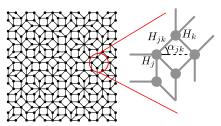
The spectral localizer for estimating bulk gaps and calculating *K*-theory

Terry A. Loring

June, 2019

Quasicrystalline Chern insulator

Aperiodic Ammann-Beenker tiling.



For Chern number -1:

$$\mu = 1$$
, $t = 1$, $\mu = 2$.

For Chern number 0:

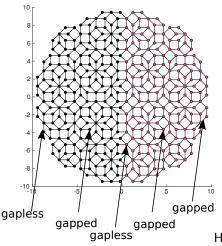
$$\mu = 1$$
, $t = \frac{1}{3}$, $\mu = 2$.

" $p_x + ip_y$ " tight binding model: H_{QC}

$$H_j = -\mu \sigma_z$$

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

Fulga, Ion Cosma, Dmitry I. Pikulin, and L. "Aperiodic Weak Topological Superconductors." Physical Review Letters 116.25 (2016): 257002.

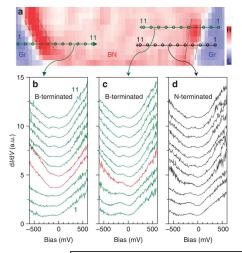


Set constants for Chern number -1 on the left (black vertices).

Set constants for Chern number 0 on the right (red vertices).

The units indicated define position operators X and Y. Using Dirichlet boundary conditions (just compress).

How can we described gapped and gapless using the same Hilbert space?



At interface of graphene surface and hexagonal boron nitride surface, expect states approximately at the Fermi level, localized at the interface.

The right shows scanning tunneling spectroscopy demonstrating this (via a scanning tunneling microscope).

Nature Comm. 5, 5403, (2015), "Spatially resolved one-dimensional boundary states in graphene-hexagonal boron nitride planar heterostructures" by Park et al.

Clamp an STM probe over position (0,0), get a combined system with no position to measure. The *localizer* abstracts this.Define

$$L_{\mathbf{0}}(X,Y,H) = \begin{pmatrix} H & X - iY \\ X + iY & -H \end{pmatrix}$$

acting on a doubled Hilbert space (electron on the surface at vertex or on the probe above vertex). One can show

$$\begin{pmatrix} H & X - iY \\ X + iY & -H \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} \approx 0 \tag{1}$$

implies that either $\psi = \frac{1}{||\psi_1||} \psi_1$ or $\psi = \frac{1}{||\psi_2||} \psi_2$ will satisfy

$$H\psi \approx 0$$
, $X\psi \approx 0$, $Y\psi \approx 0$.

Our ability to solve Eq. 1 is limited by the size of

$$\operatorname{gap}_{\mathbf{0}}(X, Y, H) = \|L_{\mathbf{0}}(X, Y, H)^{-1}\|^{-1}$$

which is the smallest absolute eigenvalue of the localizer.

Notice

$$L_{\mathbf{0}}(\kappa X, \kappa Y, H) = \begin{pmatrix} H & \kappa X - i\kappa Y \\ \kappa X + i\kappa Y & -H \end{pmatrix}$$

is equally valid. Small κ makes $H\psi\approx 0$ closer to zero at the cost of making $X\psi$ and $Y\psi$ larger.

We can also "move the probe" and shift H, so

$$L_{\lambda}(\kappa X, \kappa Y, H) = \begin{pmatrix} H - \lambda_{3} & \kappa (X - \lambda_{1}) - i\kappa (Y - \lambda_{2}) \\ \kappa (X - \lambda_{1}) - i\kappa (Y - \lambda_{2}) & - (H - \lambda_{3}) \end{pmatrix},$$

and now small

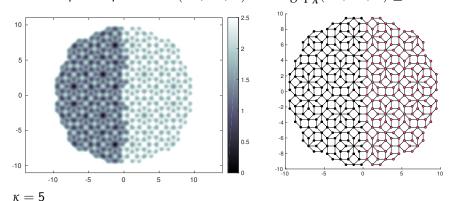
$$\operatorname{gap}_{\lambda}(X, Y, H) = \|L_{\lambda}(X, Y, H)^{-1}\|^{-1}$$

leads to

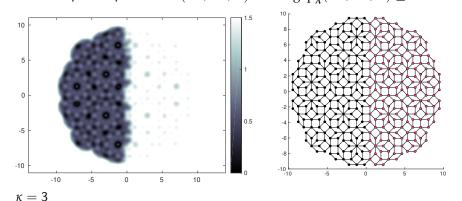
$$H\psi \approx \lambda_1 \psi$$
, $X\psi \approx \lambda_2 \psi$, $Y\psi \approx \lambda_3 \psi$.

