Quantifiable local topological protection in quantum materials

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Almost commuting operators and physics

According to von Neumann (in 1927)

> *quantum mechanics attributes to the quantities* q_k *and* p_k *the well-known operators* $\mathbf{Q}_k = q_k \cdots$ *and* $\mathbf{P}_k = \frac{\hbar}{i}\frac{\partial}{\partial q_k} \cdots$*, whose lack of commutability [...] corresponds to the lack of simultaneous measurability of these quantities. We now assume that two other, commuting, operators* $\mathbf{P}'_k, \mathbf{Q}'_k$ *exist whose difference from* $\mathbf{P}_k$ *(respectively,* $\mathbf{Q}_k$*) is so small that its size [...] does not significantly exceed the value* $\hbar/2$ *required by the uncertainty relation.*

and also (in 1932)

> *the macroscopic procedure consists of replacing all possible operators* A*,* B*,* C*, ..., which as a rule to not commute with each other, by other operators* A'*,* B'*,* C'*, ..., (of which these are functions to within a certain approximation) which do commute with each other.*

Such approximations are *not* always possible, which is why we have Chern insulators.

Almost commuting matrices and K-theory

In basis $|-s\rangle$, $|-s+1\rangle$, ..., $|s\rangle$, define

$$Z_s\,|k\rangle = \alpha_k\,|k\rangle\,, \quad L_s\,|k\rangle = \beta_k\,|k+1\rangle$$

for some $-1 = \alpha_1 < \alpha_2 < \cdots < \alpha_n = 1$, $\alpha_n^2 + \beta_n^2 \approx 1$.
Now set

$$X_s = \tfrac{1}{2}(L_s^\dagger + L_s), \quad Y_s = \tfrac{i}{2}(L_s^\dagger - L_s).$$

These almost commute and generate a "fuzzy sphere" since

$$\|[X_s, Y_s]\| \to 0,\ \|[X_s, Y_s]\| \to 0,\ \|[Y_s, Z_z]\| \to 0 \text{ and } \left\|X_s^2 + Y_s^2 + Z_s^2 - I\right\| \to 0.$$

Man-Duen Choi (in 1988) showed

$$X_s \otimes \sigma_x + Y_s \otimes \sigma_y + Z_s \otimes \sigma_z$$

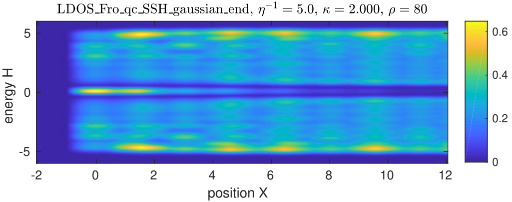
has two more positive than negative eigenvalues. He proved that X_s', Y_s', Z_s' commuting with each other implies

$$\left\|X_s' - X_s\right\| + \left\|Y_s' - Y_s\right\| + \left\|Z_s' - Z_s\right\| \geq 1 - s.$$

Theorem (Lin, 1995). $\forall \epsilon > 0$, $\exists \delta > 0$ for the following.
If H and X are n-by-n Hermitian matrices with $\|HX - XH\| \leq \delta$ then there are H' and X' commuting with $\|H - H'\| < \epsilon$ and $\|X - X'\| < \epsilon$.

Hastings (2008) – This tell us a gapped, finite, 1D system in Class A is "Wannierizable" / close to an atomic limit.

True in all 10 AZ symmetry classes if one allows zero-modes (follows from extensions of Lin's theorem by David Herrera, 2024 and others).



LDOS at the end of a quasiperiodic variation of an SSH chain. From paper on windowed LDOS, joint with Fu and Watson.

States approximately local in position and energy

For a system (non-interacting) with open boundaries, the key observables are H for energy and position observables $X_1, \ldots, X_d$.

Eigenstates ψ_1 and ψ_2 of H at slightly different energies might be delocalized in position while

$$\psi = \frac{1}{\sqrt{2}}\psi_1 + \frac{1}{\sqrt{2}}\psi_2$$

is well-localized. The LDOS can miss this.

For Hermitian observable A we have

$$\left\| A \left|\psi\right\rangle - \lambda \left|\psi\right\rangle \right\|^2 = \triangle_\psi^2 A + \left(\mathrm{E}_\psi[A] - \lambda\right)^2 .$$

A *joint approximate eigenvector* for $X_1, \ldots, X_d, H$ is a state that is approximately localized in energy and position.

