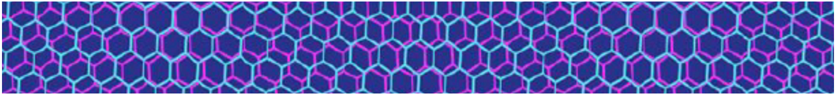
Magic Angles for Twisted Bilayer Graphene

Microlocal Analysis and Mathematical Physics
In honor of Anders Melin's 80th birthday

Maciej Zworski

September 21, 2023



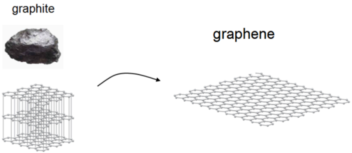
A project in the time of covid-19

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



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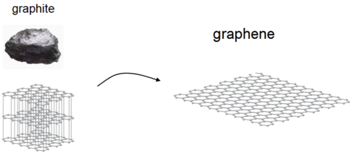

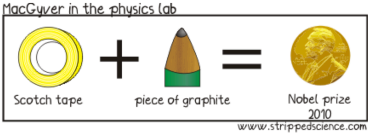

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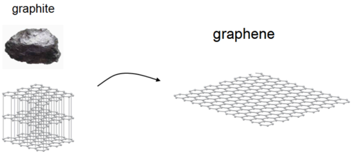

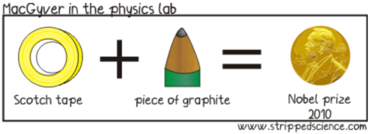

Geim–Novoselov '04

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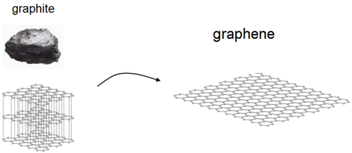

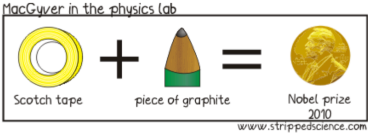

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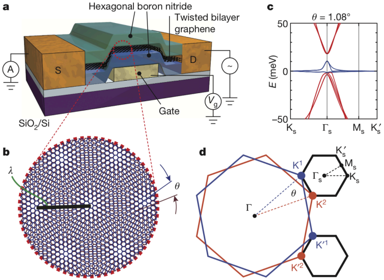

Cao et al '18, Yankovitz et al '18: superconductivity at $\theta \simeq 1.08^\circ$

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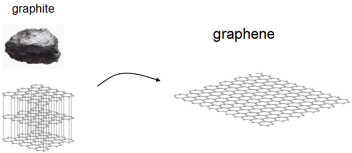

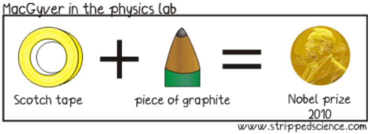

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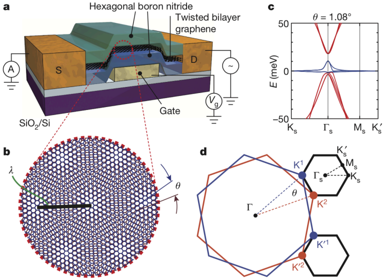

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Predicted by Bistritzer–MacDonald '11

The chiral model of TBG

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Editors' Suggestion

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The operator of today

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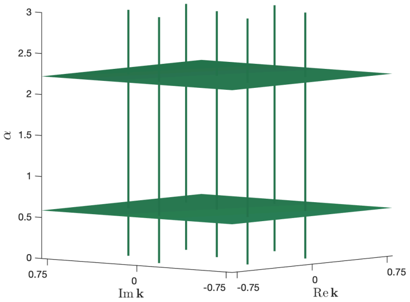

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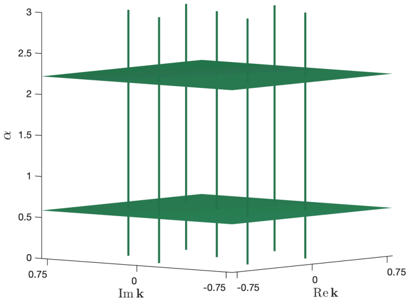

Seeley 85: $P(\alpha) = e^{ix}D_x + \alpha e^{ix}, \ x \in \mathbb{S}^1$, $\mathrm{Spec}(P(\alpha)) = \mathbb{C}, \ \alpha \in \mathbb{Z}$.