We need to tune this by adjusting κ . Too large a κ gives an abstraction of microscopy, not spectroscopy.

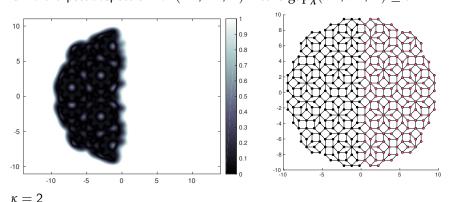
We now plot $\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$ with $\lambda_3 = 0$ as a function of (λ_1, λ_2) .



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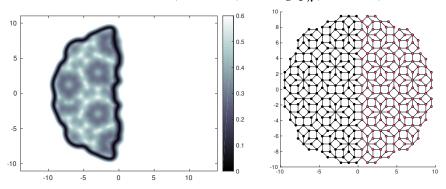


We now plot $\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$ with $\lambda_3 = 0$ as a function of (λ_1, λ_2) .

Clifford spectrum of $(\kappa X, \kappa Y, H)$ means $\text{gap}_{\lambda}(\kappa X, \kappa Y, H) = 0$.

 $\kappa = 1$

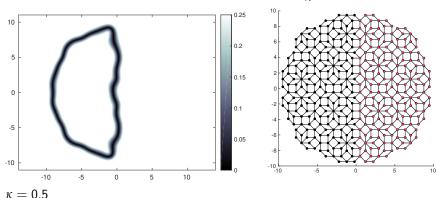
Clifford ϵ -pseudospectrum of $(\kappa X, \kappa Y, H)$ means $\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) \leq \epsilon$.



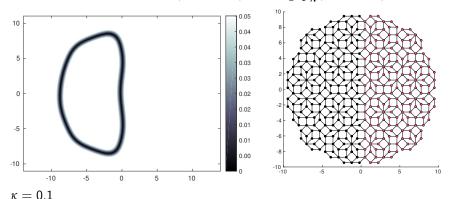
We now plot gap_{λ}(κX , κY , H) = $\|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$ with $\lambda_3 = 0$ as a function of (λ_1, λ_2) .

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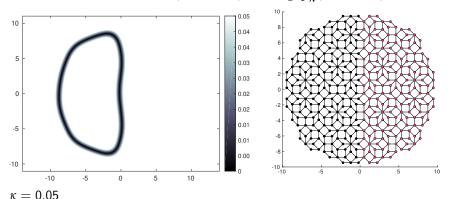
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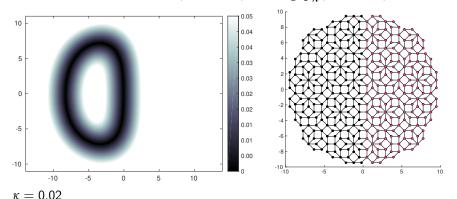
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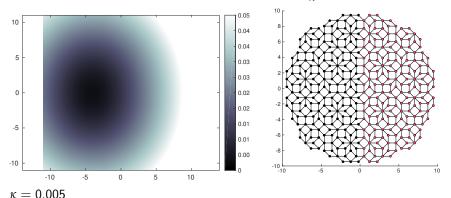
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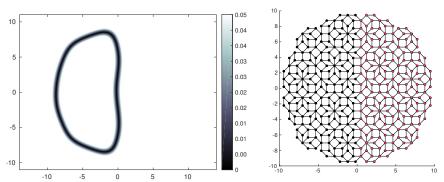


