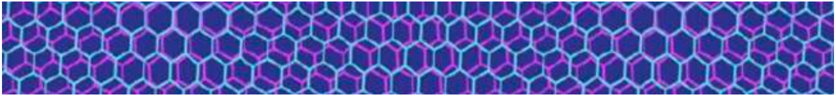
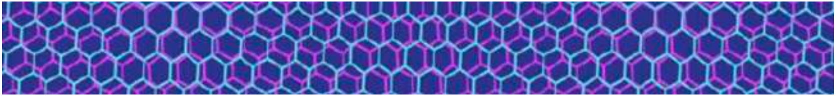
Mathematics of magic angles in twisted bilayer graphene

Herrsching, Mathematical results of many-body quantum systems

Simon Becker

June 10, 2022

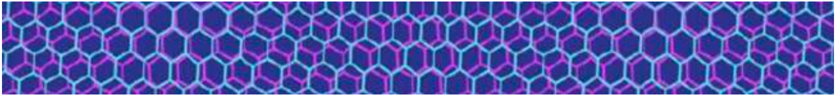




Based on joint work with

2020:, Mark Embree, Jens Wittsten, Maciej Zworski

2022: Tristan Humbert, Maciej Zworski



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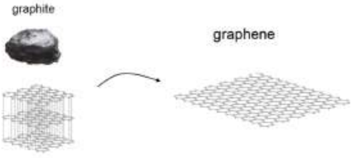
E. Brian Davies 2007: *Studying non-self-adjoint operators is like being a vet rather than a doctor: one has to require a much wider range of knowledge, and accept that one cannot expect to have as high a rate of success when confronted with particular cases.*

Motivation: bilayer graphene



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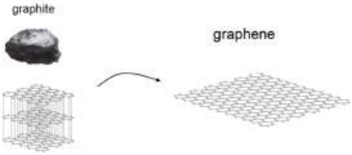

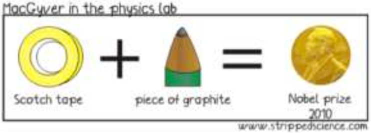

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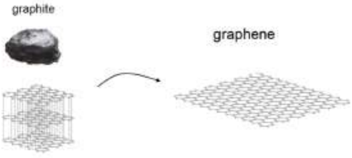

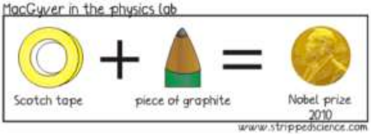

Geim–Novoselov '04

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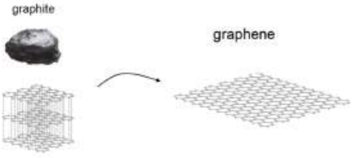

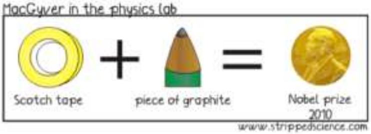

Geim–Novoselov '04

192 USD for 500 mg

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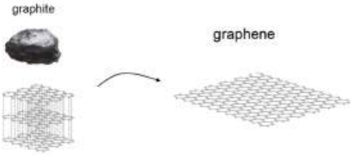

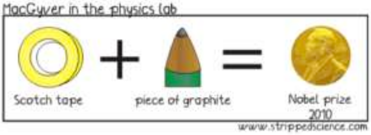

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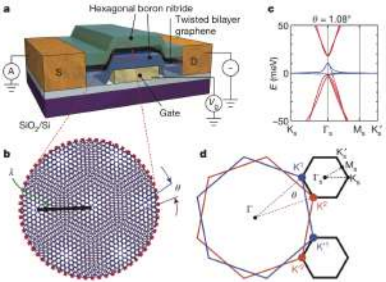

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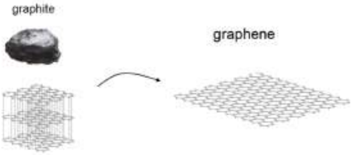

