

# Mathematics of magic angles

## CERMICS Colloquium

Maciej Zworski

April 19, 2023





A project in the time of covid-19

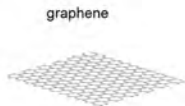
2020: Simon Becker, Mark Embree, Jens Wittsten, MZ: **BEWZ**

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

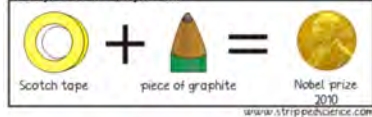
2023: Michael Hitrik, MZ: **HZ**, Simon Becker MZ: **BZ**



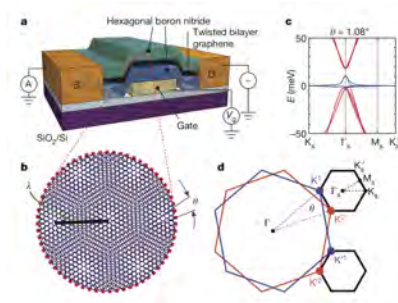
## Motivation: bilayer graphene



MacGyver in the physics lab



## Geim–Novoselov '04



Cao et al '18, Yankovitz et al '18: superconductivity at  $\theta \simeq 1.08^\circ$

Predicted by Bistritzer–MacDonald '11

## Origin of Magic Angles in Twisted Bilayer Graphene

Grigory Tarnopolsky, Alex Jura Kruchkov, and Ashvin Vishwanath  
*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*

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

$$z = x_1 + ix_2, \quad D_{\bar{z}} := \frac{1}{2i}(\partial_{x_1} + i\partial_{x_2})$$

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

$$U(z + \frac{4}{3}\pi i\omega^\ell) = \bar{\omega} U(z), \quad U(\omega z) = \omega U(z), \quad \ell = 1, 2.$$

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

Mathematical derivation:

**Cancès–Garrigue–Gontier, Watson–Kong–MacDonald–Luskin** '22

## The operator of today

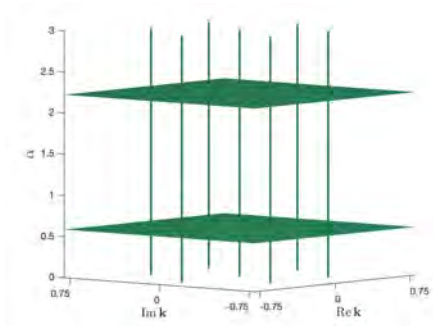
$$D(\alpha) = \begin{pmatrix} 2D_{\bar{z}} & \alpha U(z) \\ \alpha U(-z) & 2D_{\bar{z}} \end{pmatrix} \text{ on } \mathbb{C}/\Gamma, \quad D_{\bar{z}} = \frac{1}{2i}(\partial_{x_1} + i\partial_{x_2})$$

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

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

# The operator of today

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

Editors' Suggestion

## Origin of Magic Angles in Twisted Bilayer Graphene

Grigory Tarnopolsky, Alex Jura Kruchkov,<sup>\*</sup> and Ashvin Vishwanath  
*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*

Twisted bilayer graphene (TBG) was recently shown to host superconductivity when tuned to special “magic angles” at which isolated and relatively flat bands appear. However, until now the origin of the magic angles and their irregular pattern have remained a mystery. Here we report on a fundamental continuum model for TBG which features not just the vanishing of the Fermi velocity, but also the perfect flattening of the entire lowest band. When parametrized in terms of  $\alpha \sim 1/\theta$ , the magic angles recur with a remarkable periodicity of  $\Delta\alpha \approx 3/2$ . We show analytically that the exactly flat band wave functions can be constructed from the doubly periodic functions composed of ratios of theta functions—reminiscent of quantum Hall wave functions on the torus. We further report on the unusual robustness of the experimentally relevant first magic angle, address its properties analytically, and discuss how lattice relaxation effects help justify our model parameters.