The quadratic local gap

We define a local gap at position $\mathbf{x}$ and energy E as

$$\mu^{\mathsf{Q}}_{\mathbf{x},E}(X_1,\ldots,X_d,H) = \min_{\|\psi\|=1}\left(\sum_{j=1}^{d}\left\|X_j\psi - x_j\psi\right\|^2 + \|H\psi - E\psi\|^2\right)^{\frac{1}{2}},$$

and this equals the square root of the smallest eigenvalue of

$$Q_{\mathbf{x},E}(X_1,\ldots,X_d,H) = \sum_{j=1}^{d}\left(X_j - x_jI\right)^2 + (H-EI)^2\,.$$

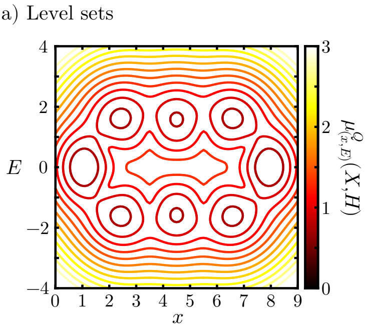
We call the function

$$(\mathbf{x},E) \mapsto \mu^{\mathsf{Q}}_{\mathbf{x},E}(X_1,\ldots,X_d,H)$$

the *quadratic pseudospectrum* of $(X_1,\ldots,X_d,H)$, or the *quadratic local gap*

Since $Q_{\mathbf{x},E}(X_1,\ldots,X_d,H)$ will generally be sparse, this is practical to compute numerically.

The Quadratic local gap in 1D



Shown is the quadratic pseudospectrum for a very short topologically non-trivial SSH system.

In practice, replace X_j by κX_j to somewhat align position units with energy units. Generally a large range of κ gives consistent results.

We seek a "square root" of $Q_{\mathbf{x},E}(X_1,\ldots,X_d,H)$ that detects K-theory.

The Clifford local gap

Pick Hermitian matrices γ_j that anticommute and so that $\gamma_j^2 = I$. The spectral localizer is

$$L_{\mathbf{x},E}(X_1,\ldots,X_d,H) = \sum_{j=1}^{d}(X_j - x_j I)\otimes\gamma_j + (H - EI)\otimes\gamma_{d+1}.$$

As long as H is local, so $[H, X_j]$ are small, we find

$$(L_{\mathbf{x},E}(X_1,\ldots,X_d,H))^2 \approx (Q_{\mathbf{x},E}(X_1,\ldots,X_d,H))\otimes I.$$

We call the function

$$(\mathbf{x},E)\mapsto \mu^{\mathsf{C}}_{\mathbf{x},E}(X_1,\ldots,X_d,H)$$

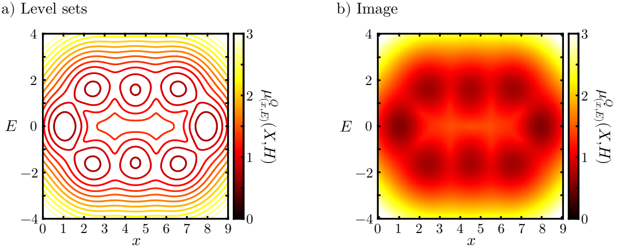
the *Clifford pseudospectrum* of $(X_1,\ldots,X_d,H)$ where

$$\mu^{\mathsf{C}}_{\mathbf{x},E}(X_1,\ldots,X_d,H)$$

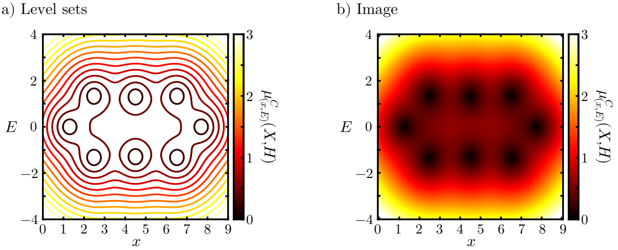
equals minimum absolute value of an eigenvalue of $L_{\mathbf{x},E}(X_1,\ldots,X_d,H)$.

- Almost as good at finding well-localized states.
- Also detects local topology.

Both local gaps for an SSH chain



The quadratic pseudospectrum.