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Bands: eigenvalues of $H_{\mathrm{k}}(\alpha) := \begin{pmatrix} 0 & D(\alpha)^* - \bar{\mathrm{k}} \\ D(\alpha) - \mathrm{k} & 0 \end{pmatrix}$, $\mathrm{k} \in \mathbb{C}/\tfrac{1}{3}\Lambda^*$

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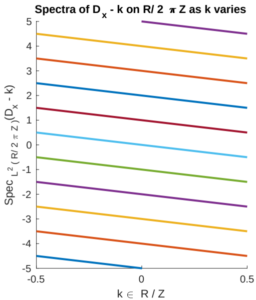

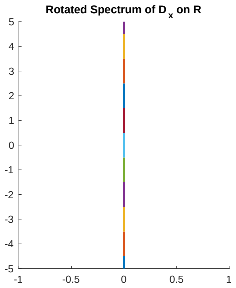

Theorem (BEWZ '20) *There exists a discrete set* $\mathcal{A} \subset \mathbb{C}$ *such that*

$$\mathrm{Spec}_{L^2_0(\mathbb{C}/\Lambda)} D(\alpha) = \begin{cases} \Lambda^* + \{K, -K\} & \alpha \notin \mathcal{A} \\ \mathbb{C} & \alpha \in \mathcal{A}, \end{cases}$$

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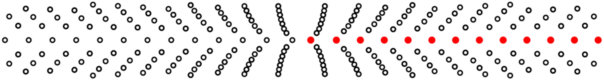

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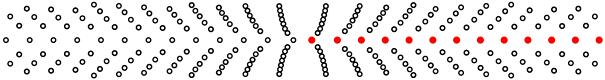

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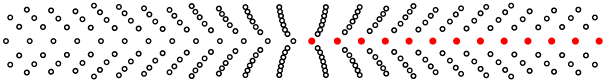

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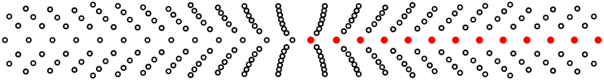

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Theorem (BEWZ '20) *There exists a discrete set $\mathcal{A} \subset \mathbb{C}$ such that*

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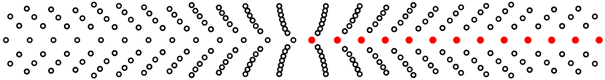

k	α_k	$\alpha_k - \alpha_{k-1}$
1	0.58566355838955	
2	2.2211821738201	1.6355
3	3.7514055099052	1.5302
4	5.276497782985	1.5251
5	6.79478505720	1.5183
6	8.3129991933	1.5182
7	9.829066969	1.5161
8	11.34534068	1.5163
9	12.8606086	1.5153
10	14.376072	1.5155
11	15.89096	1.5149
12	17.4060	1.5150
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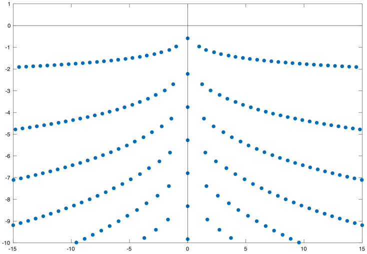
Magic angles vs. Scattering resonances



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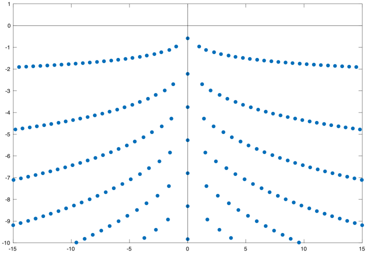