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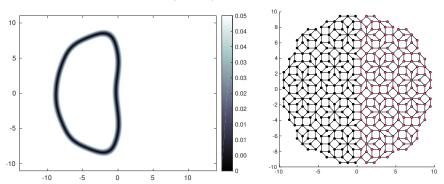
We fix $\kappa=0.1$ and varying the energy setting λ_3 . All spectral data respects the symmetry $H\mapsto -H$, so we need only look at $\lambda_3\geq 0$. Plotting

$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$



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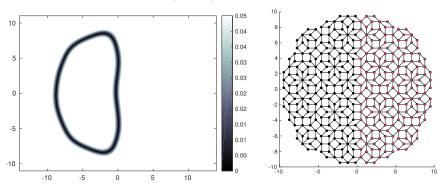
$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$



$$\kappa = 0.1, \lambda_3 = 0.2$$

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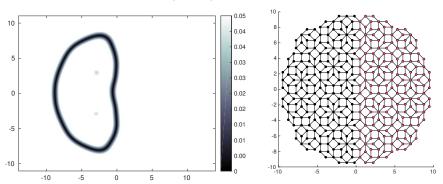
$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$



$$\kappa = 0.1, \ \lambda_3 = 0.4$$

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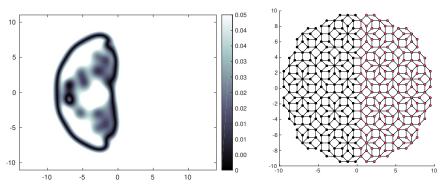
$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$



$$\kappa = 0.1, \ \lambda_3 = 0.6$$

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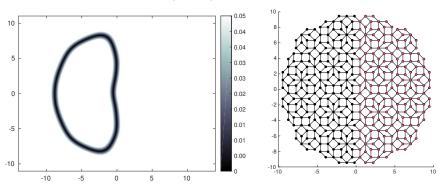
$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$



$$\kappa = 0.1, \ \lambda_3 = 0.8$$

We fix $\kappa=0.1$ and varying the energy setting λ_3 . All spectral data respects the symmetry $H\mapsto -H$, so we need only look at $\lambda_3\geq 0$. Plotting

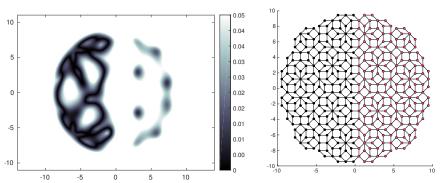
$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$



$$\kappa = 0.1, \ \lambda_3 = 1.0$$

We fix $\kappa=0.1$ and varying the energy setting λ_3 . All spectral data respects the symmetry $H\mapsto -H$, so we need only look at $\lambda_3\geq 0$. Plotting

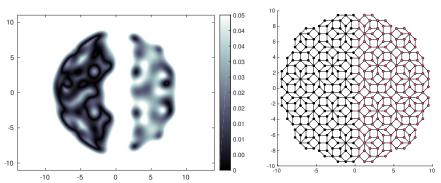
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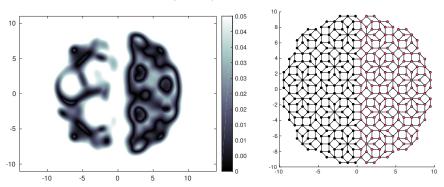
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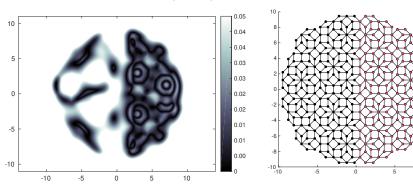
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with $\lambda_3 = 0$ as a function of (λ_1, λ_2) :

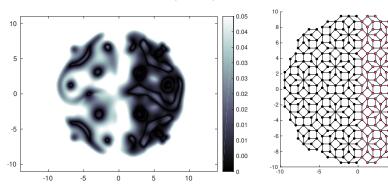


10

We fix $\kappa=0.1$ and varying the energy setting λ_3 . All spectral data respects the symmetry $H\mapsto -H$, so we need only look at $\lambda_3\geq 0$. Plotting

$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$

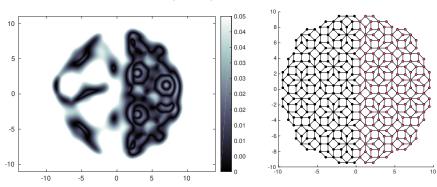
with $\lambda_3 = 0$ as a function of (λ_1, λ_2) :