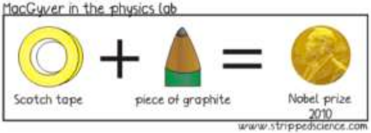

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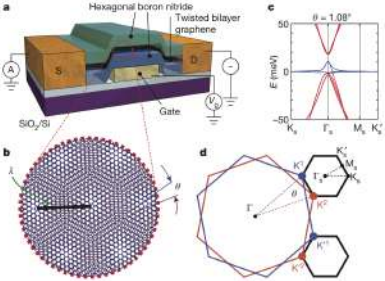
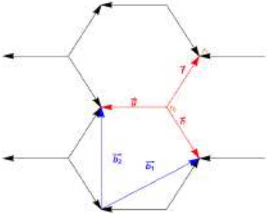


Tight-binding model-Twisted bilayer graphene



We define the discrete Laplacian on the honeycomb lattice $H : \ell^2(\mathbb{Z}^2;\mathbb{C}^2) \to \ell^2(\mathbb{Z}^2;\mathbb{C}^2)$ by

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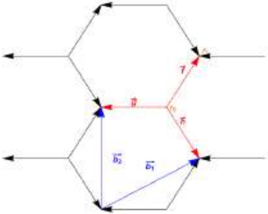

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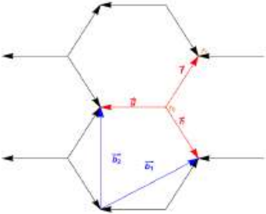

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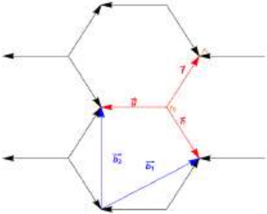

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where

$$(W_\theta\psi)_n = (w*\psi)(R_\theta n) := \sum_{m\in\mathbb{Z}^2} w(R_\theta n-m)\psi_m \text{ with } w \in \mathscr{S}(\mathbb{R}^2;\mathbb{C}^{2\times 2}).$$

The Bistritzer-MacDonald Hamiltonian

Massatt-Carr'20 showed that close to zero energy the model is effectively described by:

The Hamiltonian of two non-interacting sheets of graphene is

$$H = \begin{pmatrix} H_D & 0 \\ 0 & H_D \end{pmatrix} \text{ with } H_D = \begin{pmatrix} 0 & 2D_{\bar{z}} \\ 2D_z & 0 \end{pmatrix}.$$

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

Editors' Suggestion

Origin of Magic Angles in Twisted Bilayer Graphene

Grigory Tarnopolsky, Alex Jura Kruchkov,* and Ashvin Vishwanath
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The chiral model of TBG

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This limit is very important also for many-body effects cf. Bernevig–Vishwanath-Zaletel et al.

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Decompose into irreducible representions of this Heisenberg group:

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

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

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

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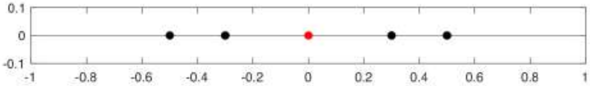

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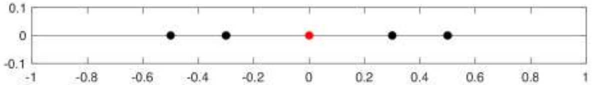

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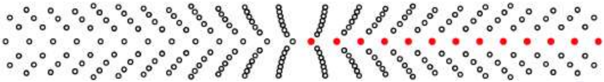

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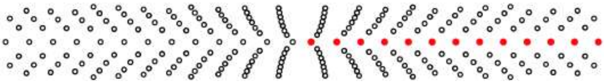

