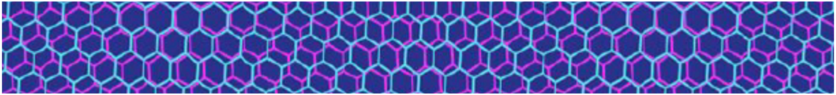
Mathematics of magic angles

CERMICS Colloquium

Maciej Zworski

April 19, 2023

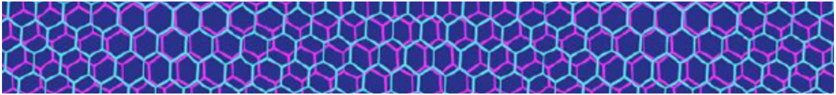


A project in the time of covid-19

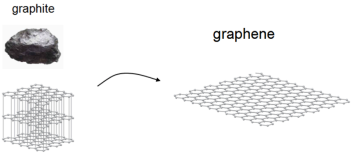
2020: Simon Becker, Mark Embree, Jens Wittsten, MZ: **BEWZ**

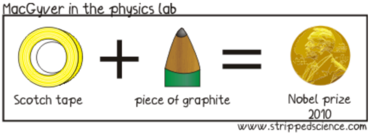
2022: Simon Becker, Tristan Humbert, MZ: **BHZ**

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

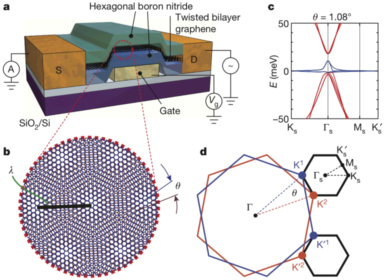


Motivation: bilayer graphene





Geim–Novoselov '04



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

Predicted by Bistritzer–MacDonald '11

The chiral model of TBG

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

Editors' Suggestion

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

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

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

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

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

Derived from the full Bistritzer–MacDonald '11 Hamiltonian

Mathematical derivation:
Cancès–Garrigue–Gontier, Watson–Kong–MacDonald–Luskin '22

The operator of today

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

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

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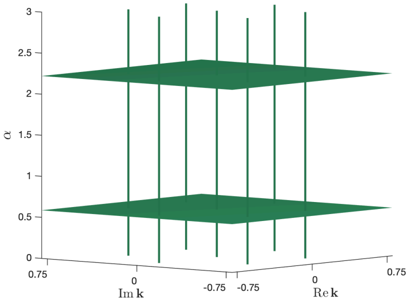

Seeley 85: $P(\alpha) = e^{ix}D_x + \alpha e^{ix}$, $x \in \mathbb{S}^1$, $\mathrm{Spec}(P(\alpha)) = \mathbb{C}$, $\alpha \in \mathbb{Z}$.

The operator of today

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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 $\Delta\alpha \simeq 3/2$. 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 $H_{\mathrm{k}}(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* - \bar{\mathrm{k}} \\ D(\alpha) - \mathrm{k} & 0 \end{pmatrix}$, $\mathrm{k} \in \mathbb{C}/\Gamma^*$

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

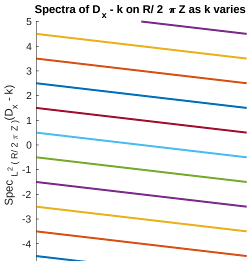
A simpler example first: $D_x := \frac{1}{i}\partial_x$

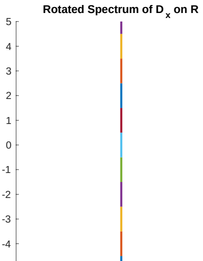
$$\mathrm{Spec}_{L^2(\mathbb{R})}(D_x) = \mathbb{R}, \qquad \mathrm{Spec}_{L^2(\mathbb{R}/2\pi\mathbb{Z})}(D_x) = \mathbb{Z}$$

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

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

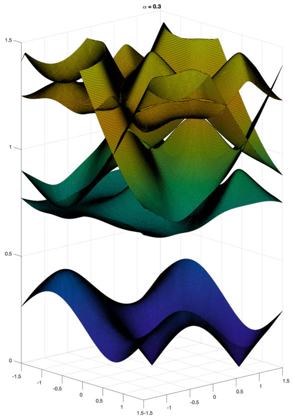
$$\mathrm{Spec}_{L^2(\mathbb{R})}(D_x) = \bigcup_{k\in\mathbb{R}/\mathbb{Z}} \mathrm{Spec}_{L^2(\mathbb{R}/2\pi\mathbb{Z})}(D_x - k)$$