10

We fix $\kappa=0.1$ and varying the energy setting λ_3 . All spectral data respects the symmetry $H\mapsto -H$, so we need only look at $\lambda_3\geq 0$. Plotting

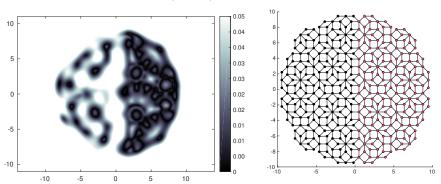
$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$



$$\kappa = 0.1, \lambda_3 = 2.2$$

We fix $\kappa=0.1$ and varying the energy setting λ_3 . All spectral data respects the symmetry $H\mapsto -H$, so we need only look at $\lambda_3\geq 0$. Plotting

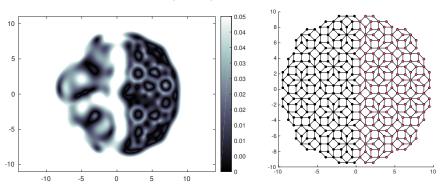
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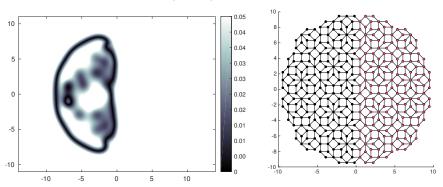
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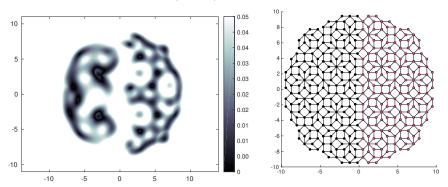
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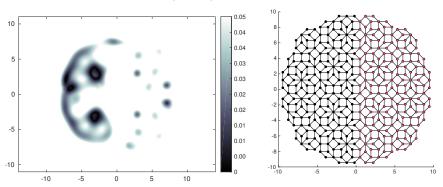
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$$\kappa = 0.1, \lambda_3 = 3.0$$

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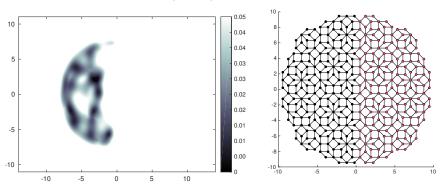
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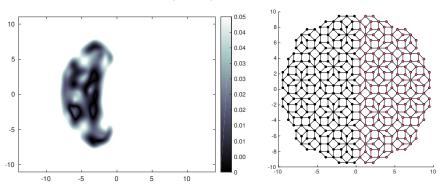
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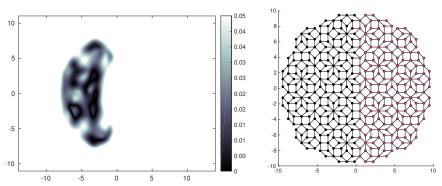
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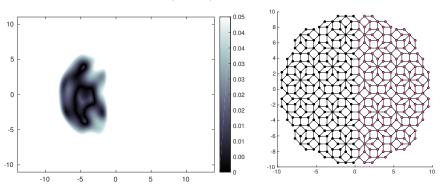
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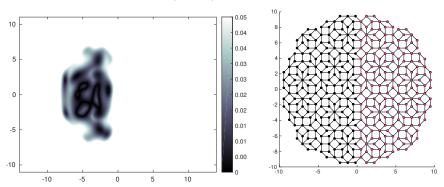
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$$\kappa = 0.1, \lambda_3 = 4.0$$

We fix $\kappa=0.1$ and varying the energy setting λ_3 . All spectral data respects the symmetry $H\mapsto -H$, so we need only look at $\lambda_3\geq 0$. Plotting

