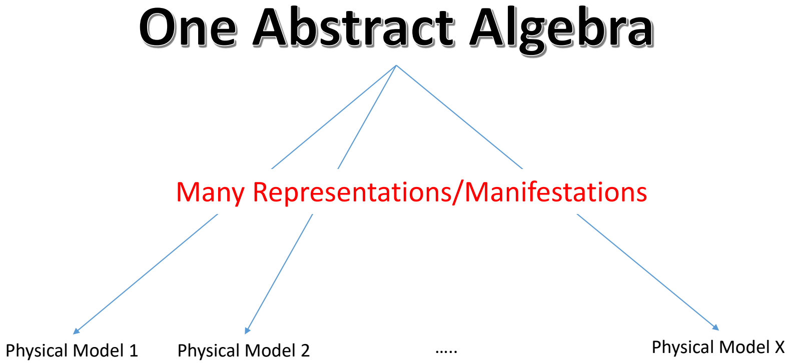
$$\mathcal{A}_\Phi \ni h = \sum_{q\in\mathbb{Z}^d} u_q\, w_q \mapsto H_\omega = \sum_{q,n\in\mathbb{Z}^d} S_q|n\rangle\langle n| \otimes w_q(\tau_n\omega).$$

Dynamics of electrons hopping on a 2d-lattice in a magnetic field:

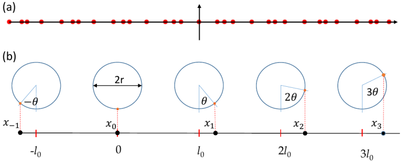


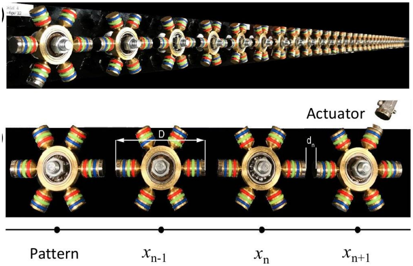


All Representations are Interesting



Physical System 2 ($h \in C(\mathbb{T}^1) \rtimes_\tau \mathbb{Z} \simeq \mathcal{A}_{\Phi_2}$)





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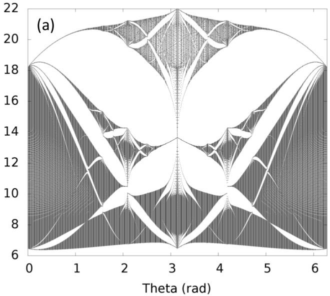
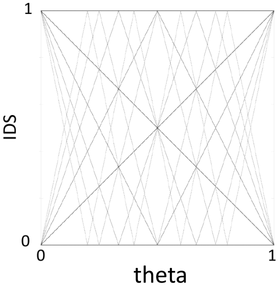
$$h = \sum_q u_q \, e^{-|x_{\tau_q \omega} - x_\omega + q l_0|}$$

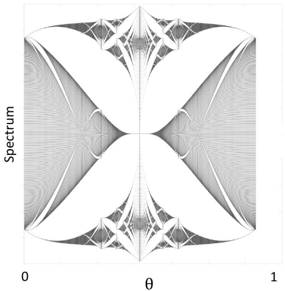


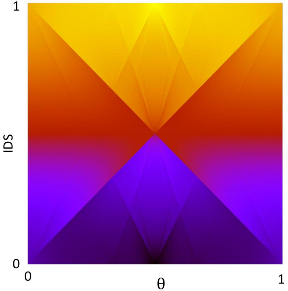
$$H = \sum_{n,m} e^{-|x_n - x_m|} |n\rangle\langle m|$$

For any gap projection p_G:

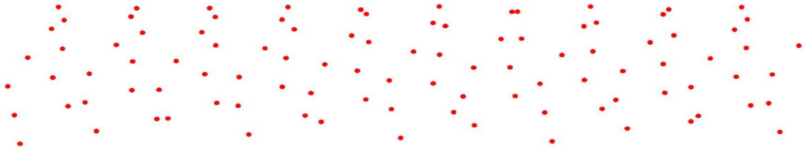
$$\mathcal{T}(p_G) \in \{n + m\theta,\ \ n, m \in \mathbb{Z}\} \cap [0, 1].$$