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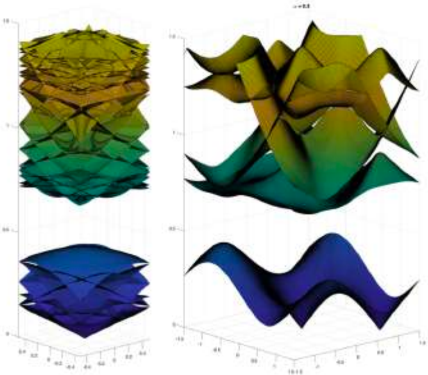
The bands are eigenvalues of $H_{\mathbf{k}}(\alpha)$ on $L^2_{\mathbf{0}}(\mathbb{C}/\Gamma)$, $\mathbf{k} \in \mathbb{C}/3\Gamma^*$:



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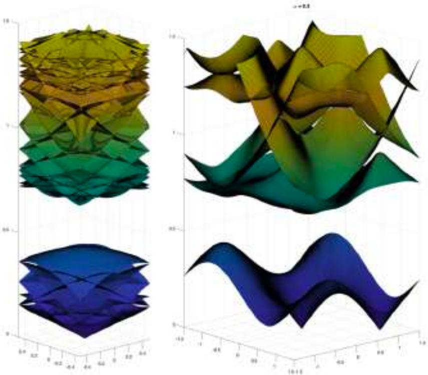

Theorem (BHZ '22; implicit in BEWZ '20)

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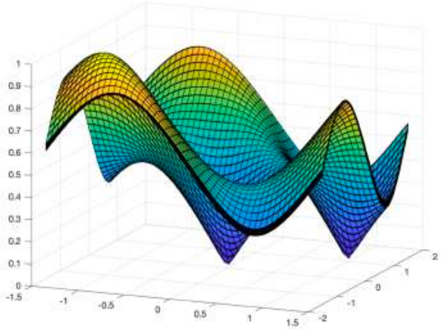

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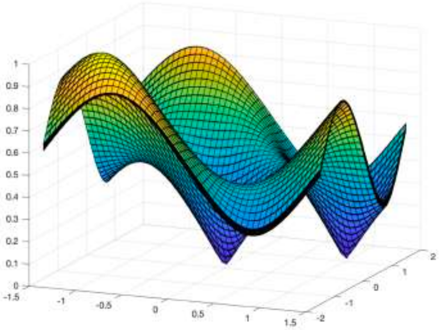

Rescaled plots remain almost fixed at $\mathbf{k} \longmapsto |U(-4\sqrt{3}\pi i\mathbf{k}/9)|$

Exponential squeezing of bands

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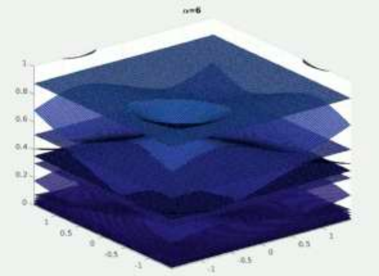

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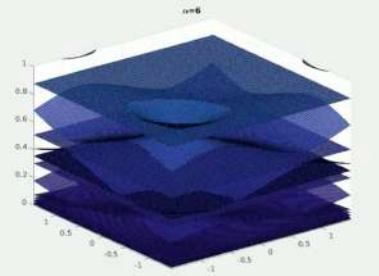

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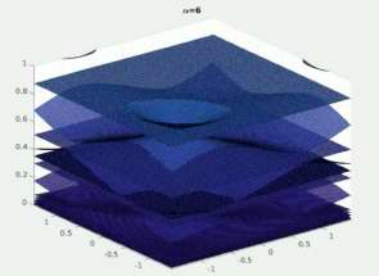

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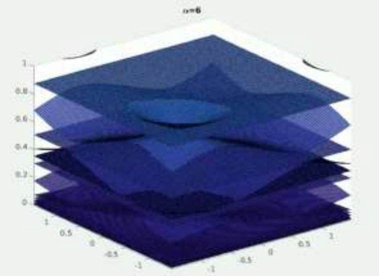

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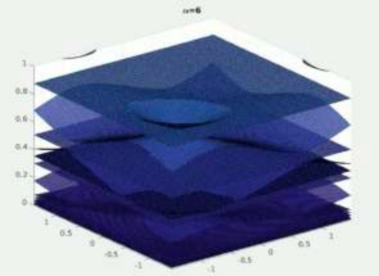

