

Mathematics of magic angles

Maxwell Institute Mini-symposium in Analysis and PDE

Maciej Zworski

March 31, 2023







A project in the time of covid-19

2020: Simon Becker, Mark Embree, Jens Wittsten, MZ: **BEWZ**

2022: Simon Becker, Tristan Humbert, MZ: **BHZ**

2023: Michael Hitrik, MZ: **HZ**, Simon Becker MZ: **BZ**

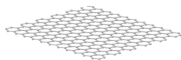


Motivation: bilayer graphene

graphite



graphene

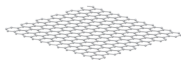


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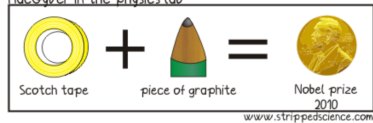
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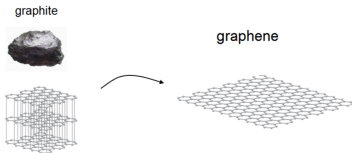
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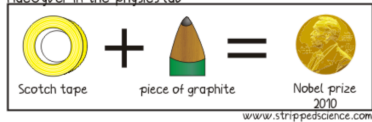
MacGyver in the physics lab



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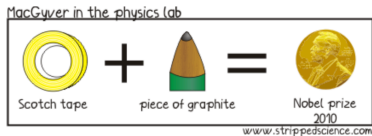
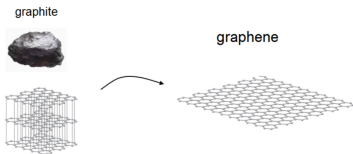


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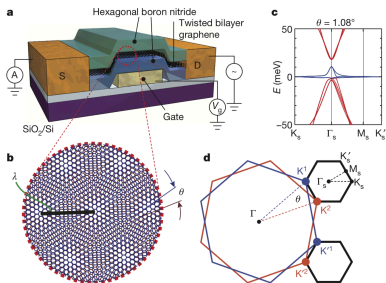


Geim–Novoselov '04

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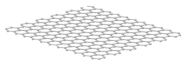
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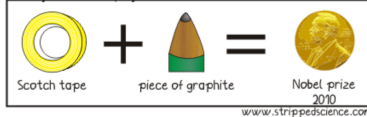
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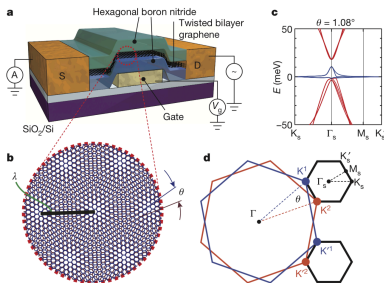
graphene



MacGyver in the physics lab



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Predicted by Bistritzer–MacDonald '11

The chiral model of TBG

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PHYSICAL REVIEW LETTERS **122**, 106405 (2019)

Editors' Suggestion

Origin of Magic Angles in Twisted Bilayer Graphene

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$$U(z) := \sum_{k=0}^2 \omega^k e^{\frac{1}{2}(z\bar{\omega}^k - \bar{z}\omega^k)}, \quad \omega := e^{2\pi i/3}.$$

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Derived from the full **Bistritzer–MacDonald** '11 Hamiltonian

The operator of today

$$D(\alpha) = \begin{pmatrix} 2D_{\bar{z}} & \alpha U(z) \\ \alpha U(-z) & 2D_{\bar{z}} \end{pmatrix} \text{ on } \mathbb{C}/\Gamma, \quad D_{\bar{z}} = \frac{1}{2i}(\partial_{x_1} + i\partial_{x_2})$$

$$U(z + \gamma) = U(z), \quad \gamma \in \Gamma, \text{ a (very specific) lattice}$$