The Clifford pseudospectrum.

Local topology in Chern insulators

When $d = 2$ we generally use $\gamma_1 = \sigma_x$, $\gamma_2 = \sigma_y$, $\gamma_3 = \sigma_z$.

In class A, the invariant is

$$\frac{1}{2}\mathrm{Sig}\left(L_{x,y,E}(X, Y, H)\right)$$

where the signature is the number of eigenvalues that are positive minus the number that are negative.

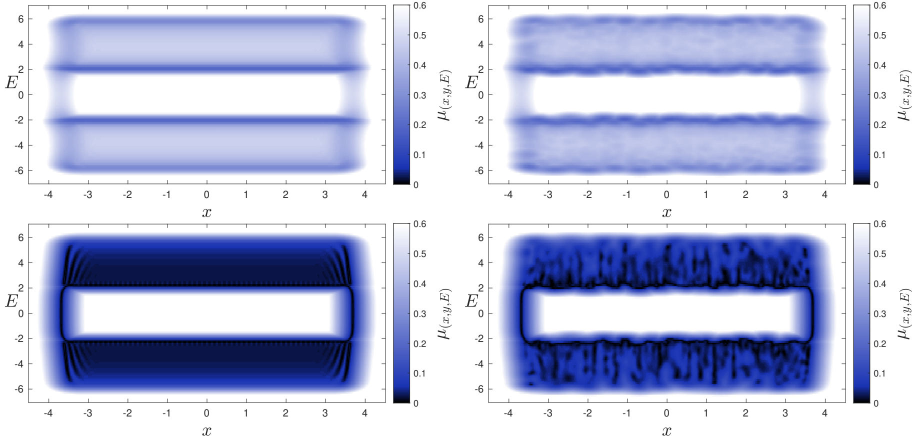
The signature can change only when $L_{x,y,E}(X, Y, H)$ becomes singular. When $\mu^{\mathrm{C}}_{x,y,E}(X_1, \ldots, X_d, H)$ is large a large change in H will be required to change the local index.

If $XH = HX$ and $HY = YH$ we are in "an atomic limit" and we find

$$\frac{1}{2}\mathrm{Sig}\left(L_{x,y,E}(X, Y, H)\right) = 0.$$

If signature is zero then there is a path (X_t, Y_t, H_t), almost commuting at every t, from (X_t, Y_t, H_t) to an atomic limit. Can be a long path.

Both local gaps of a Chern insulator



Shown are $y = 0$ slices. Units are adjusted, replacing X and Y by κX and κY.

Top is quadratic, bottom is Clifford. Left is clean. Right is with disorder.

1D in Class AIII

If Π implements Chiral-symmetry then we have $X\Pi = \Pi X$ and $\Pi H = -H\Pi$. Here

$$L_{x,E}(X,H) = (X - xI) \otimes \sigma_x + (H - EI) \otimes \sigma_y$$

Shifting H to $H - EI$ ruins symmetry, unless $E = 0$.

At $E = 0$ the local invariant is

$$\frac{1}{2}\text{Sig}\left(((X - xI) + iH)\Pi\right).$$

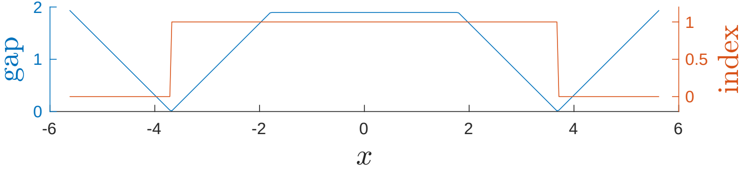
Notice $((X - xI) + iH)$ is a block out of the spectral localizer

$$L_{x,0}(X,H) = \begin{bmatrix} 0 & (X - xI) - iH \\ (X - xI) + iH & 0 \end{bmatrix}.$$

Local measure of strength of topological protection

Studying materials, only need to track $L_{\boldsymbol{\lambda}}(X, Y, H)$ as $\boldsymbol{\lambda}$ moves on a line.

Need only compute the index formula (K-theory) and the eigenvalue closest to zero (local gap).