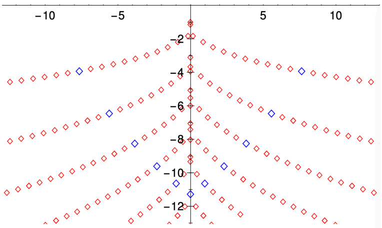

Magic α's

Resonances for $B_{\mathbb{H}^2}(0, 1)$

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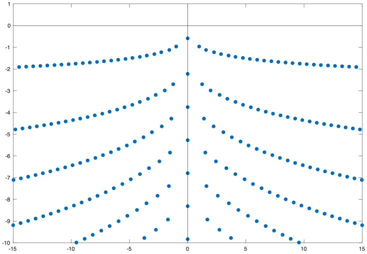

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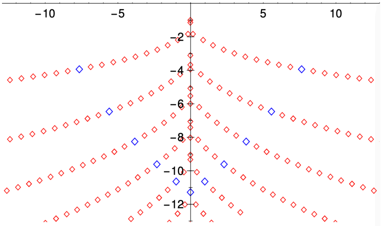

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$$|\{\alpha \in \mathcal{A} : |\alpha| \leq r\}| \leq Cr^2$$

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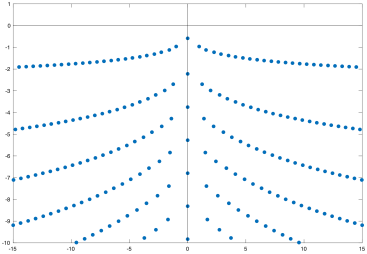

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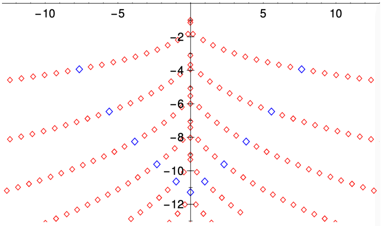

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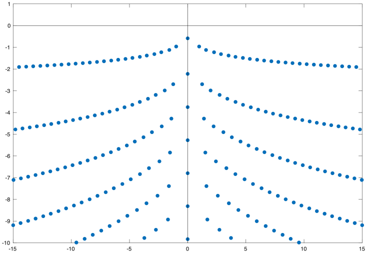

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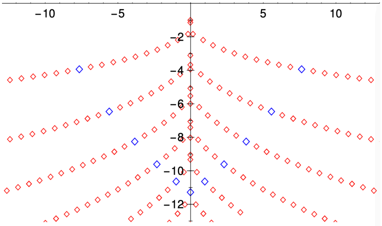

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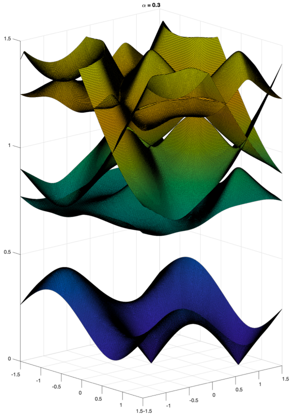
(Known for obstacles in hyperbolic plane: Vodev, Borthwick...)

Flat bands

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



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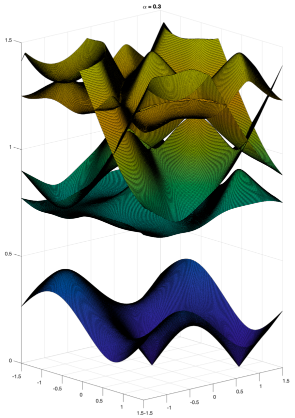

Theorem (BHZ '22; implicit in BEWZ '20)

$$\exists\, \mathrm{k} \notin \Lambda^* + \{K, -K\} \;\; E_1(\alpha, \mathrm{k}) = 0 \implies \forall\, \mathrm{k} \;\; E_1(\alpha, \mathrm{k}) = 0.$$

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

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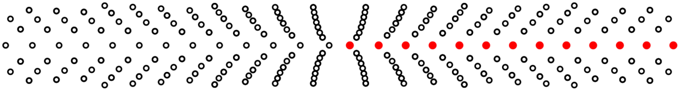