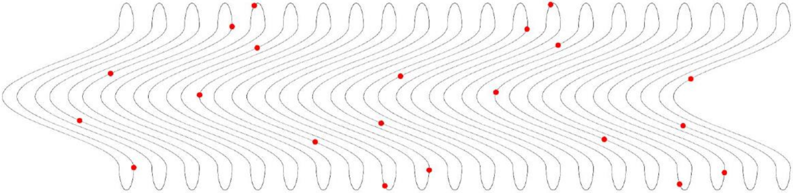


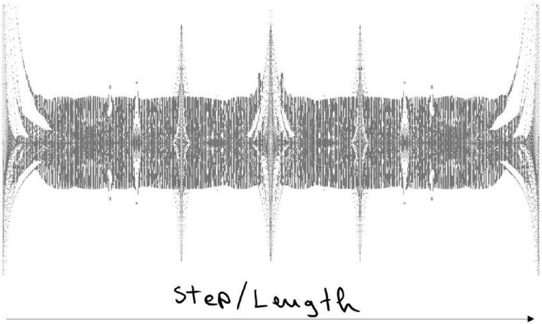
Place identical resonators at each point and let them interact pair-wise



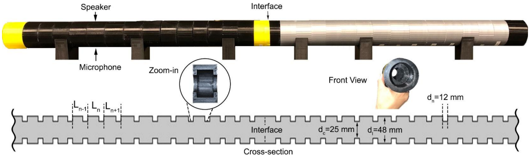
Lets try with the same Hamiltonian $$H = \sum_{n,m} e^{-|x_n - x_m|} |n\rangle\langle m|$$

Physical System 3





Physical System 4 $((\Delta - \lambda)^{-1} \in \mathbb{K} \otimes C(\mathbb{T}^2) \rtimes \mathbb{Z} \simeq \mathbb{K} \otimes \mathcal{A}_{\Phi_3})$



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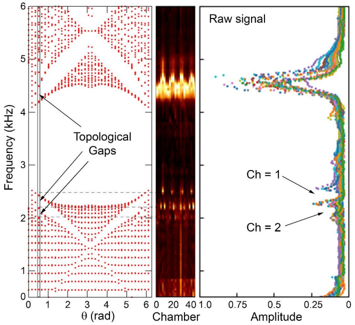
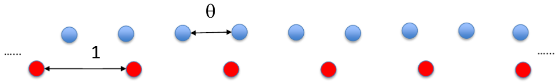
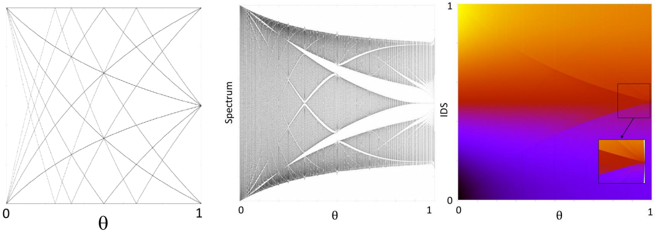


Physical System 5

For any gap projection p_G:

$$\mathcal{T}(p_G) \in \left\{n + \frac{m\theta}{1+\theta},\ \ n, m \in \mathbb{Z}\right\} \cap [0, N] \cap [0, 1]$$

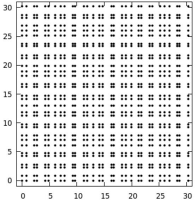


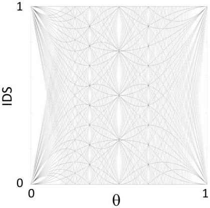


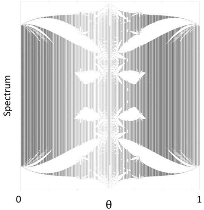
For any gap projection p_G:

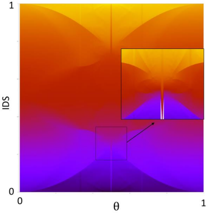
$$\mathcal{T}(p_G) \in \{n + m\theta_1 + k\theta_2 + l\theta_1\theta_2,\ n, m, k, l \in \mathbb{Z}\} \cap [0, 1]$$

$$\boldsymbol{p}_n = \boldsymbol{n} + r\left(\sin(n_1\theta_1 + \omega_1) - \sin(\omega_1)\right)\boldsymbol{e}_1 + r\left(\sin(n_2\theta_2 + \omega_2) - \sin(\omega_2)\right)\boldsymbol{e}_2,$$