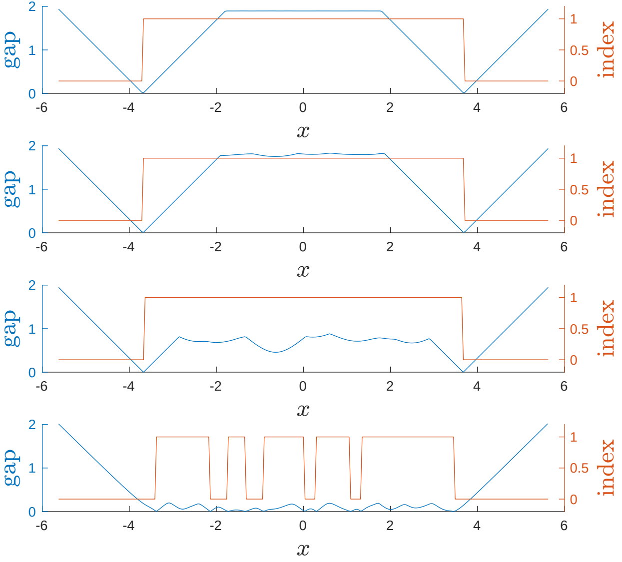
No disorder.

The localizer gap inceases (up to a point) as (x, y) moves away from the edge of the system.

Small disorder can move the edge state a little.

Moving or eliminating the edge state takes a larger permutation.

Adding disorder



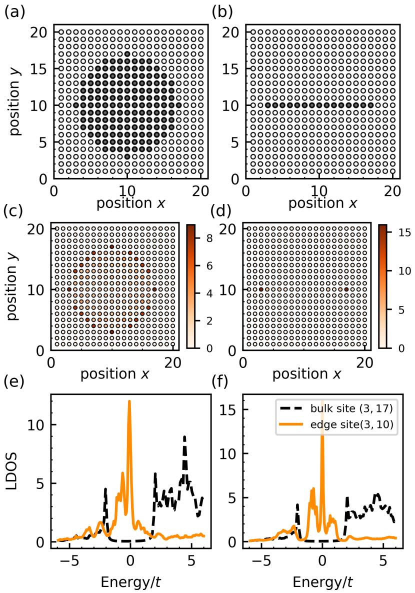
Disorder 0% of size of bulk gap.

Disorder 12% of size of bulk gap.

Disorder 60% of size of bulk gap.

Disorder 120% of size of bulk gap.

Consider a Shiba lattice, in class D. Atop the surface of a superconductor, place pattern of magnetic atoms.



Consider a Shiba lattice, in class D. Atop the surface of a superconductor, place pattern of magnetic atoms.

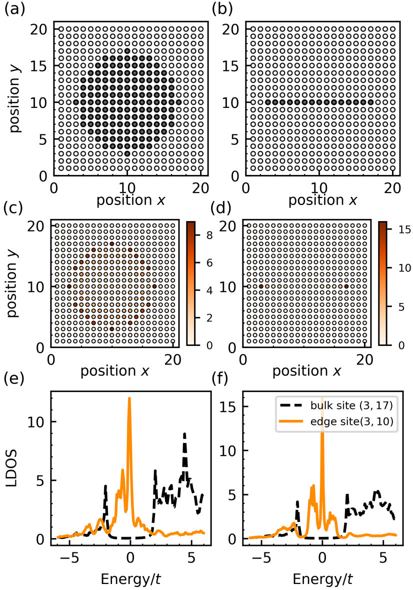
For line in x-direction, use as local invariant

$$\text{sign}\left(\det\left((X - xI) + iH\right)\right)$$

and

$$\frac{1}{2}\text{Sig}\left(L_{x,y,E}(X,Y,H)\right)$$

for a disk or square.



Dimension cross-over in class D

Consider a Shiba lattice, in class D. Atop the surface of a superconductor, place pattern of magnetic atoms.