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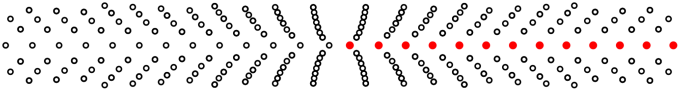

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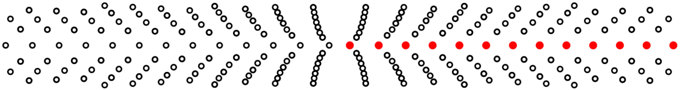

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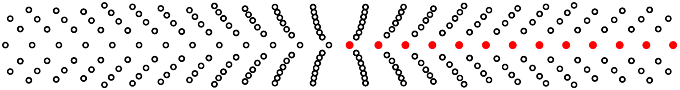

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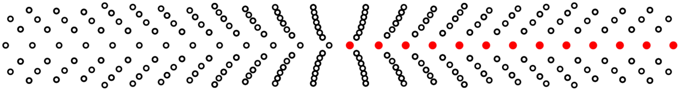

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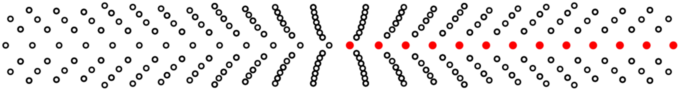

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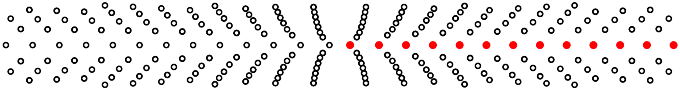

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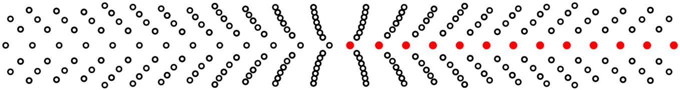

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Remark: Luskin–Watson '21 showed $|\mathcal{A} \cap (0.583, 0.589)| \geq 1$

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Example $Q(\alpha, k) = D(\alpha) + k$, $m(\alpha_0, k) = \mathbb{1}_{\{K, -K\} + \Lambda^*}$ (symmetry protected states!)

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Example $Q(\alpha, k) = (2D_{\bar{z}} + k)^2 - \alpha^2 U(z) U(-z)$: a scalar model in which $m(0, k) = 2\,\mathbb{1}_{\Lambda^*}(k) > \dim \ker Q(0, k)$.

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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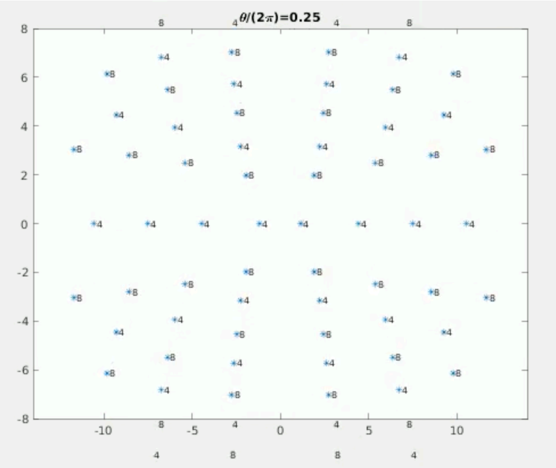

Structure of eigenfunctions at the flat band

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Consider the (rescaled) Green function of $2D_{\bar{z}}$ on $\mathbb{C}/\Lambda$:

$$(2D_{\bar{z}} + k) F_k(z) = a(k)\delta_0(z), \qquad k \mapsto F_k \text{ holomorphic}$$

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Theorem (BHZ '22) *If $\alpha \in \mathcal{A}$ is simple then the unique zero has to appear at the stacking point $z_S := -z(K) = \sqrt{3}/i$.*

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$$F_k(z) = e^{\frac{i}{2}(z-\bar{z})k}\frac{\theta(z - z(k))}{\theta(z)}, \quad a(k) = \frac{2\pi\theta(z(k))}{\theta'(0)}, \quad z(k) = \frac{\sqrt{3}}{4\pi i}k,$$