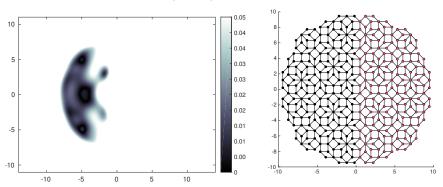
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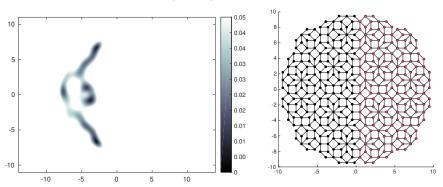
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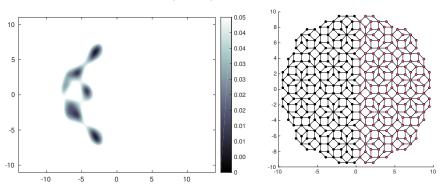
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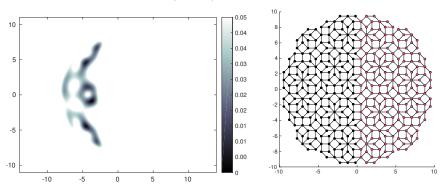
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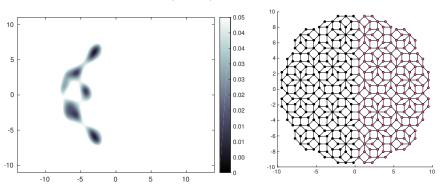
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$$\kappa = 0.1, \lambda_3 = 5.0$$

We fix $\kappa=0.1$ and varying the energy setting λ_3 . All spectral data respects the symmetry $H\mapsto -H$, so we need only look at $\lambda_3\geq 0$. Plotting

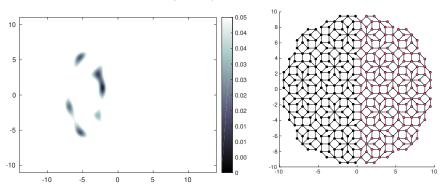
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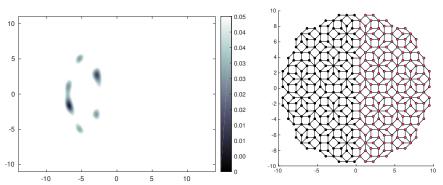
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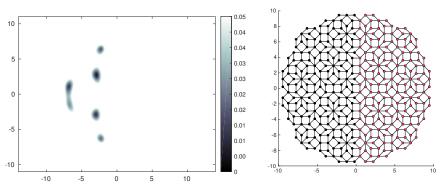
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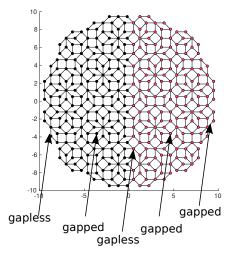


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$$\operatorname{gap}_{\lambda}(\kappa X, \kappa Y, H) = \|L_{\lambda}(\kappa X, \kappa Y, H)^{-1}\|^{-1}$$



$$\kappa = 0.1, \lambda_3 = 5.8$$



Left to right, we have, very approximately, localized spectrum as follows:

$$[-1.6, 1.6]$$

$$[-5.6, -0.8] \cup [0.8, 5.6]$$

$$[-2.8, 2.8]$$

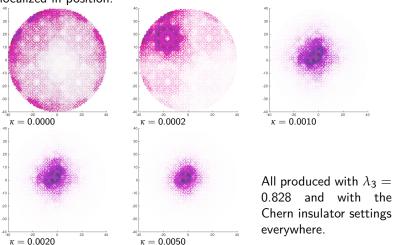
$$[-3.2, -1.2] \cup [1.2, 3.2]$$

$$[-3.2, -1.6] \cup [1.6, 3.2]$$

Larger samples will allow for smaller κ and better localization.

Approximate eigenvectors

When $\operatorname{gap}_{\lambda}(\kappa X,\kappa Y,H)\approx 0$, say with $\lambda_1=\lambda_2=0$, we obtain unit vector ψ with $H\psi\approx \lambda_3\psi$, $X\psi\approx 0$, $Y\psi\approx 0$. Bigger κ means more localized in position.



Approximate eigenvectors

We examine four of these, for deviation of ψ in the Hamiltonian H_{ρ} (radius ρ here is 40) and radial position $R_{\rho} = \sqrt{X^2 + Y^2}$.