For line in x-direction, use as local invariant

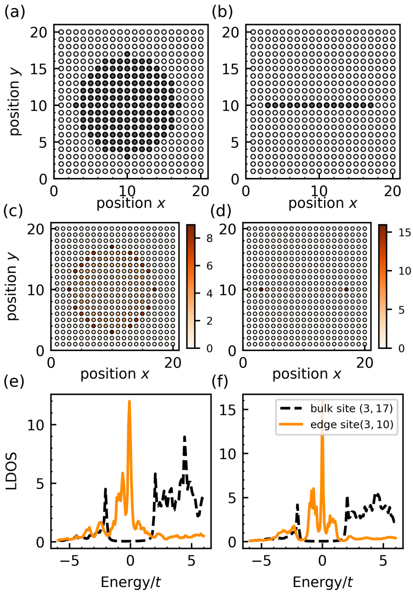
$$\text{sign}\left(\det\left((X - xI) + iH\right)\right)$$

and

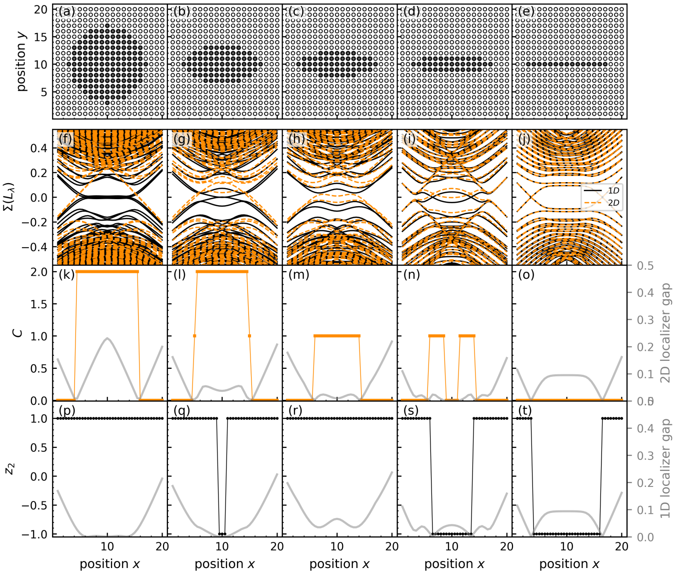
$$\frac{1}{2}\text{Sig}\left(L_{x,y,E}(X, Y, H)\right)$$

for a disk or square.

For other shapes, we can use both.
This is on the Arxiv, joint with Cerjan and Rodriguez-Vega.



Dimension cross-over in Class D



From a disk to a line of adatoms.

Spectrum of 1D and 2D localizers as x-position varies.

2D local invariant and local gap.

1D local invariant and local gap.

Quantum spin Hall systems

For a class AII system in 2D, we assume $\mathcal{T}^2 = -I$ and that X, Y and H all commute with $\mathcal{T}$. Typically $\mathcal{T} = U \circ \mathcal{K}$ where $U = I \otimes i\sigma_y$. For fixed x, y and H,

$$L_{x,y,E}(X, Y, Z)$$

is in class D in 0D for the time-reversal operator

$$(I \otimes i\sigma_y \otimes i\sigma_y) \circ \mathcal{K}$$

which is, in some basis, just $\mathcal{K}$ (complex conjugation). Theory says there is a unitary Q so that

$$Q\left(L_{x,y,E}(X, Y, Z)\right) Q^{\dagger}$$

is anti-symmetric. Then we compute Fermionic parity, here a local $\mathbb{Z}_2$ index,

$$\text{Sign}\left(\text{Pf}\left(Q\left(L_{x,y,E}(X, Y, Z)\right) Q^{\dagger}\right)\right).$$

The Pfaffian can only change sign by going through zero, so only when the spectral localizer becomes singular.

A crafty unitary

Suppose $\mathcal{T} = U \circ \mathcal{K}$ and $U^2 = I$. We seek a unitary Q so that

$$Q \circ \mathcal{K} \circ Q^\dagger = \mathcal{T}.$$

Since $Q \circ \mathcal{K} \circ Q^\dagger = QQ^\top \circ \mathcal{K}$ what is required is $QQ^\top = U$.
In the case of

$$U = (i\sigma_y) \otimes (i\sigma_y) = \begin{bmatrix} 0 & 0 & 0 & -I \\ 0 & 0 & I & 0 \\ 0 & I & 0 & 0 \\ -I & 0 & 0 & 0 \end{bmatrix}$$

we can use

$$Q = \frac{e^{-\frac{i\pi}{4}}}{\sqrt{2}} \begin{bmatrix} I & 0 & 0 & iI \\ 0 & I & -iI & 0 \\ 0 & -iI & I & 0 \\ iI & 0 & 0 & I \end{bmatrix}.$$

Thus $QL_{x,y,E}(X,Y,Z)Q^\dagger$ is skew-symmetric and purely imaginary. Where there is a local gap, the Pfaffian of this is well-defined and takes a real, non-zero value.