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

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

A simpler example first:  $D_x := \frac{1}{i} \partial_x$

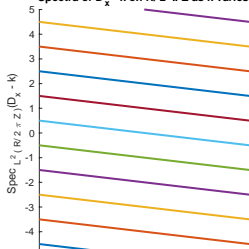
$$\text{Spec}_{L^2(\mathbb{R})}(D_x) = \mathbb{R}, \quad \text{Spec}_{L^2(\mathbb{R}/2\pi\mathbb{Z})}(D_x) = \mathbb{Z}$$

$$L^2(\mathbb{R}) \simeq L^2(\mathbb{R}/\mathbb{Z}; L^2(\mathbb{R}/2\pi\mathbb{Z})), \quad D_x|_{L^2(\mathbb{R})} \simeq \bigoplus_{k \in \mathbb{R}/\mathbb{Z}} (D_x - k)|_{L^2(\mathbb{R}/2\pi\mathbb{Z})}$$

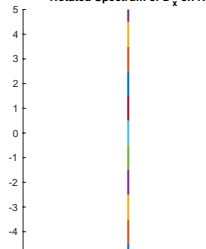
$$u(x) \mapsto U(x, k) := \sum_{m \in \mathbb{Z}} e^{-2\pi i(x-m)k} u(x-m), \quad D_x u \mapsto (D_x - k)U$$

$$\text{Spec}_{L^2(\mathbb{R})}(D_x) = \bigcup_{k \in \mathbb{R}/\mathbb{Z}} \text{Spec}_{L^2(\mathbb{R}/2\pi\mathbb{Z})}(D_x - k)$$

Spectra of  $D_x - k$  on  $\mathbb{R}/2\pi\mathbb{Z}$  as  $k$  varies

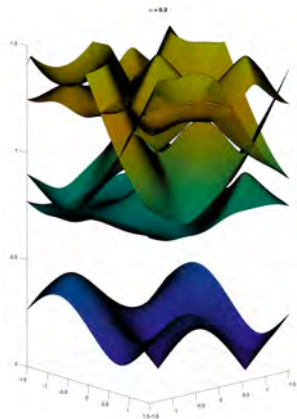


Rotated Spectrum of  $D_x$  on  $\mathbb{R}$



## Flat bands

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

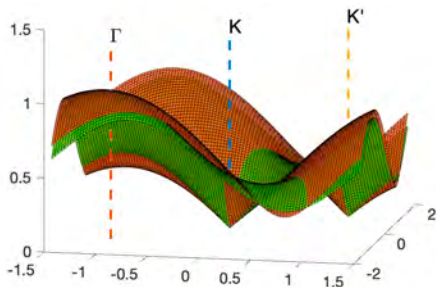


Theorem (BHZ '22; implicit in BEWZ '20)

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

## A curious structure of the first band

$$k \mapsto E_1(\alpha, k) / (\max_k E_1(\alpha, k)), \quad 0.4 < \alpha < 0.6$$



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

## Symmetries play a crucial role!

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

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

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

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

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

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

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

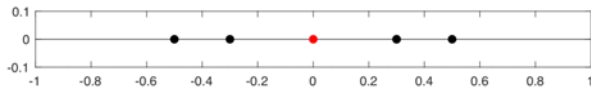
## Symmetry protected states

$$\ker_{L^2(\mathbb{C}/\Gamma)} H(0) = \mathbb{C}^4, \quad \Gamma = 4i\pi(\omega a_1 + \omega^2 a_2)$$

$$e_1 \in L^2_{\rho_{1,0}}, \quad e_2 \in L^2_{\rho_{0,0}}, \quad e_3 \in L^2_{\rho_{1,1}}, \quad e_4 \in L^2_{\rho_{0,1}}.$$

$$H(\alpha) = -\mathcal{W} H(\alpha) \mathcal{W}^*, \quad \mathcal{W} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \mathcal{W} \mathcal{C} = \mathcal{C} \mathcal{W}, \quad \mathcal{L}_a \mathcal{W} = \mathcal{W} \mathcal{L}_a$$