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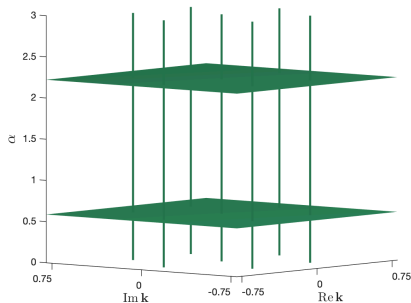
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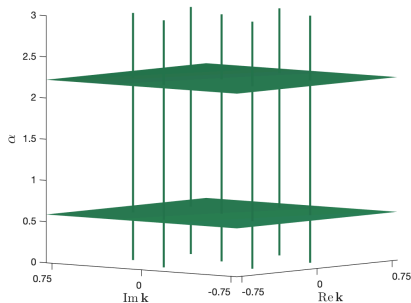
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Seeley 85: $P(\alpha) = e^{ix} D_x + \alpha e^{ix}$, $x \in \mathbb{S}^1$, $\text{Spec}(P(\alpha)) = \mathbb{C}$, $\alpha \in \mathbb{Z}$.

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Bands: eigenvalues of $H_{\mathbf{k}}(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* - \bar{\mathbf{k}} \\ D(\alpha) - \mathbf{k} & 0 \end{pmatrix}$, $\mathbf{k} \in \mathbb{C}/\Gamma^*$

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A flat band at 0 energy means that $\text{Spec}_{L^2(\mathbb{C}/\Gamma)}(D(\alpha)) = \mathbb{C}$

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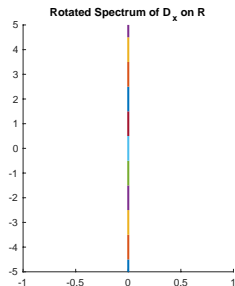
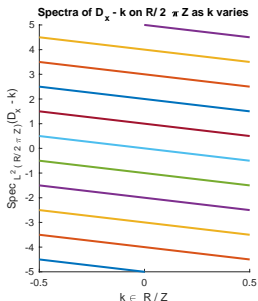
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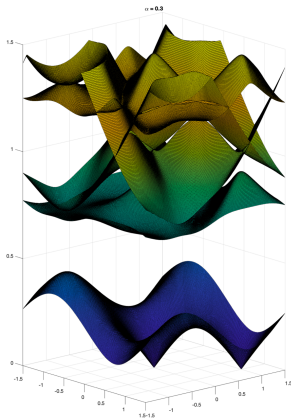
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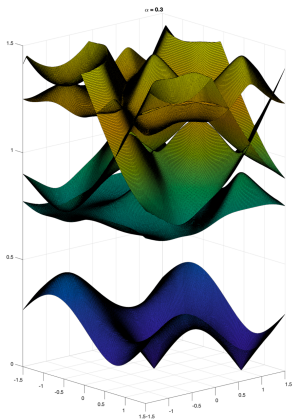
Flat bands

The bands are eigenvalues of $H_k(\alpha)$ on $L_0^2(\mathbb{C}/\Gamma)$, $k \in \mathbb{C}/3\Gamma^*$:



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Theorem (BHZ '22; implicit in BEWZ '20)

$$\exists k \notin 3\Gamma^* + \{0, -i\} \quad E_1(\alpha, k) = 0 \implies \forall k \quad E_1(\alpha, k) = 0.$$

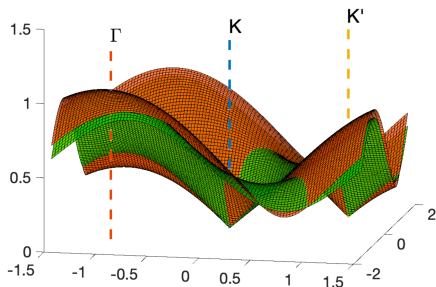
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$$k \mapsto \tilde{E}_1(\alpha, k) / (\max_k \tilde{E}_1(\alpha, k)), \quad 0.4 < \alpha < 0.6$$

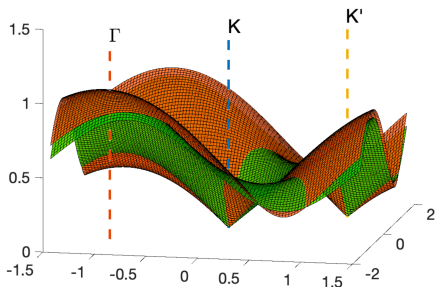
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Rescaled plots remain almost fixed at $k \mapsto |U(-4\sqrt{3}\pi ik/9)|$