Calculating these invariants

Good software to compute the sign of a Pfaffian is in development. Expect to compute this effectively for Hilbert space dimension N up to about 1 million on a powerful workstation.

The other local indices, in any dimension, any AZ class, end up with

- sig $\left(\widetilde{L}\right) \rightarrow$ use sparse `LDLT` factorization
- sign $\left(\det(\widetilde{L})\right) \rightarrow$ use sparse `LU` factorization
- sign $\left(\mathrm{Pf}(\widetilde{L})\right) \rightarrow$ stuck with dense Hessenberg factorization, for a little longer.

Matlab code for all these are in an online supplement to my 2015 paper. In all cases, $\widetilde{L}$ is built from the full spectral localizer.

Avoid computing all the eigenvalues.

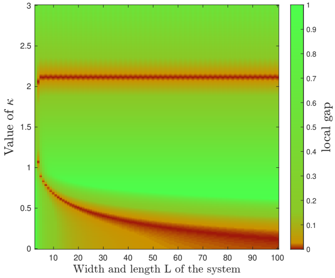
When can we link these invariant to established invariants?

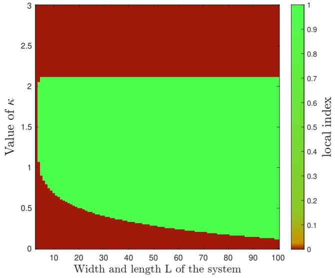
Schulz-Baldes, with me or Nora Doll, proved roughly the following.

If infinite-volume system is gapped, and we use κX_j for small κ, and if we truncate to a large radius ρ, then at the center the local index of (X_ρ, Y_ρ, H_ρ) agrees with the established bulk index of (X, Y, H).

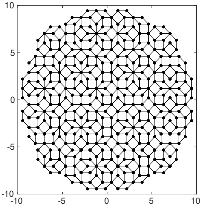
To know how big we we need ρ, and how small κ, we need an estimate on the spectral gap of H, i.e. $g = \|H^{-1}\|^{-1}$.

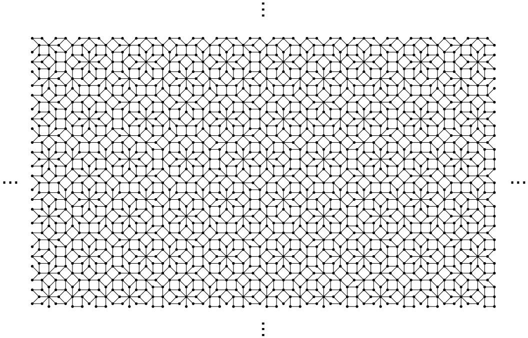
In practice, we can use smaller ρ and a wider range of κ than theorems indicate.





Truncating infinite-area topological insulator

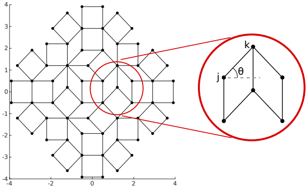




No gap in spec(H_ρ) (due to spectral pollution / interesting edge states) so this is no help in computing spec(H).

For correct ρ and κ, the local gap will approximate the distance of κ to the spectrum of H.

$p_x + ip_y$ tight-binding model on an Ammann-Beenker tiling

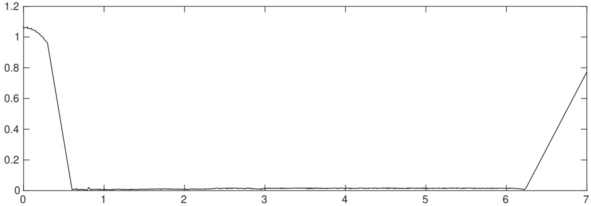


The Hilbert space is $\ell^2(\mathcal{V}) \otimes \mathbb{C}^2$ where $\mathcal{G} = (\mathcal{E}, \mathcal{V})$ is the graph based on an Ammann-Beenker tiling.