κ	Deviation of ψ in H_{ρ}	Deviation of ψ in R_{ρ}
0.0002	0.0032	7.8981
0.0010	0.0032	4.1666
0.0020	0.0083	3.7527
0.0050	0.0227	3.001

Varying κ and using large ρ , we calculated approximate eigenvectors for various H_{ρ} that could be tapered to produce approximate eigenvectors for the infinite area Hamiltonian H_{QC} . The spectrum seems to be

$$[-6.227, -0.604] \cup [0.604, 6.227]$$

with error in Hausdorff distance less that 0.044. (A semi-rigorous result.)

K-theory

For the infinite system, Bellissard, van Elst, and Schulz-Baldes showed that the Chern number is the index of the Fredholm operator

$$\operatorname{ind}(H_{QC}, X, Y) = \operatorname{ind}\left(\Pi_{v}\left(\frac{X + iY}{|X + iY|}\right)\Pi_{v} + (I - \Pi_{v})\right)$$

where Π_{ν} is the spectral projector of H_{QC} for to the valence band.

There is an index for a finite system, which can be centered at any point.

$$\operatorname{ind}_{\lambda}(H_{\rho}, \kappa X, \kappa Y) = \frac{1}{2} \operatorname{Sig}(L_{\lambda}(H_{\rho}, \kappa X, \kappa Y))$$

where Sig(X) is the number of positive eigenvalues minus the number of negative eigenvalues.

Typically we take λ_3 in the center of the gap or at the Fermi level, so here $\lambda_3=0$. For a round or square sample that is built with consistent constants, best to use $\lambda_1=0$, $\lambda_2=0$.

K-theory

Theorem(L-Schulz-Baldes). If ρ is large enough, and κ is a certain range,

$$\frac{1}{2}\operatorname{Sig}\left(L_{\lambda}\left(H_{\rho},\kappa X,\kappa Y\right)\right)=\operatorname{ind}\left(\Pi_{\nu}\left(\frac{X+iY}{|X+iY|}\right)\Pi_{\nu}+(I-\Pi_{\nu})\right)$$

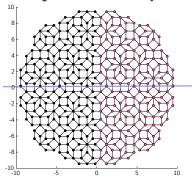
Our proof depends on the nice formula, in complex, ungraded case, for the boundary map $\partial_1: \mathcal{K}_1(\mathcal{Q}) \to \mathcal{K}_0(\mathbb{K})$

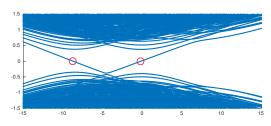
($\mathbb K$ the compact operators and $\mathcal Q$ the Caulkin algebra).

The usual picture starts with unitary u in B, lifts to $\|a\| \le 1$ in A and then $\partial_1\left([u]\right) = [p] - [1]$ where

$$\begin{split} p &= \left(\begin{array}{cc} a & -\sqrt{1-aa^*} \\ \sqrt{1-a^*a} & a^* \end{array} \right) \left(\begin{array}{cc} 1 & 0 \\ 0 & 0 \end{array} \right) \left(\begin{array}{cc} a & -\sqrt{1-aa^*} \\ \sqrt{1-a^*a} & a^* \end{array} \right)^* \\ &= \frac{1}{2} \left(\begin{array}{cc} 2aa^* - 1 & a2\sqrt{1-a^*a} \\ a^*2\sqrt{1-aa^*} & 1-2a^*a \end{array} \right) + \frac{1}{2} \left(\begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) \end{split}$$

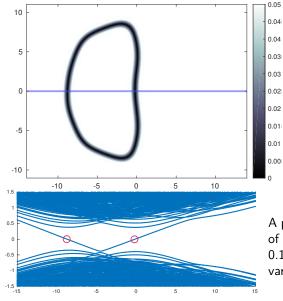
K-theory from the spectrum of the localizer





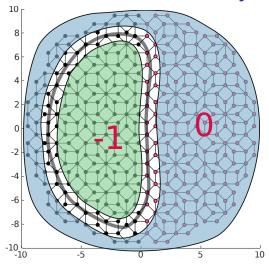
A portion of the spectrum of the localizer, with $\kappa=0.1,\ \lambda_2=\lambda_3=0$ and varying $\lambda_1.$

K-theory from the spectrum of the localizer



A portion of the spectrum of the localizer, with $\kappa=0.1,\ \lambda_2=\lambda_3=0$ and varying $\lambda_1.$

K-theory



The Clifford spectrum must appear between the regions of different K-theory.