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



$$\dim \ker_{L^2(\mathbb{C}/\Gamma)}(H(\alpha)) \geq 4, \quad \dim \ker_{L^2(\mathbb{C}/\Gamma)}(D(\alpha)) \geq 2$$

## Spectral characterization of flat bands

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

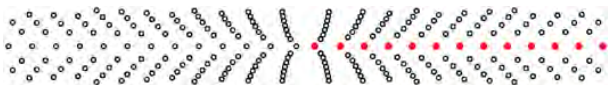
$$L_0^2(\mathbb{C}/\Gamma) := \{u \in L^2(\mathbb{C}/\Gamma) : \mathcal{L}_a u = u, \quad a \in \frac{1}{3}\Gamma/\Gamma\}.$$

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

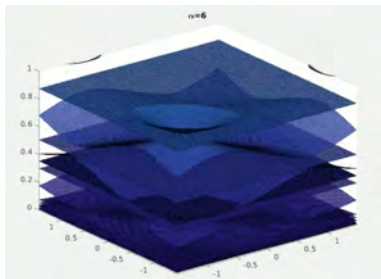
**Flat band at 0**  $\iff \text{Spec}_{L_0^2(\mathbb{C}/\Gamma)}(D(\alpha)) = \mathbb{C}$

**Theorem (BEWZ '20)** *There exists a discrete set  $\mathcal{A} \subset \mathbb{C}$  such that*

$$\text{Spec}_{L_0^2(\mathbb{C}/\Gamma)} D(\alpha) = \begin{cases} 3\Gamma^* + \{0, -i\} & \alpha \notin \mathcal{A} \\ \mathbb{C} & \alpha \in \mathcal{A}, \end{cases}$$



## Exponential squeezing of bands



**Theorem.** (BEWZ '20) *There exist  $c_j > 0$  such that for all  $k \in \mathbb{C}$ ,*

$$|E_j(\alpha, k)| \leq c_0 e^{-c_1 \alpha}, \quad j \leq c_2 \alpha, \quad \alpha > 0.$$

In practice,  $c_1 = 1$  and  $c_2$  can be taken arbitrarily large

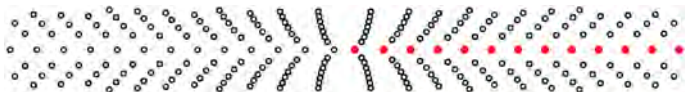
Consequence of general results about **quasimodes** for semiclassical ( $h = 1/\alpha$ ) non-normal operators:

Hörmander '69 ( $\{q, \bar{q}\} \neq 0$ ), Sato–Kawai–Kashiwara '73 ...

Dencker–Sjöstrand–Z '04

$$\text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \begin{cases} \Gamma^* & \alpha \notin \mathcal{A} \\ \mathbb{C} & \alpha \in \mathcal{A}, \end{cases}$$

**flat band** at  $\alpha \iff \text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \mathbb{C} \iff 1/\alpha \in \text{Spec}(T_k)$



We did **not** prove that  $\mathcal{A} \cap \mathbb{R}_+ \neq \emptyset$ . However,  $\mathcal{A} \neq \emptyset$  **BEWZ** '21:

$$\sum_{\alpha \in \mathcal{A}} \alpha^{-4} = \text{tr } T_k^4 = \frac{72\pi}{\sqrt{3}}, \quad \text{combinatorics} + \wp \text{ function}$$

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

$$\text{Spec}_{L^2(\mathbb{C}/\Gamma)} D(\alpha) = \begin{cases} \Gamma^* & \alpha \notin \mathcal{A} \\ \mathbb{C} & \alpha \in \mathcal{A}, \end{cases}$$

**Theorem (BHZ '22)** For all  $p > 1$

$$\sum_{\alpha \in \mathcal{A}} \alpha^{-2p} \in \frac{\pi}{\sqrt{3}} \mathbb{Q} \quad \text{and as a consequence } |\mathcal{A}| = \infty.$$

$$\sigma_p := \frac{1}{18} \text{tr } T_k^{2p}, \quad F_k(\alpha) := \det_2(I - \alpha^2 T_k^2)$$