Define H as an infinite matrix with $H_j = -\mu\sigma_z$ associated with each vertex and a hopping term for each edge

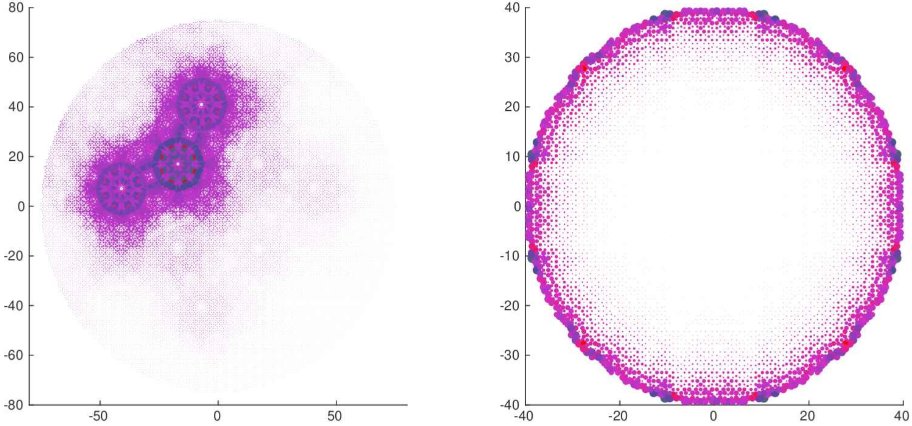
$$H_{jk} = -t\sigma_z - \frac{i}{2}\Delta\sigma_x \cos(\theta_{jk}) - \frac{i}{2}\Delta\sigma_y \sin(\theta_{jk})$$

Estimate on distance from to the spectrum of H:



$p_x + ip_y$ tight-binding model, a bulk and an edge state

These methods work by finding approximate eigenvalues of H_ρ that avoid the edges.

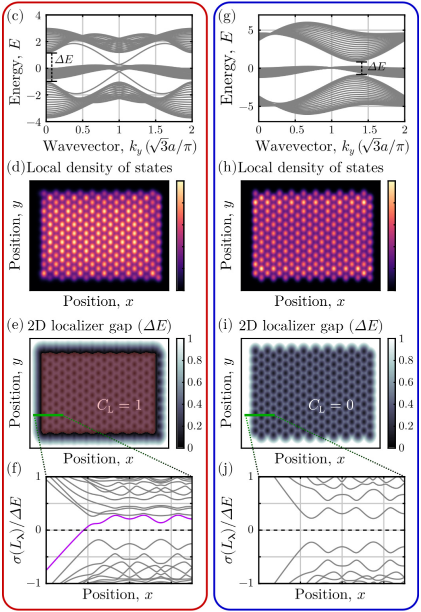


Better methods in infinite-dimensional numerical linear algebra have been developed since this work. See Hege, Moscolari and Teufel, 2025.

Some places where the spectral localizer finds local topology

- Models of photonic Quasicrystals, not just tight-binding (with Wong and Cerjan).
- Topological semimetals (Stoiber and Schulz-Baldes)
- Topological metals, if we find a local gap (with Cerjan)
- Fragile topology given $C_2\mathcal{T}$ symmetry (with Lee, Wong, Vaidya, Cerjan).
- Metal-isulator heterostructures
- With modifications, pseudospectral methods work with periodic boundary conditions.

A topological Chern metal

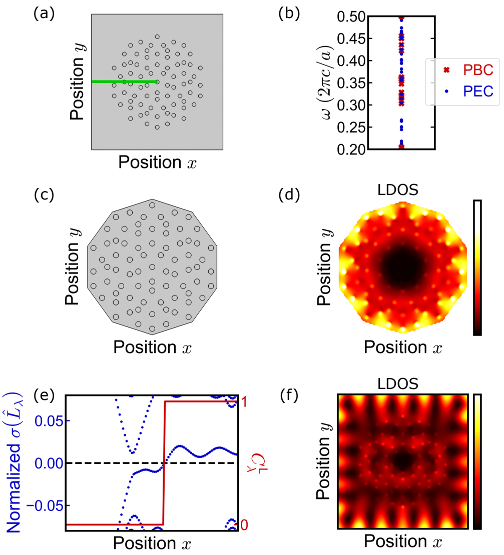


The LDOS cannot distinguish topological and trivial metals.

The Clifford pseudospectrum shows a clear edge effect in the topological case. (Hue shows the local index).