Universal C^*-algebra $\widehat{\mathcal{A}}_\Phi = C^*(C_N(\Omega), \hat{u}_1, \ldots, \hat{u}_d)$ with same relations except for:

$$\hat{u}_1^* \hat{u}_1 = 1, \quad \hat{u}_1 \hat{u}_1^* = 1 - \hat{e} \quad (\hat{e} = \text{projection})$$

Generic element:

$$\hat{a} = \sum_{n,m \in \mathbb{N}} \hat{u}_1^n (\hat{u}_1^*)^m \, \hat{a}_{nm}, \quad \hat{a}_{nm} \in \mathcal{A}_{\tilde{\Phi}} \quad \tilde{\Phi} = \Phi_{d-1}$$

Canonical representations $\hat{\pi}_\omega$:

$$f \mapsto \sum_{n \in \mathbb{N} \times \mathbb{Z}^{d-1}} |n\rangle\langle n| \otimes f(\tau_n \omega), \quad \hat{u}_q \mapsto \Pi S_q \Pi^*, \quad \Pi : \mathbb{Z}^d \to \mathbb{N} \times \mathbb{Z}^{d-1},$$

supply all homogeneous physical models with a boundary. Note that:

$$\hat{\pi}_\omega(\hat{e}) = \sum_{n \in \{0\} \times \mathbb{Z}^{d-1}} |n\rangle\langle n|.$$

The principal ideal generated by $\hat{e}$

$$\widetilde{\mathcal{A}}_{\tilde{\Phi}} = \widehat{\mathcal{A}}_{\Phi}\, \hat{e}\, \widehat{\mathcal{A}}_{\Phi} \simeq \mathbb{K} \otimes \mathcal{A}_{\tilde{\Phi}}$$

serves as the algebra of the boundary observables and

$$0 \longrightarrow \widetilde{\mathcal{A}}_{\tilde{\Phi}} \xrightarrow{\ i\ } \widehat{\mathcal{A}}_{\Phi} \underset{i'}{\overset{\mathrm{ev}}{\rightleftarrows}} \mathcal{A}_{\Phi} \longrightarrow 0$$

The exact sequence between the linear spaces is split, hence:

$$\widehat{\mathcal{A}}_{\Phi} \ni \hat{a} = i'(a) + \tilde{a}, \quad \text{with unique pair } a \in \mathcal{A}_{\Phi},\ \tilde{a} \in \widetilde{\mathcal{A}}_{\tilde{\Phi}}.$$

Furthermore:

$$\hat{\pi}_\omega\big(i'(a)\big) = \Pi \pi_\omega(a) \Pi \quad \text{(Dirichlet boundary condition)}$$

$$\hat{\pi}(\tilde{a}) = \text{boundary condition}$$

The K-Groups and Generators

$$\begin{array}{ccccc} K_0(\widetilde{\mathcal{A}}_{\tilde\Phi}) & \xrightarrow{i_*} & K_0(\widehat{\mathcal{A}}_\Phi) & \xrightarrow{\mathrm{ev}_*} & K_0(\mathcal{A}_\Phi) \\ \mathrm{Ind}\uparrow & & & & \downarrow \mathrm{Exp} \\ K_1(\mathcal{A}_\Phi) & \xleftarrow{\mathrm{ev}_*} & K_1(\widehat{\mathcal{A}}_\Phi) & \xleftarrow{i_*} & K_1(\widetilde{\mathcal{A}}_{\tilde\Phi}) \end{array}$$

- The generators of $K_0(\mathcal{A}_\Phi)$ and $K_0(\widetilde{\mathcal{A}}_{\tilde\Phi})$ can be indexed as:

$$[e_J]_0 \text{ and } [\tilde e_{J'}]_0, \quad J,\ \{1\}\cup J' \subseteq \{1,\dots,d\}, \quad |J|, |J'| = \text{even}$$

- The generators of $K_1(\mathcal{A}_\Phi)$ and $K_1(\widetilde{\mathcal{A}}_{\tilde\Phi})$ can be indexed as:

$$[v_J]_1 \text{ and } [\tilde v_{J'}]_1, \quad J,\ \{1\}\cup J' \subseteq \{1,\dots,d\}, \quad |J|, |J'| = \text{odd}$$

and chosen such that:

- $$\mathrm{Exp}[e_{\{1\}\cup J}]_0 = [\tilde v_J]_1$$

- $$\mathrm{Ind}[v_{\{1\}\cup J}]_1 = [\tilde e_J]_0$$

K-Theoretic Bulk-Boundary Principle Supplied by Exp Map

Consider $(\hat{h}, h, G)$ given and let $p_G = \chi_{(-\infty,G]}(h)$ be the gap-projection.