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Hörmander'69, Sato-Kawai-Kashiwara'73...Dencker-Sjöstrand-Z'04

Exponential squeezing of bands via solvability of PDE

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$$\{p, \bar{p}\} := \sum_{j=1}^{n} \partial_{\xi_j} p \partial_{x_j} \bar{p} - \partial_{\xi_j} \bar{p} \partial_{x_j} p|_{(x_0, \xi_0)} \neq 0$$

$\Longrightarrow$ $Pu = f$ is not solvable near x_0 for a generic $f \in C^\infty$

Essential step: $\exists\, u_h$ supported in $B(x_0, h^{\frac{1}{2}-})$ such that

$$\forall\, N\, \exists C_N \quad \|Pu_h\|_{L^2} \leq C_N h^N, \quad \|u_h\|_{L^2} = 1$$

Sato–Kawai–Kashiwara '73, Dencker–Sjöstrand–Z '04: if a_α's are analytic functions then

$$\exists\, c > 0 \quad \|Pu_h\|_{L^2} \leq e^{-c/h}, \quad \|u_h\|_{L^2} = 1$$

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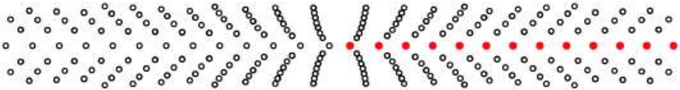

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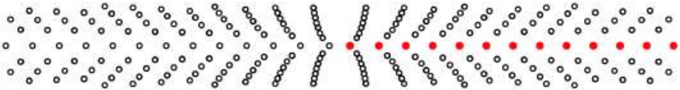

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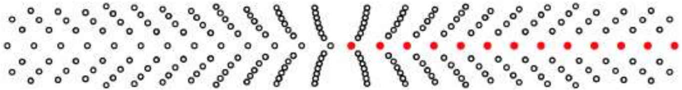

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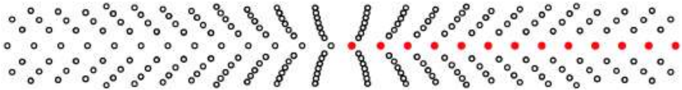

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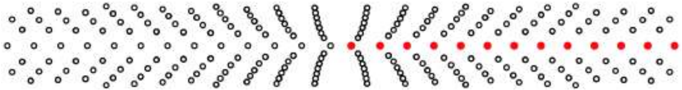

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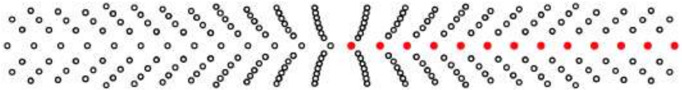

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BEWZ '21 (motivated by LW): $|\mathcal{A} \cap \mathbb{R}_+| \geq 2$

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6	8.3129991933	1.5182
7	9.829066969	1.5161
8	11.34534068	1.5163
9	12.8606086	1.5153
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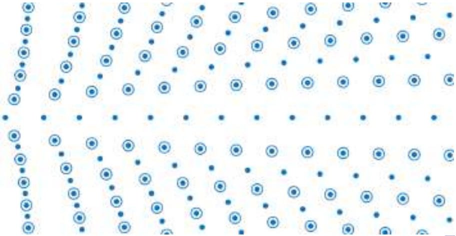

Works for general potentials with $\mathbb{Z}_3^2 \rtimes \mathbb{Z}_3$ symmetries

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

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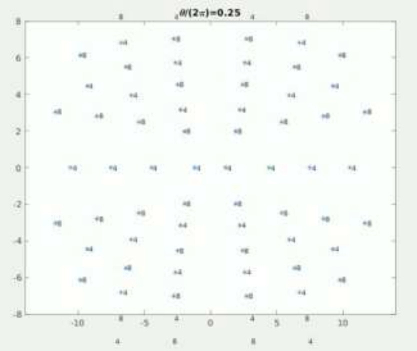