$p$	$\sqrt{3}\sigma_p/3^p\pi$
2	4/9
3	32/63
4	40/81

$p$	$\sqrt{3}\sigma_p/3^p\pi$
5	9560/20007
6	245120/527877
7	1957475168/4337177481

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

Spectral characterization allows accurate computation of more  $\alpha$ 's:

$k$	$\alpha_k$	$\alpha_k - \alpha_{k-1}$
1	0.58566355838955	
2	2.2211821738201	1.6355
3	3.7514055099052	1.5302
4	5.276497782985	1.5251
5	6.79478505720	1.5183
6	8.3129991933	1.5182
7	9.829066969	1.5161
8	11.34534068	1.5163
9	12.8606086	1.5153
10	14.376072	1.5155
11	15.89096	1.5149
12	17.4060	1.5150
13	18.920	1.5147

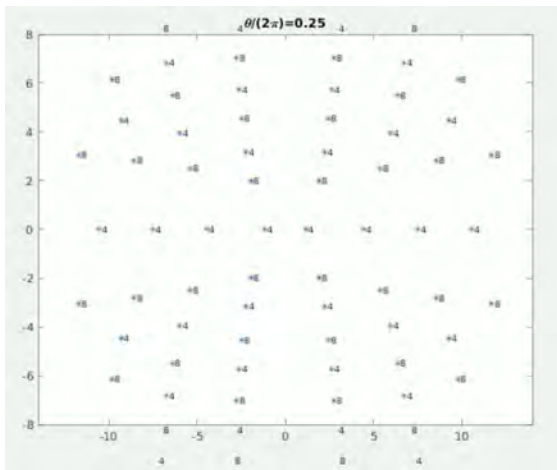
Tarnopolsky et al '19 observed that  $\alpha_k - \alpha_{k-1} \simeq \frac{3}{2}$  ( $0 < k \leq 8$ )

Ren-Gao-MacDonald-Niu '20 "exact" WKB:

$$\alpha_k - \alpha_{k-1} \simeq 1.47 \quad ???$$

Works for general potentials with  $\mathbb{Z}_3^2 \times \mathbb{Z}_3$  symmetries

$$U_\theta(z) := \sum_{k=0}^2 \omega^k (\cos^2 \theta e^{\frac{1}{2}(\bar{z}\omega^k - z\bar{\omega}^k)} + \sin^2 \theta e^{\bar{z}\omega^k - z\bar{\omega}^k})$$



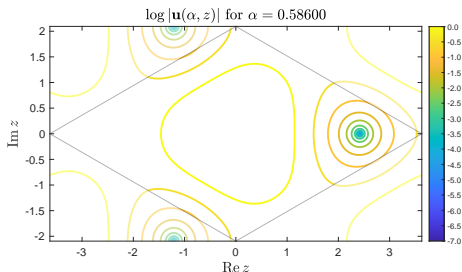
## Flat bands from theta functions

Tarnopolsky et al '19: consider  $u \in L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma; \mathbb{C}^2)$ ,  $D(\alpha)u = 0$

$$u_k(z) := e^{\frac{i}{2}(z\bar{k} + \bar{z}k)} f_k(z) u(z), \quad z \mapsto e^{\frac{i}{2}(z\bar{k} + \bar{z}k)} f_k(z) \text{ periodic}, \quad \partial_{\bar{z}} f_k = 0$$
$$(D(\alpha) - k)u_k(z) = 0$$

**Problem:**  $f_k$  with these properties will have poles

**Solution:** Look for  $\alpha$ 's at which  $u$  has a zero!



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**Problem:**  $f_k$  with these properties will have poles

**Solution:** Look for  $\alpha$ 's at which  $u$  has a zero!

$$u(\alpha, z_S) = 0, \quad \alpha \in \mathcal{A}, \quad z_S = \frac{4\sqrt{3}}{9}\pi, \quad z_S \equiv \omega z_S \pmod{\Gamma/3}$$

$$e^{\frac{i}{2}(z\bar{k} + \bar{z}k)} f_k(z) = e^{2\pi(\zeta - \bar{\zeta})k/\sqrt{3}} \frac{\theta_1(\zeta + k|\omega)}{\theta_1(\zeta|\omega)}, \quad z = \frac{4}{3}\pi i \omega \zeta$$