Exp map in terms of this data:

Consider a continuous $f : \mathbb{R} \to \mathbb{R}$ with $f = 0/1$ below/above G. Then:

$$\mathrm{Exp}[p_G]_0 = \left[e^{-2\pi\imath f(\hat{h})}\right]_1 \qquad (1 - f(\hat{h}) \text{ supplies a lift for } p_G)$$

The big statement: Let

$$K_0(\mathcal{A}_\Phi) \ni [p_G]_0 = \sum_{|J|=\text{even}} c_J \, [e_J]_0$$

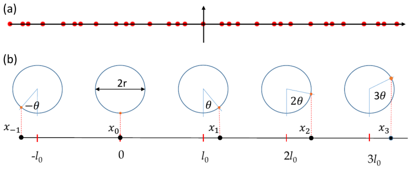
If any of c_J's with $\{1\} \subset J$ are nonzero, then:

$$G \subset \mathrm{Spec}(\hat{h}).$$

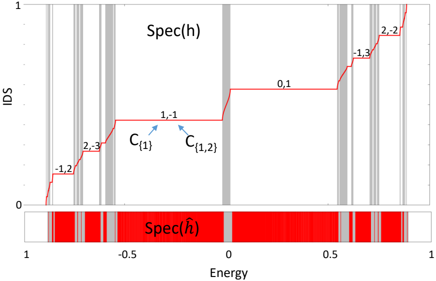
Proof.

- If $\mathrm{Spec}(\hat{h})$ is not the whole G, then we can concentrate the variation of f in $\rho(\hat{h})$.
- But then $e^{-2\pi\imath f(\hat{h})} = 1$ and we know this is not possible.

Example 1

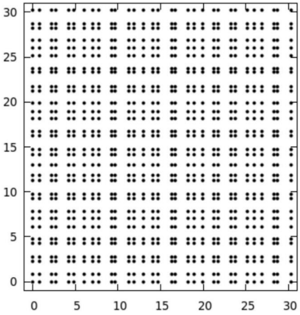


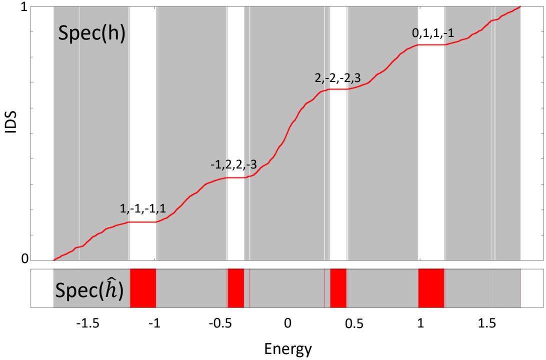
(a)
(b)
2r
$-\theta$
θ
2θ
3θ
x_{-1}
x_0
x_1
x_2
x_3
$-l_0$
0
l_0
$2l_0$
$3l_0$

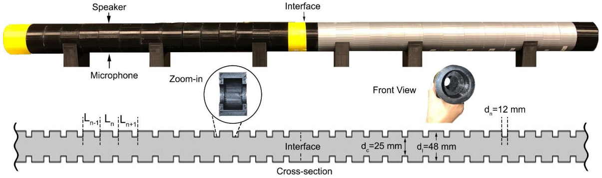


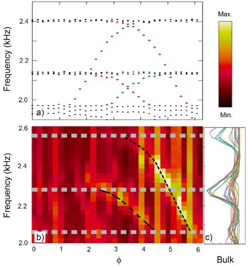
Spec(h)
IDS
1
0
-1,2
2,-3
1,-1
0,1
-1,3
2,-2
$C_{\{1\}}$
$C_{\{1,2\}}$
Spec($\hat{h}$)
1
-0.5
0
0.5
1
Energy

Example 2






Speaker
Interface
Microphone
Zoom-in
Front View
d_n=12 mm
L_{n-1} L_n L_{n+1}
Interface
d_c=25 mm
d_i=48 mm
Cross-section