The larger the gap of the localizer in those regions, the more robust the Clifford spectrum and approximate eigenvectors.

Now one position observable X and Hamiltonian H, say on $\ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$. Also finite systems using open boundary conditions (X_{ρ}, H_{ρ}) .

In class BDI have two symmetries, and M_{2n} becomes real and graded: $a\mapsto a^{\tau}$ giving the real structure and $a\mapsto a^{\sigma}$ the grading, so $a^{\tau}=a^*$ means real, $a^{\sigma}=a$ means even.

The localizer is, at (0,0),

$$L_{\mathbf{0}}(\kappa X, H) = \left(\begin{array}{cc} 0 & \kappa X - iH \\ \kappa X + iH & 0 \end{array} \right).$$

We note that $v = \kappa X - iH$ is invertible with symmetries

$$v^{\tau} = v^*$$
. $v^{\sigma} = v^*$.

If we set $u = v(v^*v)^{-\frac{1}{2}}$, we get a unitary with symmetries

$$u^{\tau} = u^*$$
. $u^{\sigma} = u^*$.

This defines directly a K_0 class in the Trout picture of K_0 .

To get an index from the infinite system, one can consider

$$W = PQP + (I - P)$$

where P is projection on the the space X>0 and Q is the spectral projection for H corresponding to $[0,\infty)$. If we take w as the image of 2W-I in the Caulkin algebra Q, then w will be unitary with symmetries

$$w^{\sigma} = -w, \ w^{\tau} = w^*.$$

This defines directly a K_1 class in the Van Daele picture of K_1 .

Claim: Using the Trout picture in even degrees and the Van Daele picture in odd degrees gives the easiest formulas for the boundary maps in K-theory of real, graded C^* -algebras.

First, a look at the complex, graded case...

K-theory for complex, graded C^* -algebras

This is a current project with Hermann Shulz-Baldes. Here $\sigma:A\to A$ is an order-2 *-automorphism.

	with unitaries	with invertibles	due to
$K_1(A,\sigma)$	$u^{\sigma} = -u, u^* = u, u^2 = 1$	$u^{\sigma}=-u, u^*=u$	Van Daele
$K_0(A, \sigma)$	$u^{\sigma}=u^*$	$u^{\sigma}=u^*$	Trout

From $0 \rightarrow I \rightarrow A \rightarrow B \rightarrow 0$ we get a *natural* six-term exact sequence

$$K_0(I) \longrightarrow K_0(A) \longrightarrow K_0(B)$$

$$\downarrow^{\partial_0} \qquad \qquad \downarrow^{\partial_0}$$
 $K_1(B) \longleftarrow K_1(A) \longleftarrow K_1(I)$

Theorem (Kubota). Given $u^{\sigma} = -u$, $u^* = u$, $u^2 = 1$ in B lift to $-1 \le a \le 1$ in A with $a^{\sigma} = -a$ and then

$$\partial_1([u]) = [-\exp(-\pi i a)]$$

This works only if $A \cong A_0 \hat{\otimes} \mathcal{C}\ell^2$, small modifications needed in general. Kubata also proved this in the real and graded case.

K-theory for complex, graded C^* -algebras

Theorem(L-Schulz-Baldes). Given $u^* = u^{-1} = u^{\tau}$ in B lift to $||a|| \le 1$ in A with $a^{\tau} = a^*$ and then

$$\partial_0\left(\left[u
ight]
ight) = \left[W\left(egin{array}{cc} 2aa^*-1 & a2\sqrt{1-a^*a} \ a^*2\sqrt{1-aa^*} & 1-2a^*a \end{array}
ight)W^*
ight]$$

where W is a scalar unitary chosen to give this the correct symmetry for the desired grading on $\mathbf{M}_2(\tilde{I})$.