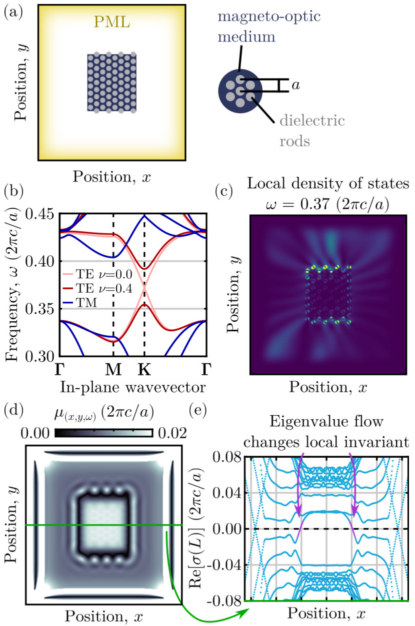
From paper written with Cerjan.

Photonic crystal slabs



From a paper with Stephan Wong and Alexander Cerjan.

Metal-insulator heterostructures



(a) A photonic crystal with Perfectly Matched Layer to simulate light lost to free space.

(b) Bandstructure.

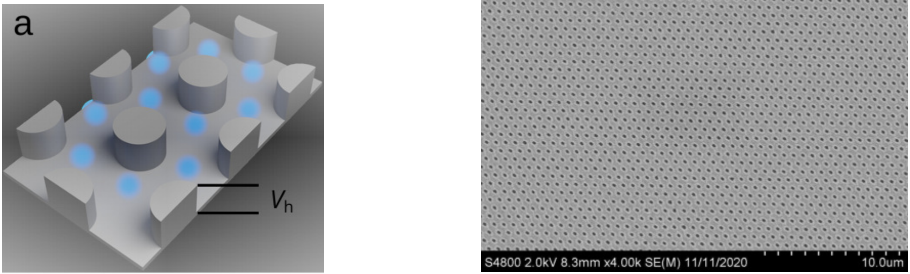
(c) Real part of local density of states.

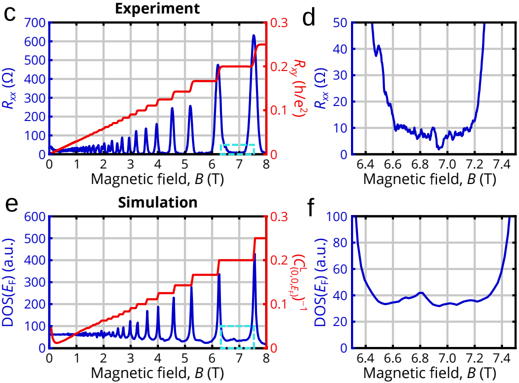
(d) Localizer gap data, at fixed E[1]

(e) Flow of eigenvalues of spectral localizer – crossing indicate change in local topology.

Dixon, Kahlil Y., et al. "Classifying Topology in Photonic Heterostructures with Gapless Environments." Physical Review Letters, 131:21 (2023), 213801.

Patterned semiconductor





(a) (b) Patterned etching in semiconductor.

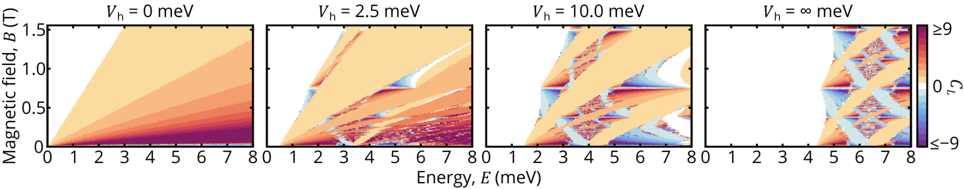
(c d) As magnetic field increases we see the Landau levels.

(e f) Local index in model matches well.

Next slide: Hofstadter butterfly.

Simulated data[2]. Local K-theory illustrated in color. Not a simple tight-binding model, but a discretized version of the single-particle Hamiltonian:

$$H = \frac{1}{2m^*}\left(-i\hbar\nabla + e\mathbf{A}(x)\right)^2 + V(x) + \frac{\mu_B g}{\hbar} s_z B$$



[2] C. Spataru, W. Pan, A. Cerjan, PRL, 2025.

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Hege, Paul; Moscolari, Massimo and Teufel, Stefan. ”Computing the spectrum and pseudospectrum of infinite-volume operators from local patches.” Mathematics of Computation (2025).

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