Frequency (kHz)
2.4
2.2
2.0
a)
Max.
Min.
2.6
2.4
2.2
2.0
b)
c)
0 1 2 3 4 5 6
ϕ
Bulk

K-Theoretic Bulk-Boundary Principle Supplied by Ind Map

Consider $(\hat{h}, h, G)$ and assume chiral symmetry $(N \to 2N)$:

$$J = \begin{pmatrix} 1_N & 0 \\ 0 & -1_N \end{pmatrix}, \quad J(h-G)J^{-1} = -(h-G)$$

then

$$p_G = \tfrac{1}{2}\begin{pmatrix} 1 & -u_G^* \\ -u_G & 1 \end{pmatrix}, \quad \mathrm{sgn}(h-G) = \begin{pmatrix} 0 & u_G^* \\ u_G & 0 \end{pmatrix}$$

Ind map in terms of this data:

Consider a continuous $g : \mathbb{R} \to \mathbb{R}$ with $g = \pm 1$ above/below G and $g - G$ odd. Then:

$$\mathrm{Ind}[u_G]_1 = \left[e^{-\imath \frac{\pi}{2} g(\hat{h})} \mathrm{diag}(1_N, 0_N) e^{\imath \frac{\pi}{2} g(\hat{h})}\right]_0 - [\mathrm{diag}(1_N, 0_N)]_0$$

Note:

$$e^{-\imath \frac{\pi}{2} g(\hat{h})} \mathrm{diag}(1_N, 0_N) e^{\imath \frac{\pi}{2} g(\hat{h})} = \tfrac{1}{2} J(e^{\imath \pi g(\hat{h})} + 1) + \mathrm{diag}(0_N, 1_N).$$

K-Theoretic Bulk-Boundary Principle Supplied by Ind Map

$$\mathrm{Ind}[u_G]_1 = \left[e^{-\imath\frac{\pi}{2}g(\hat{h})}\mathrm{diag}(1_N, 0_N)e^{\imath\frac{\pi}{2}g(\hat{h})}\right]_0 - [\mathrm{diag}(1_N, 0_N)]_0$$

Note:

$$e^{-\imath\frac{\pi}{2}g(\hat{h})}\mathrm{diag}(1_N, 0_N)e^{\imath\frac{\pi}{2}g(\hat{h})} = \tfrac{1}{2}J(e^{\imath\pi g(\hat{h})} + 1) + \mathrm{diag}(0_N, 1_N).$$

The big statement:

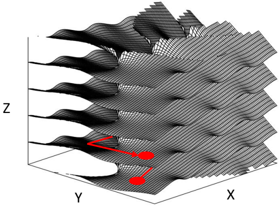
$$K_1(\mathcal{A}_\Phi) \ni [u_G]_1 = \sum_{|J|=\text{odd}} c_J\,[v_J]_1$$

If any of c_J's with $J \cap \{1\}$ are nonzero, then:

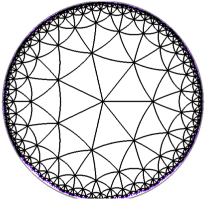
$$\{G\} \subset \mathrm{Spec}(\hat{h}) \quad \text{(mid-gap point belongs to the spectrum)}$$

Proof.

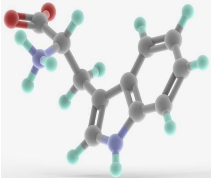
- If $\{G\}$ is not inside $\mathrm{Spec}(\hat{h})$, then we can concentrate the variation of g in this missing interval.
- But then $\frac{1}{2}J(e^{\imath\pi g(\hat{h})} + 1) = 0$ and we know this is not possible.



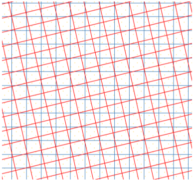
Group C*-algebras and crossed products by Heisenberg group



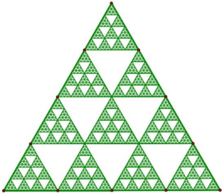
Group C*-algebras and crossed products by Fucshian groups



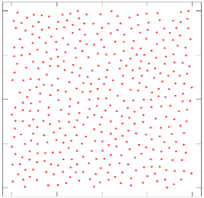
Graph Algebras



Moire patterns



Fractal patterns



Grupoid Algebras

A Word About Quasi-Crystals

Quasi-Crystal