In the real, graded case, one needs to replace $\mathbf{M}_2(A)$ with $A \hat{\otimes} \mathcal{C} \ell^{2,0}$.

Also, if $A\cong A_0\hat{\otimes}\mathcal{C}\ell^{1,1}$ is not true then one starts with u in $B\hat{\otimes}\mathcal{C}\ell^{1,1}$ and ends up in $\tilde{I}\hat{\otimes}\mathcal{C}\ell^{3,1}$, but always the formula uses $2aa^*-1$ and $a2\sqrt{1-a^*a}$.

In class BDI, the grading comes from a self-adjoint grading operator Γ , so $A^{\sigma} = \Gamma A \Gamma$. The class in $K_0(\boldsymbol{M}_{2n}(\mathbb{C}), \sigma, \tau)$ determined by

$$\kappa X - iH$$
.

Under the isomotphism $K_0(\mathbf{M}_{2n}(\mathbb{C}), \sigma, \tau) \cong \mathbb{Z}$ this works out to be

$$\frac{1}{2}\mathrm{Sig}\left(\kappa X\Gamma + H\right)$$

which was one of the formulas guessed in 2015.

Note: Both $\kappa X\Gamma + H$ and

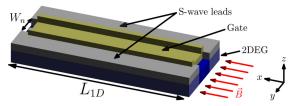
$$L_{\mathbf{0}}(\kappa X, H) = \begin{pmatrix} 0 & \kappa X - iH \\ \kappa X + iH & 0 \end{pmatrix}$$

are hermitian, and fiddling with singular value decomposition shows

$$\lambda \in \sigma(L_0(\kappa X, H)) \iff \pm \lambda \in \sigma(\kappa X \Gamma + H).$$

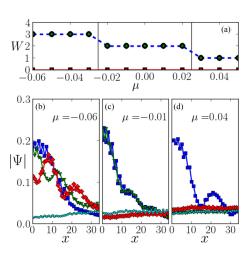
L. "K-theory and pseudospectra for topological insulators." Annals of Physics 356 (2015): 383-416.

Liu, Shabani, and Mitra were able to map a 2D system to a 1D, class BDI system in a study of Majorana Fermions.

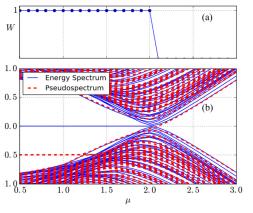


"A 2DEG with strong spin-orbit coupling is contacted with s-wave superconducting leads that have a phase difference ϕ and The top gate can be used an in-plane longitudinal magnetic field, \overrightarrow{B} . The top gate can be used to tune the chemical potential. Majorana edge modes appear at either end of the 1D normal channel." from Liu, Shabani, and Mitra (2018).

Liu, Shabani, and Mitra. "Long-range Kitaev chains via planar Josephson junctions." Physical Review B 97.23 (2018): 235114.



(top) "Comparison of the topological invariant computed via a winding number in 2D system (dashed line) and via the realspace invariant in the 1D model (circles) defined in Eq. (15)." (bottom) "The amplitude of four positive energy modes closest to zero [...] in the three topological phases shown." "The amplitudes are averaged over disorder realizations [...] that there are as many edge modes as the invariant predicts." from Liu, Shabani, and Mitra (2018).



Again from Liu, Shabani, and Mitra (2018).

On the bottom is a plot of the spectrum of H (blue dots) and the spectrum of $\kappa X\Gamma + H$ red squares as a parameter μ moves the system from an topological insulator ($\mu < 2$) to an ordinary insulator.

On top is a plot of the finite index $\frac{1}{2}$ Sig $(\kappa X\Gamma + H)$.

The Localizer

- Defined in any dimension, any Atland Zirnbauer symmetry class
- ② Defines the Clifford (pseudo)spectrum emergent topology from tuples of hermitian matrices
- Enables numerical algorithm to find spectrum of infinite area, quasiperiodic Hamiltonians.
- **1** Defines a local K-theory index use $\kappa = C$
- **1** Defines a global *K*-theory index use $\kappa = \frac{C}{\text{system radius}}$
- Gradually the indices are getting proven correct
- Not clear how to modify localizer for interacting fermions