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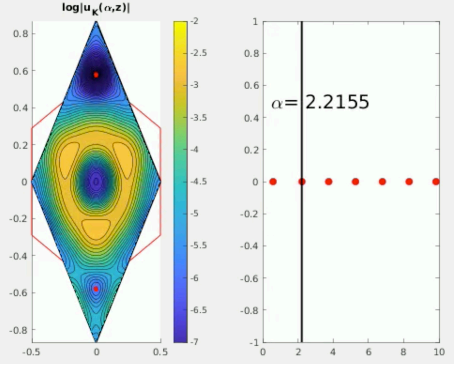

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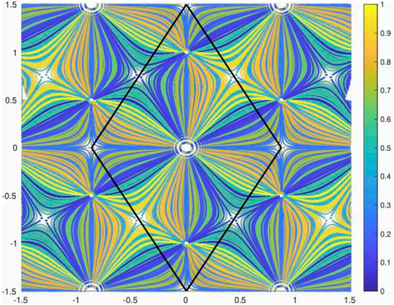

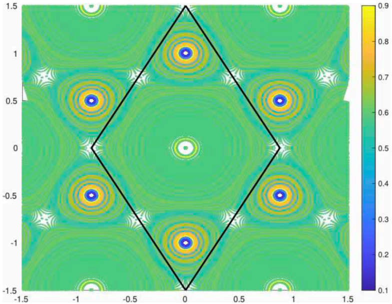

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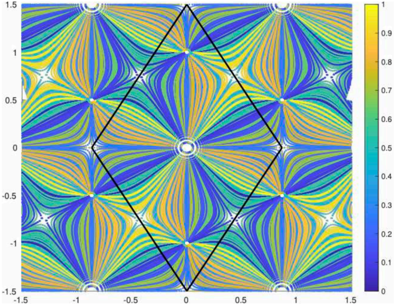

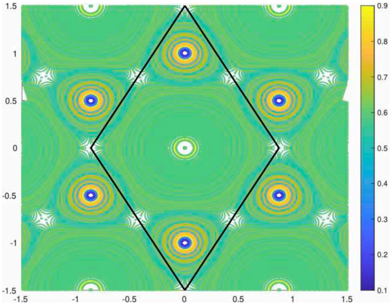

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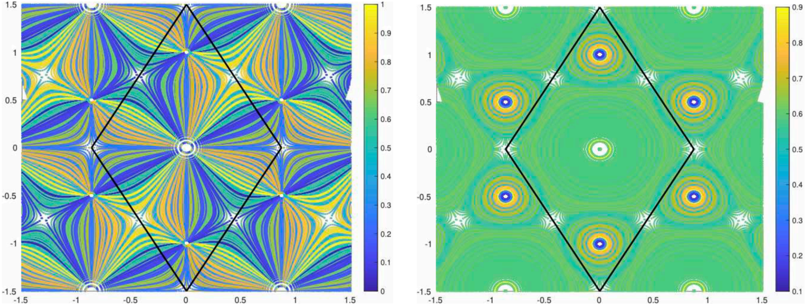

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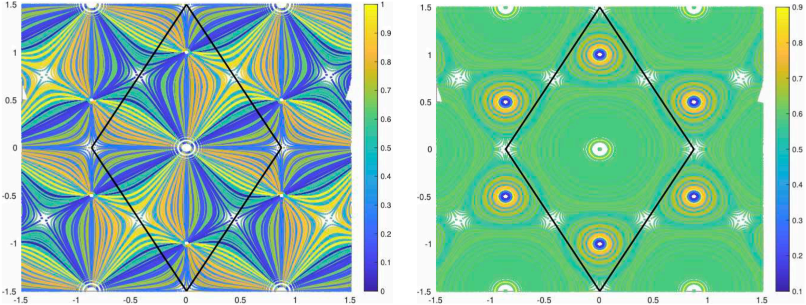

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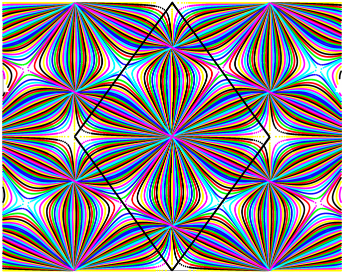