Flat bands

The bands are eigenvalues of $H_k(\alpha)$ on $L^2_0(\mathbb{C}/\Gamma)$, $k \in \mathbb{C}/3\Gamma^*$:

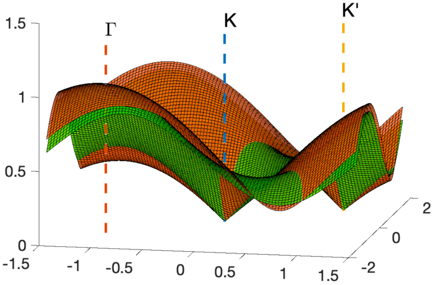


Theorem (BHZ '22; implicit in BEWZ '20)

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

A curious structure of the first band

$$\mathrm{k} \mapsto E_1(\alpha, \mathrm{k})/(\max_{\mathrm{k}} E_1(\alpha, \mathrm{k})), \quad 0.4 < \alpha < 0.6$$



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

Symmetries play a crucial role!

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

$$\mathscr{L}_{\mathrm{a}} \mathrm{u} = \mathrm{diag}(\omega^{a_1+a_2}, 1, \omega^{a_1+a_2}, 1)\mathrm{u}(z + \tfrac{4}{3} i\pi(\omega a_1 + \omega^2 a_2)), \quad \mathrm{a} \in \mathbb{Z}_3^2,$$

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

$$\mathscr{L}_{\mathrm{a}} H = H \mathscr{L}_{\mathrm{a}}, \quad \mathscr{C} H = H \mathscr{C}, \quad \mathscr{C} \mathscr{L}_{\mathrm{a}} = \mathscr{L}_{M\mathrm{a}} \mathscr{C}, \quad M = \begin{pmatrix} 0 & -1 \\ 1 & -1 \end{pmatrix}.$$

Decompose into irreducible representions of this Heisenberg group:

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

$$\rho_{k,p} \quad \longleftrightarrow \quad \mathscr{L}_{\mathrm{a}} \equiv \omega^{k(a_1+a_2)}, \quad \mathscr{C} \equiv \bar{\omega}^p$$

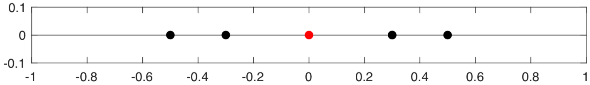
Symmetry protected states

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

$$\mathrm{e}_1 \in L^2_{\rho_{1,0}}, \quad \mathrm{e}_2 \in L^2_{\rho_{0,0}}, \quad \mathrm{e}_3 \in L^2_{\rho_{1,1}}, \quad \mathrm{e}_4 \in L^2_{\rho_{0,1}}.$$

$$H(\alpha) = -\mathscr{W} H(\alpha) \mathscr{W}^*, \ \ \mathscr{W} := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \ \mathscr{W}\mathscr{C} = \mathscr{C}\mathscr{W}, \ \mathscr{L}_{\mathrm{a}}\mathscr{W} = \mathscr{W}\mathscr{L}_{\mathrm{a}}$$

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

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

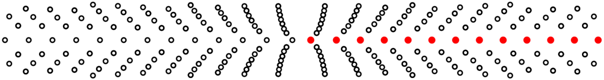
$$L_0^2(\mathbb{C}/\Gamma) := \{\mathrm{u} \in L^2(\mathbb{C}/\Gamma) : \mathscr{L}_{\mathrm{a}}\mathrm{u} = \mathrm{u}, \quad \mathrm{a} \in \tfrac{1}{3}\Gamma/\Gamma\}.$$

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

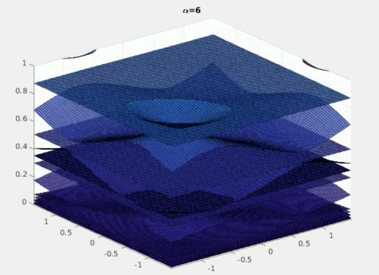
Flat band at 0 $\iff$ $\mathrm{Spec}_{L_0^2(\mathbb{C}/\Gamma)}(D(\alpha)) = \mathbb{C}$

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

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



Exponential squeezing of bands



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

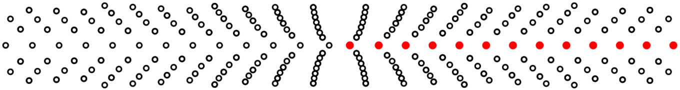
$$|E_j(\alpha, \mathrm{k})| \leq c_0 e^{-c_1 \alpha}, \quad j \leq c_2 \alpha, \quad \alpha > 0.$$