Symmetries play a crucial role!

$$D(\alpha) = \begin{pmatrix} 2D_{\bar{z}} & \alpha U(z) \\ \alpha U(-z) & 2D_{\bar{z}} \end{pmatrix}, \quad H(\alpha) = \begin{pmatrix} 0 & D^* \\ D & 0 \end{pmatrix}$$

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$$\mathcal{L}_a u = \text{diag}(\omega^{a_1+a_2}, 1, \omega^{a_1+a_2}, 1) u(z + \frac{4}{3}i\pi(\omega a_1 + \omega^2 a_2)), \quad a \in \mathbb{Z}_3^2,$$

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Decompose into irreducible representations of this **Heisenberg** group:

$$L^2(\mathbb{C}/\Gamma) = \bigoplus_{k,p \in \mathbb{Z}_3} L^2_{\rho_{k,p}}(\mathbb{C}/\Gamma; \mathbb{C}^2) \oplus L^2_{\rho_{(1,0)}}(\mathbb{C}/\Gamma; \mathbb{C}^2) \oplus L^2_{\rho_{(2,0)}}(\mathbb{C}/\Gamma; \mathbb{C}^2)$$

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$$\mathcal{C}^k u(z) = \text{diag}(1, 1, \bar{\omega}^k, \bar{\omega}^k) u(\omega^k z), \quad k \in \mathbb{Z}_3$$

$$\mathcal{L}_a H = H \mathcal{L}_a, \quad \mathcal{C} H = H \mathcal{C}, \quad \mathcal{C} \mathcal{L}_a = \mathcal{L}_{M_a} \mathcal{C}, \quad M = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}.$$

Decompose into irreducible representations of this **Heisenberg** group:

$$L^2(\mathbb{C}/\Gamma) = \bigoplus_{k,p \in \mathbb{Z}_3} L^2_{\rho_{k,p}}(\mathbb{C}/\Gamma; \mathbb{C}^2) \oplus L^2_{\rho_{(1,0)}}(\mathbb{C}/\Gamma; \mathbb{C}^2) \oplus L^2_{\rho_{(2,0)}}(\mathbb{C}/\Gamma; \mathbb{C}^2)$$

$$\rho_{k,p} \longleftrightarrow \mathcal{L}_a \equiv \omega^{k(a_1+a_2)}, \quad \mathcal{C} \equiv \bar{\omega}^p$$

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This implies that the spectrum of $H(\alpha)|_{L^2_{\rho_{k,\ell}}(\mathbb{C}/\Gamma)}$ is **even**

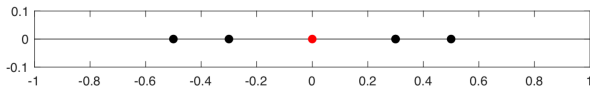
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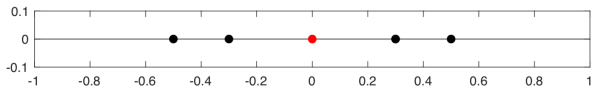
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Spectral characterization of flat bands

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$$H_k(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* - \bar{k} \\ D(\alpha) - k & 0 \end{pmatrix} : H_0^1(\mathbb{C}/\Gamma) \rightarrow L_0^2(\mathbb{C}/\Gamma),$$

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Bands: $\{E_j(\alpha, k)\}_{j \in \mathbb{Z} \setminus \{0\}} = \text{Spec}_{L_0^2} H_k(\alpha), \quad E_{\pm 1}(\alpha, 0) = E_{\pm 1}(\alpha, -i) = 0.$