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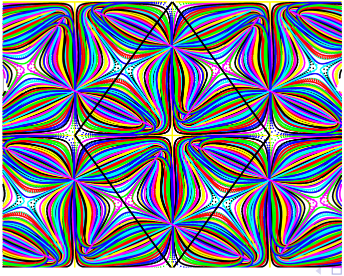

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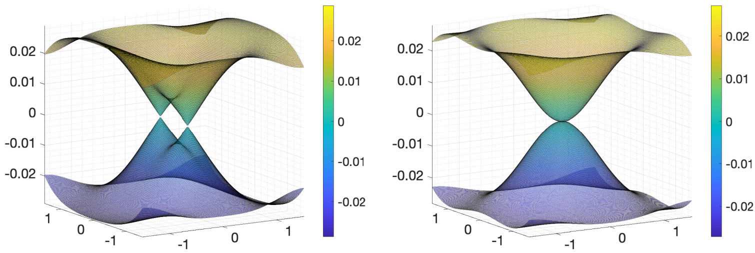

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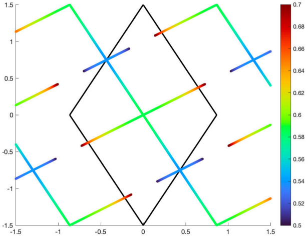

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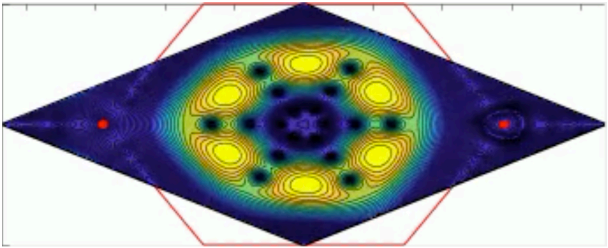

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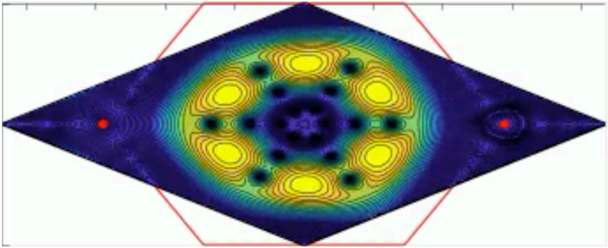

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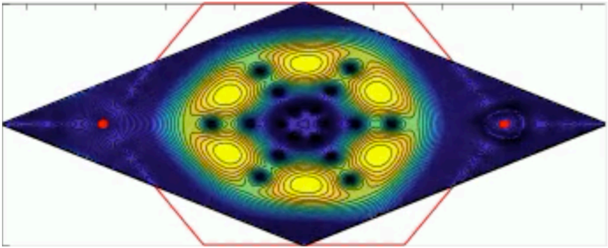

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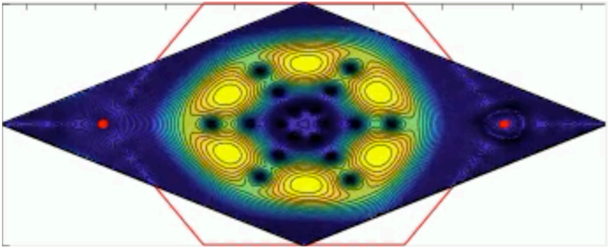

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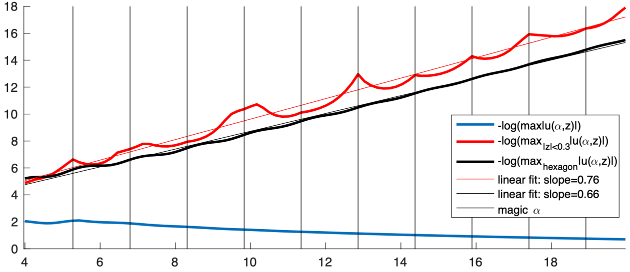