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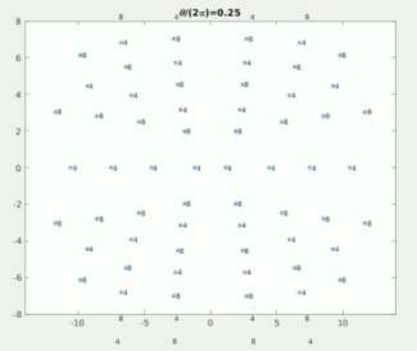

Theorem (BHZ '22) *For a generic potential flat bands are simple.*

Flat bands from theta functions

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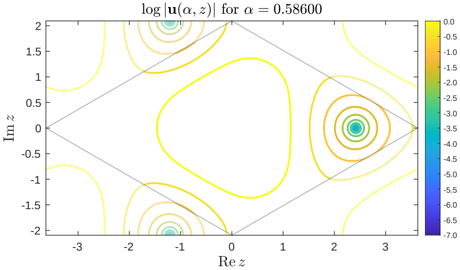

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Theorem (BHZ '22) $\alpha \in \mathcal{A}$ simple $\Rightarrow$ z_S *is the only zero of* $\mathbf{u}$.

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Felix Klein 1920: *When I was a student, abelian functions were, as an effect of the Jacobian tradition, considered the uncontested summit of mathematics, and each of us was ambitious to make progress in this field. And now? The younger generation hardly knows abelian functions.*

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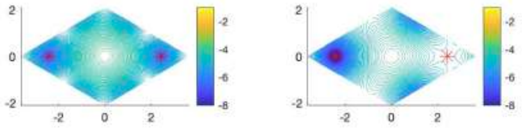

$\log |w|$ of the two component of $\mathbf{u_0} \in L^2_{\rho_{0,0}} \subset L^2_{\mathbf{0}}$, both vanishing at $-z_S$. Except for vanishing at $-z_S$ this eigenstate exists for all α's.

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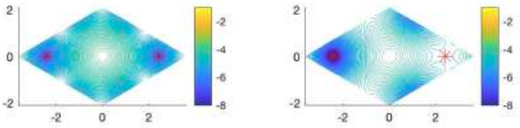

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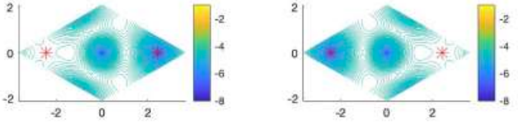

$\log|w|$ of components of $\mathbf{u_i} \in L^2_{\rho_{2,1}} \subset L^2_{\mathbf{i}}$.

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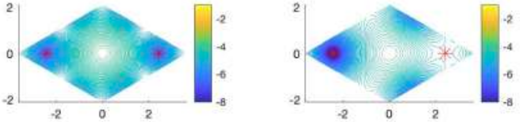

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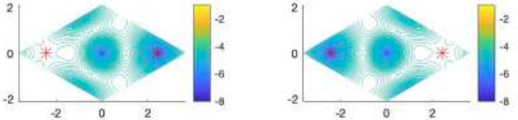

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This is the state considered by Cano et al '21 with additional symmetry $[\psi(z), \varphi(z)] \mapsto [-\varphi(-z), \psi(-z)]$.

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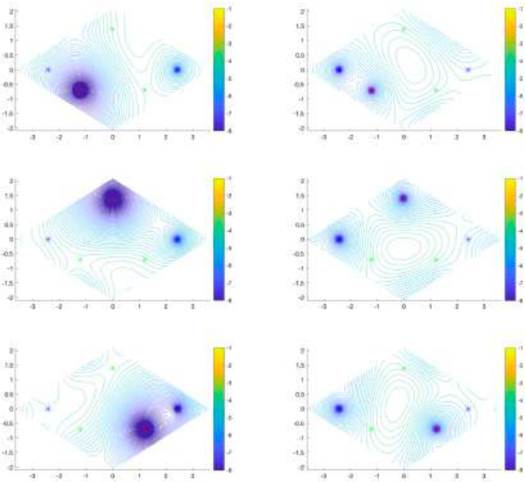
Three dimensional representations come from $\{\pm\omega^k/\sqrt{3}\}_{k=0}^2$:



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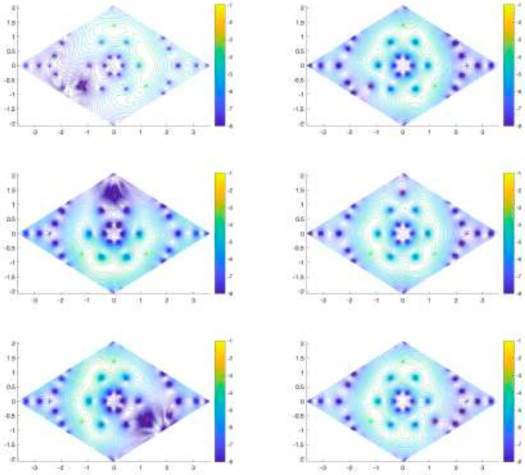

$\alpha = \alpha_5$ (fifth magic angle): vanishing determines symmetries; despite appearances $\mathbf{u}_{\omega^k/\sqrt{3}}$ do not vanish at other points.

Chern connection and curvature

$\mathbb{C}/3\Gamma^* \ni \mathbf{k} \to u_{\mathbf{k}} \in L^2_{\mathbf{0}}(\mathbb{C}/\Gamma)$ defines a holomorphic line bundle

Ledwith et al '21

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Magic angle	0.58	2.22	3.75	5.27	6.79	8.31
std	0.2834	0.1502	0.1333	0.1611	0.1965	0.2362
Magic angle	9.82	11.34	12.86	14.37	15.89	17.40
std	0.2674	0.2904	0.3518	0.3835	0.3346	0.2790

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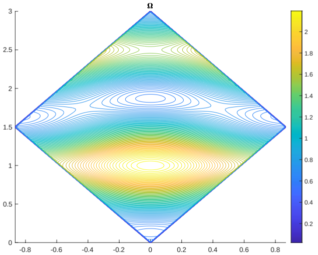

$\alpha_1 \simeq 0.58$; concentration at $\mathbf{i}$

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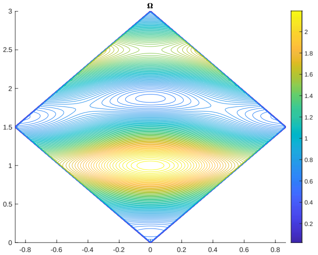

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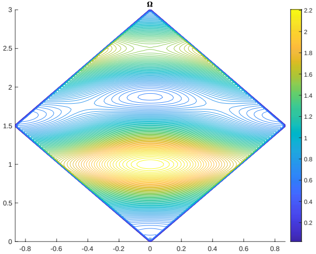

$\alpha_2 \simeq 2.22$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

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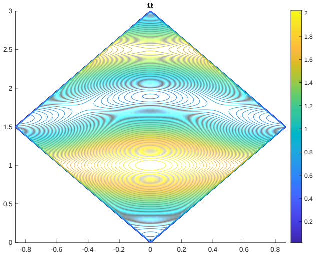

$\alpha_3 \simeq 3.75$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

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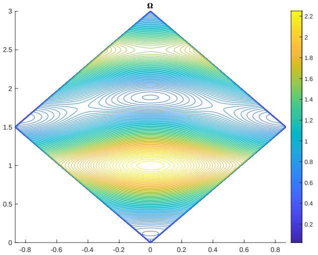

$\alpha_4 \simeq 5.27$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

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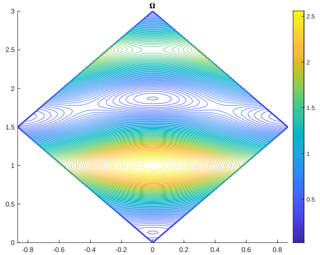