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

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

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



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

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

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

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

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

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

$$\sigma_p := \tfrac{1}{18} \operatorname{tr} T_{\mathrm{k}}^{2p}, \quad F_{\mathrm{k}}(\alpha) := \det_2(I - \alpha^2 T_{\mathrm{k}}^2)$$

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 α's:

k	α_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

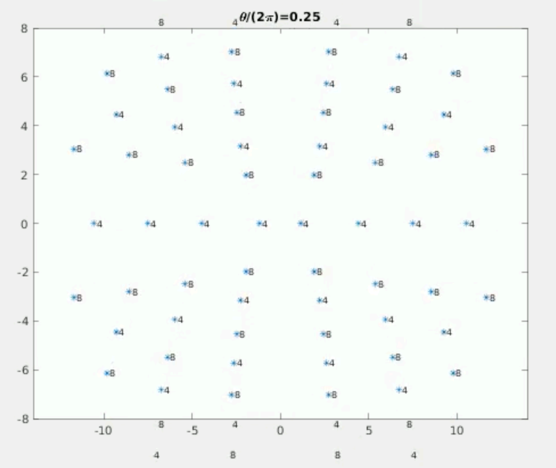
Tarnopolsky et al '19 observed that $\alpha_k - \alpha_{k-1} \simeq \frac{3}{2}$ $(0 < k \leq 8)$

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

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

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

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



Flat bands from theta functions

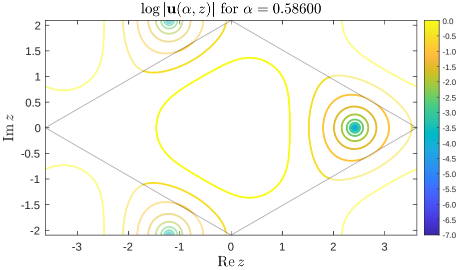
Tarnopolsky et al '19: consider $\mathrm{u} \in L^2_{\rho_{1,0}}(\mathbb{C}/\Gamma; \mathbb{C}^2)$, $D(\alpha)\mathrm{u} = 0$

$$\mathrm{u}_k(z) := e^{\frac{i}{2}(z\bar{\mathrm{k}}+\bar{z}\mathrm{k})} f_{\mathrm{k}}(z)\mathrm{u}(z), \;\; z \mapsto e^{\frac{i}{2}(z\bar{\mathrm{k}}+\bar{z}\mathrm{k})} f_{\mathrm{k}}(z) \text{ periodic}, \;\; \partial_{\bar{z}} f_{\mathrm{k}} = 0$$

$$(D(\alpha) - \mathrm{k})\mathrm{u}_k(z) = 0$$

Problem: f_{k} with these properties will have poles

Solution: Look for α's at which u has a zero!



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

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

Similar argument in Dubrovin–Novikov '80

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

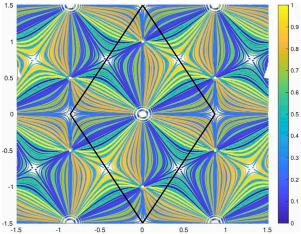
New direction: in-plane magnetic field

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 α and θ change?

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



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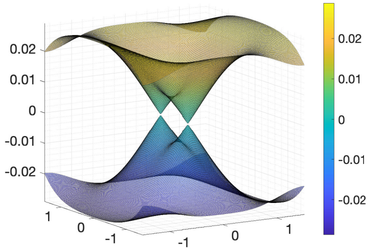

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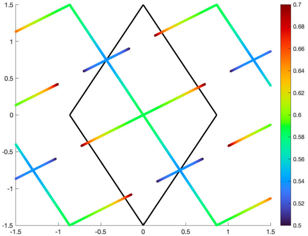
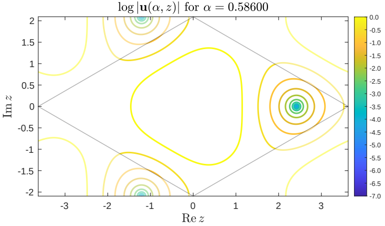
Theorem (BZ '23) *If $\underline{\alpha} \in \mathcal{A} \cap \mathbb{R}$ is simple and $0 < B_0 \ll 1$ then*