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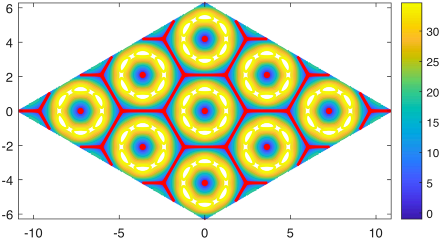
Principally scalar reduction

$$P(-\lambda)P(\lambda) = q(x, hD)I_{\mathbb{C}^2} + hR(x)$$

$$q(x,\xi) = 4\bar{\zeta}^2 - \lambda^2 U(z)U(-z), \quad z = x_1 + ix_2, \quad \bar{\zeta} = \tfrac{1}{2}(\xi_1 + i\xi_2)$$

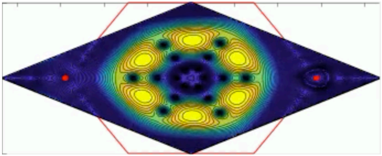
$$R(x) = \begin{pmatrix} 0 & 2\lambda D_{\bar{z}} U(z) \\ -\lambda D_{\bar{z}} U(-z) & 0 \end{pmatrix}$$

$\{q, \bar{q}\}|_{q^{-1}(0)}$ measures the "complexity" of $q(x,\xi) \in \mathbb{C}$

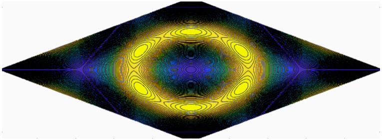


A contour plot of $|\{q, \bar{q}\}|$ over $\mathbb{C}/3\Lambda$

The rôle of the Poisson bracket



$$(q(x, hD) + hR)u = 0$$



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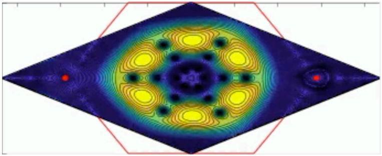

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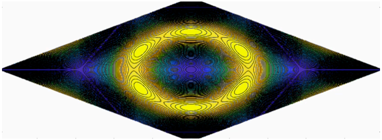

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Hörmander'60, Sato-Kawai-Kashiwara'73, Dencker-Sjöstrand-Z'04:

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$\exists\, u$ microlocalized to (x_0, ξ_0), $\quad q(x, hD)u = \mathcal{O}(e^{-c/h})$

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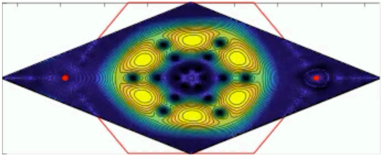

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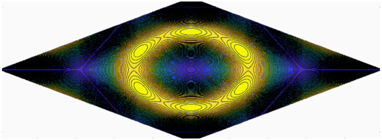

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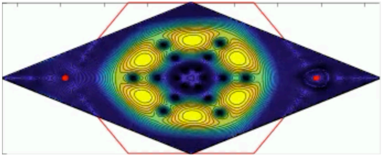

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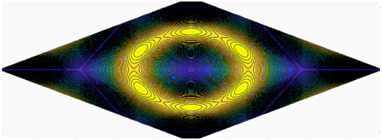

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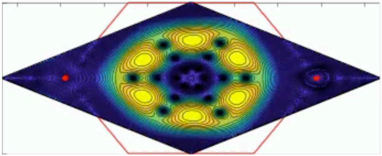

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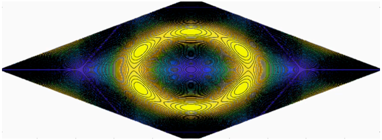

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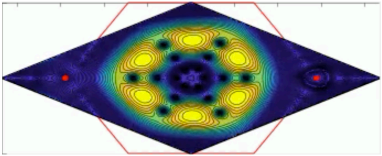

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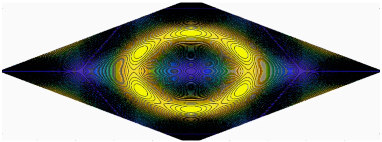