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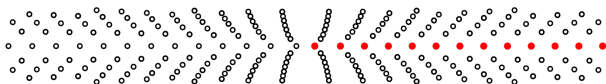
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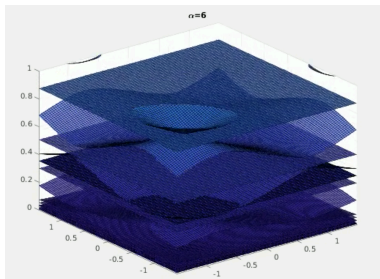
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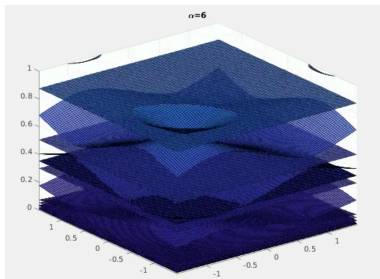


Exponential squeezing of bands

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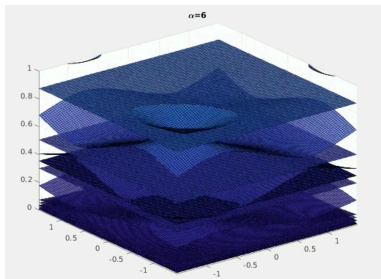
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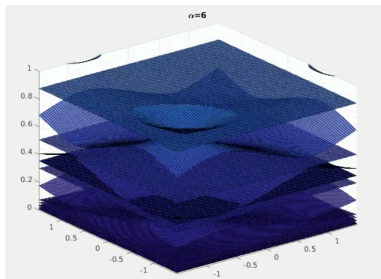


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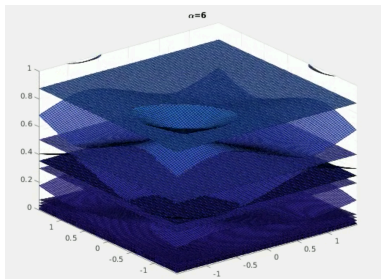
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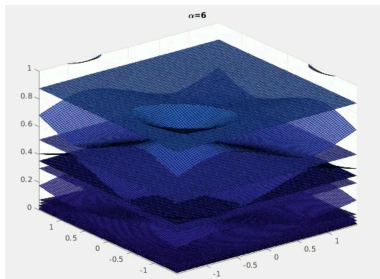
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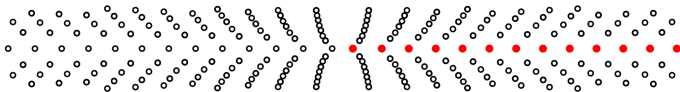
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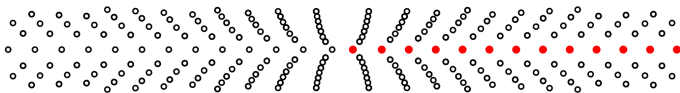
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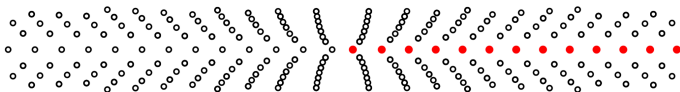
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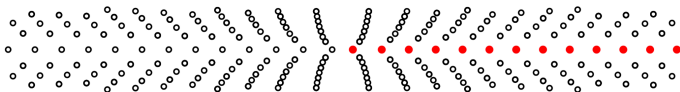


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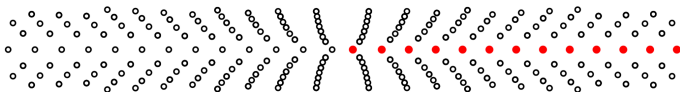


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Luskin-Watson '21: $|\mathcal{A} \cap (0.583, 0.589)| \geq 1$

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Theorem (BHZ '22) The largest real eigenvalue of T_k , $1/\alpha_*$, is *simple* and $\alpha_* \in (0.583, 0.589)$.