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

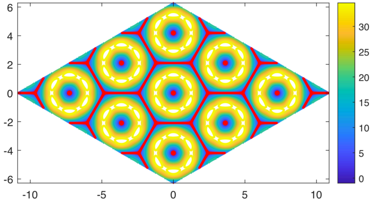
$$\mathscr{R}_\ell := \omega^\ell(2\pi(i\mathbb{R}+\mathbb{Z}) \cup \tfrac{2\pi}{\sqrt{3}}(\mathbb{R}+i\mathbb{Z})) \qquad \ell = 1 \text{ in the figure}$$



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



Countour plots of $z \mapsto \log |\mathrm{u}(\alpha, z)|$

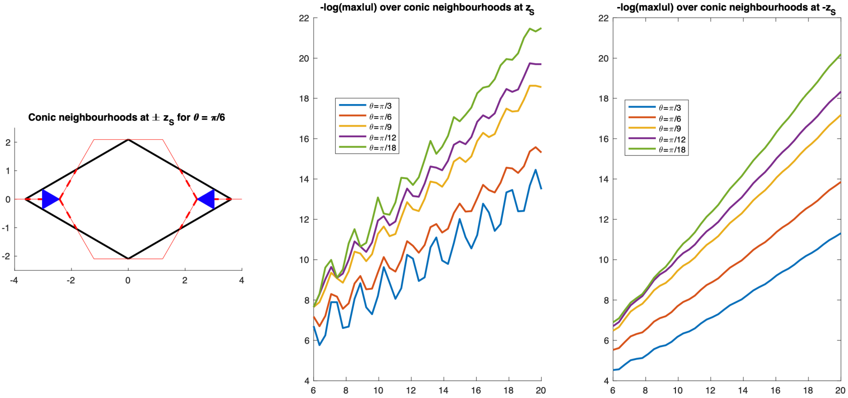


A contour plot of $|\{q, \bar{q}\}|$, $q = (2\bar{\zeta})^2 - U(z)U(-z)$

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

Fine structure of eigenfunctions

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



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

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

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

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

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

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

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 $\Omega = \mathrm{neigh}_{\mathbb{C}}(\mathrm{z}_0)$.

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.

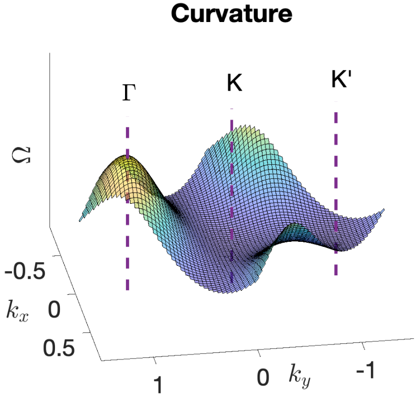
Another numerical observation (BHZ): Curvature

$\mathbb{C}/3\Gamma^* \ni \mathrm{k} \to u_{\mathrm{k}} \in L^2_0(\mathbb{C}/\Gamma)$ s holomorphic (Ledwith et al '21) and defines a natural line bundle

Chern connection: $\eta := \partial_{\mathrm{k}} \log \|u_{\mathrm{k}}\|^2 = \|\mathrm{u_k}\|^{-2} \langle \partial_{\mathrm{k}} \mathrm{u_k}, \mathrm{u_k} \rangle d\mathrm{k}$

Curvature: $\Omega = d\eta = \bar{\partial}_{\mathrm{k}} \partial_{\mathrm{k}} \log \|u_{\mathrm{k}}\|^2 = H(\mathrm{k}) d\bar{\mathrm{k}} \wedge d\mathrm{k}, \quad H(\mathrm{k}) \geq 0.$

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



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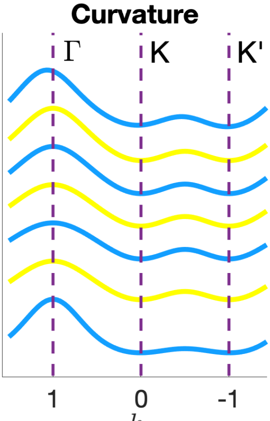
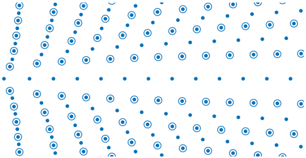


Many mathematical open problems

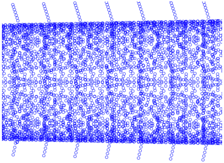
- Multiplicity issues; a stronger generic simplicity statement



- The fixed "shape" of the first band; what is a heuristic explanation?

- Significance and explanation of the curvature "peak" at $\mathsf{k} = \mathsf{i}$

- 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!