$\alpha_5 \simeq 6.79$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

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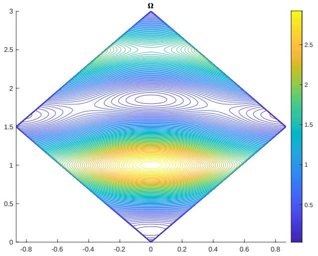

$\alpha_6 \simeq 8.31$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

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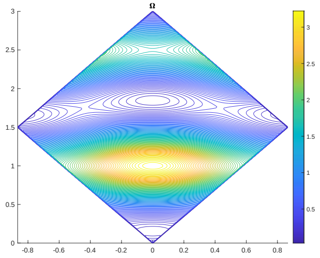

$\alpha_7 \simeq 9.82$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

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Ledwith et al '21

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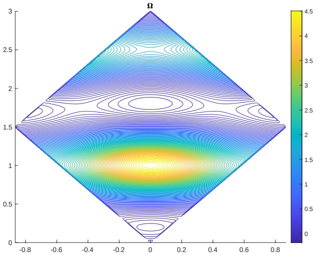
Curvature: $\Omega = d\eta = \bar{\partial}_{\mathbf{k}} \partial_{\mathbf{k}} \log \| u_{\mathbf{k}} \|^2 = H(\mathbf{k}) d\bar{\mathbf{k}} \wedge d\mathbf{k}, \quad H(\mathbf{k}) \geq 0.$

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

Standard deviation: $|\mathbb{C}/3\Gamma^*|^{-1} \int_{\mathbb{C}/3\Gamma^*} (H(k)/2\pi + c_1)^2 dm(\mathbf{k})$



$\alpha_8 \simeq 11.34$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

Chern connection and curvature

$\mathbb{C}/3\Gamma^* \ni \mathbf{k} \to u_{\mathbf{k}} \in L^2_{\mathbf{0}}(\mathbb{C}/\Gamma)$ defines a holomorphic line bundle

Ledwith et al '21

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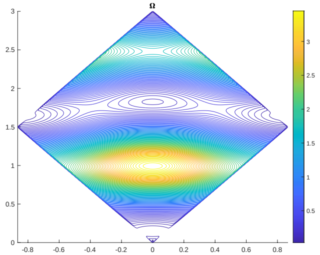

$\alpha_9 \simeq 12.96$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

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Ledwith et al '21

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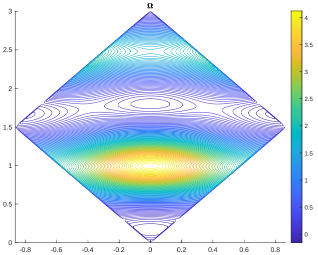
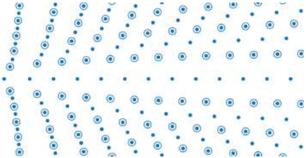


$\alpha_{10} \simeq 14.37$; concentration at $\mathbf{i} \equiv \omega i \mod 3\Gamma^*$

- Multiplicity issues; a stronger generic simplicity statement

Some mathematical open problems

- Multiplicity issues; a stronger generic simplicity statement



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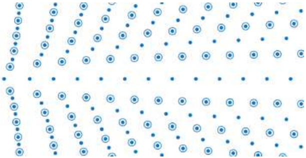

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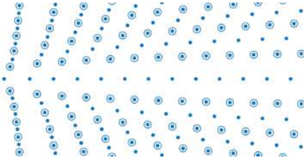

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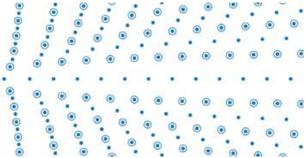

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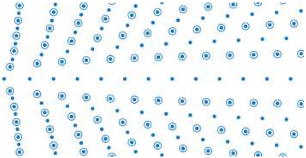

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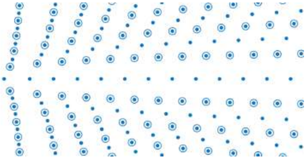

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