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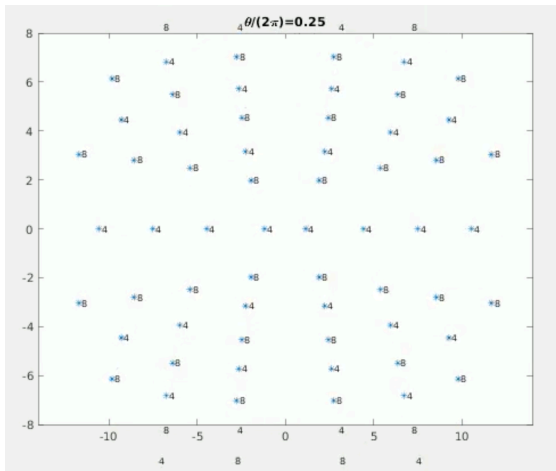
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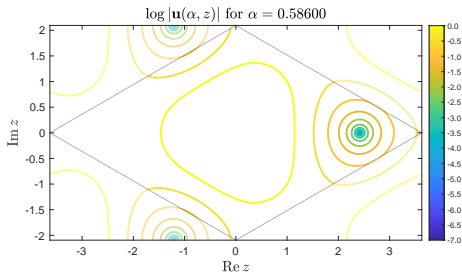
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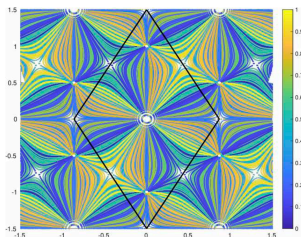
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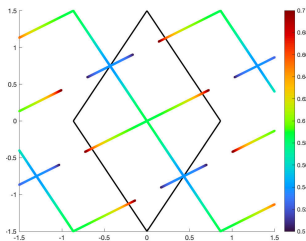
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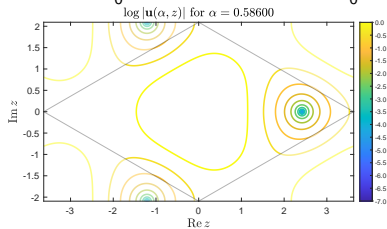
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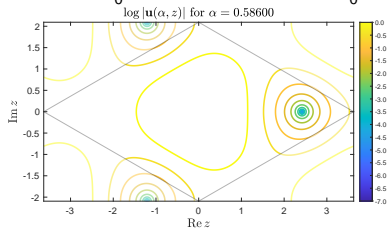
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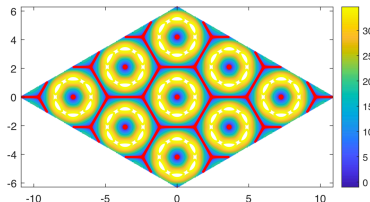


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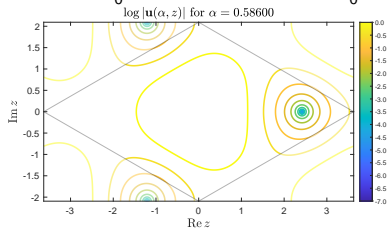


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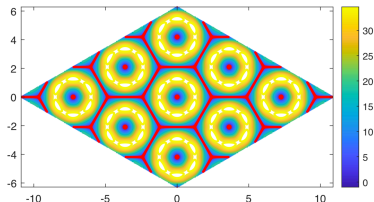


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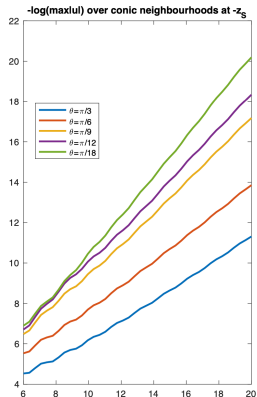
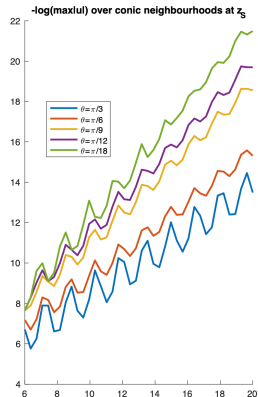
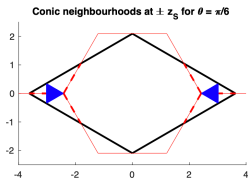