Similar argument in Dubrovin–Novikov '80

**Theorem** (BHZ '22)  $\alpha \in \mathcal{A}$  simple  $\Rightarrow z_S$  is the only zero of  $u$ .

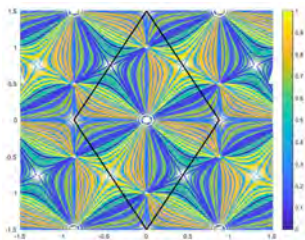
## New direction: in-plane magnetic field

Kwan et al '20, Qin–MacDonald '21:

$$D_B(\alpha) := D(\alpha) + \mathcal{B}, \quad \mathcal{B} := \begin{pmatrix} B & 0 \\ 0 & -B \end{pmatrix}, \quad B = B_0 e^{2\pi i \theta}.$$

How do the **Dirac points** move as  $\alpha$  and  $\theta$  change?

**Theorem (BZ '23)** *If  $\underline{\alpha} \in \mathcal{A}$  is simple (+ one more condition) and  $0 < B \ll 1$  then there are no flat bands and for  $\alpha \sim \underline{\alpha}$  Dirac points (eigenvalues of  $D_B(\alpha)$ ) are close to the  $\Gamma$  point.*



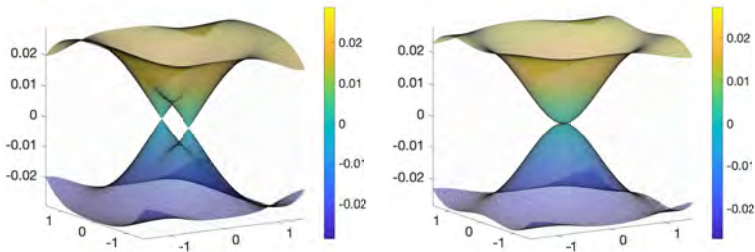
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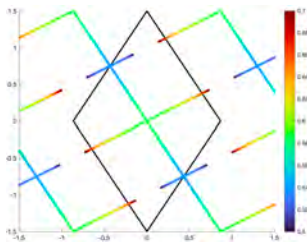
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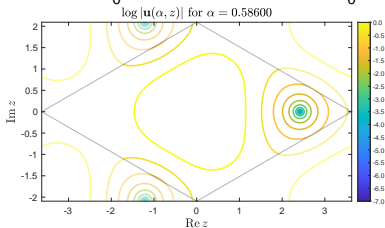
**Theorem (BZ '23)** If  $\underline{\alpha} \in \mathcal{A} \cap \mathbb{R}$  is simple and  $0 < B_0 \ll 1$  then

$$\mathcal{R}_\ell \setminus \bigcup_{k \neq K, K} D(k, \epsilon) \subset \bigcup_{\underline{\alpha} - \delta < \alpha < \underline{\alpha} + \delta} \text{Spec}_{L^2_0}(D_{\omega^\ell B}(\alpha)) \subset \mathcal{R}_\ell,$$

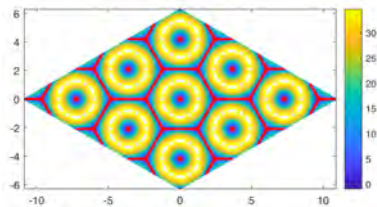
$$\mathcal{R}_\ell := \omega^\ell(2\pi(i\mathbb{R} + \mathbb{Z}) \cup \frac{2\pi}{\sqrt{3}}(\mathbb{R} + i\mathbb{Z})) \quad \ell = 1 \text{ in the figure}$$



Fine structure of  $u \in \ker_{H_0^1} D(\alpha)$  ( $\dim \ker_{H_0^1} D(\alpha) = 1$ ,  $\alpha \notin \mathcal{A}$ )



Contour plots of  $z \mapsto \log |u(\alpha, z)|$



A contour plot of  $|\{q, \bar{q}\}|$ ,  $q = (2\bar{\zeta})^2 - U(z)U(-z)$

Numerically,  $|u(\alpha, z)| \leq e^{-c_0\alpha}$  near the set where  $|\{q, \bar{q}\}| = 0$  !