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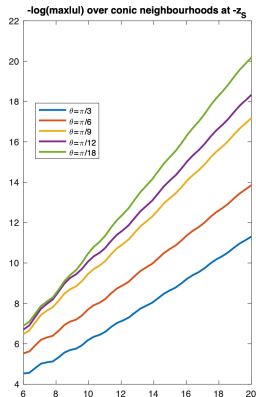
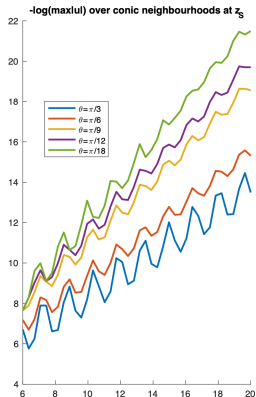
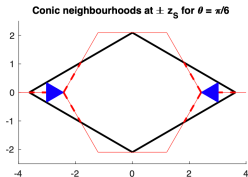
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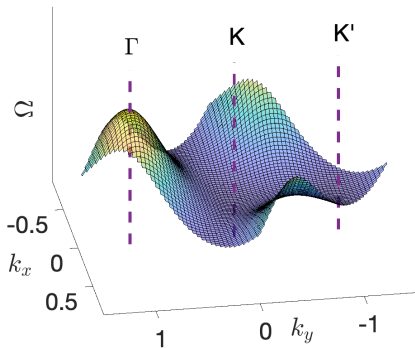
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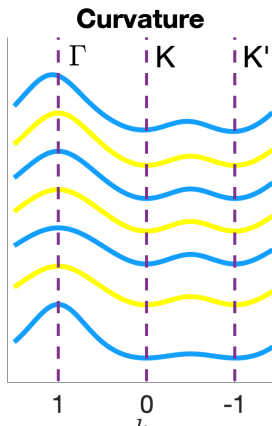
Another numerical observation (BHZ): **Curvature**

$\mathbb{C}/3\Gamma^* \ni k \rightarrow u_k \in L_0^2(\mathbb{C}/\Gamma)$ s holomorphic (Ledwith et al '21) and defines a natural line bundle

Chern connection: $\eta := \partial_k \log \|u_k\|^2 = \|u_k\|^{-2} \langle \partial_k u_k, u_k \rangle dk$

Curvature: $\Omega = d\eta = \bar{\partial}_k \partial_k \log \|u_k\|^2 = H(k) d\bar{k} \wedge dk, \quad H(k) \geq 0.$

Chern class: $c_1 = \frac{i}{2\pi} \int_{\mathbb{C}/3\Gamma^*} \Omega = -1$

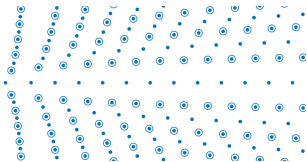


Many mathematical open problems

- ▶ Multiplicity issues; a stronger generic simplicity statement

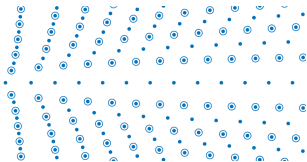
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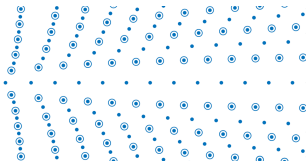
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- ▶ The fixed “shape” of the first band; what is a heuristic explanation?

Many mathematical open problems

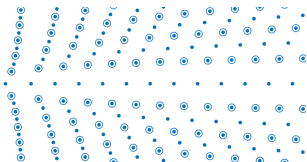
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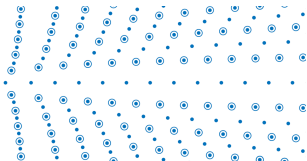
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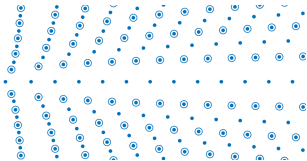
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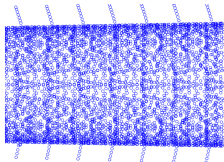
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Thanks for your attention!