**Theorem (HZ '22)** Any point on the *open* edges of the hexagon has an open neighbourhood  $\Omega \subset \mathbb{R}^2$  such that

$$|u(\alpha, z)| \leq e^{-c_\Omega/h}, \quad z \in \Omega, \quad c_\Omega > 0, \quad h = \alpha^{-1}$$

Reduction to the *principally scalar* case:  $q = (2\bar{\zeta})^2 - U(z)U(-z)$ :

$$\begin{pmatrix} 2hD_{\bar{z}} & U(z) \\ \alpha U(-z) & 2hD_{\bar{z}} \end{pmatrix} u = 0 \implies ((2hD_{\bar{z}})^2 - U(z)U(-z) + hR)u = 0$$

This allows an adaptation of (to some, v esoteric) hypoellipticity methods of **Kashiwara**, **Sjöstrand**, **Trepreau**, **Himonas**... (the 80's):

$$\{q, \bar{q}\}|_{\pi^{-1}(z_0) \cap q^{-1}(0)} = 0, \quad \{q, \{q, \bar{q}\}\}|_{\pi^{-1}(z_0) \cap q^{-1}(0)} \neq 0$$

implies the conclusion of the theorem for  $\Omega = \text{neigh}_{\mathbb{C}}(z_0)$ .

At the corners, it is trickier and does not fit into existing theories. Near the center of the hexagon  $q$  is not of principal type.

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

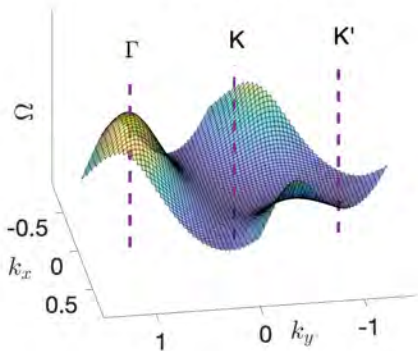
$\mathbb{C}/3\Gamma^* \ni k \rightarrow u_k \in L_0^2(\mathbb{C}/\Gamma)$  s holomorphic (Ledwith et al '21) and defines a natural line bundle

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

### Curvature



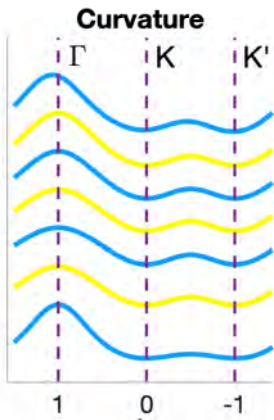
Another numerical observation (BHZ): **Curvature**

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

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

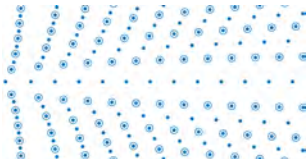
Curvature:  $\Omega = d\eta = \bar{\partial}_k \partial_k \log \|u_k\|^2 = H(k) d\bar{k} \wedge dk, \quad H(k) \geq 0.$

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

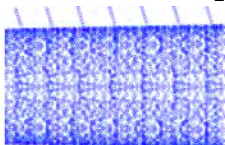


## Many mathematical open problems

- ▶ Multiplicity issues; a stronger generic simplicity statement



- ▶ The fixed “shape” of the first band; what is a heuristic explanation?
- ▶ Significance and explanation of the curvature “peak” at  $k = i$
- ▶ Asymptotics of  $\alpha \in \mathcal{A} \cap \mathbb{R}_+$ ; in particular  $\Delta\alpha \simeq \frac{3}{2}$ ? Help from **Hitrik–Sjöstrand** '04... '?



Thanks for your attention!