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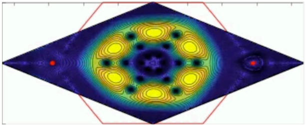
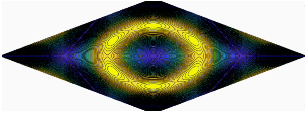
Passage to PDE with analytic coefficients has its complications

The rôle of the Poisson bracket





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Classically forbidden region when $\{q, \bar{q}\} = 0$

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then there exists an h-independent neighbourhood of x_0, Ω, *such that*

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Application to the chiral model of TBG

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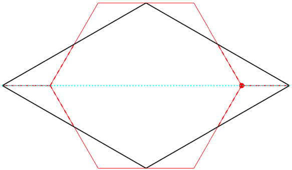

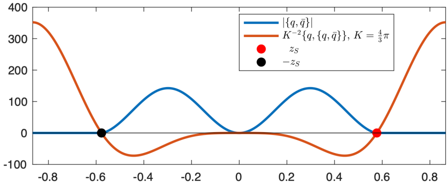

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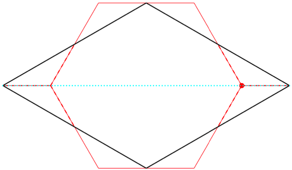

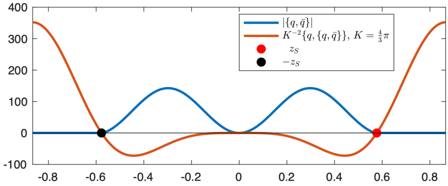

$$\{q,\{q,\bar q\}\}=\frac{128}{9}\pi^2(c-1)^2(2c+1)(2c-9),\quad c:=\cos(2\pi\sqrt{3}t/3)$$

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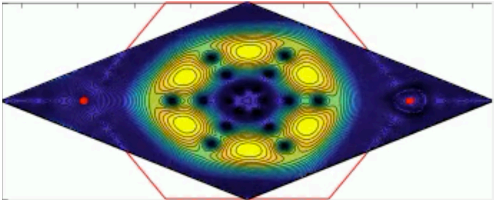

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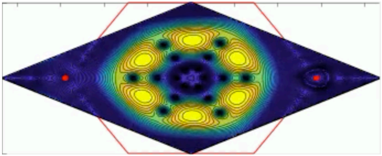
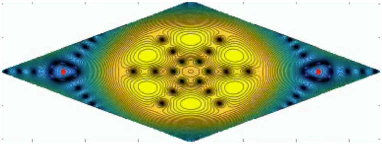


chiral model



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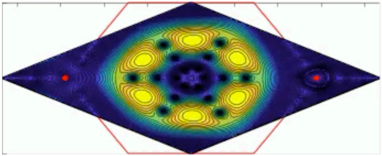

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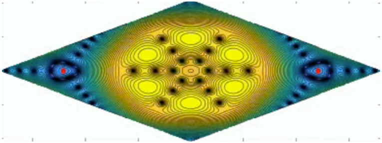
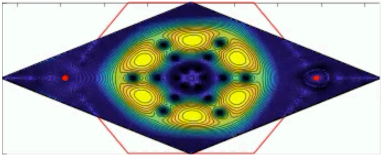


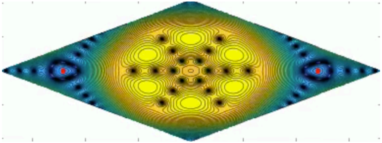
scalar model

$$\{q, \{q, \bar{q}\}\}(\pm z_S, 0) = 0$$

Application to the chiral model of TBG



chiral model



scalar model

$$\{q,\{q,\bar{q}\}\}(\pm z_S,0)=0 \quad \text{but} \quad \{q,\{q,\{q,\{q,\bar{q}\}\}\}\}(\pm z_S,0)\neq 0$$

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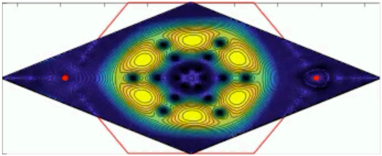

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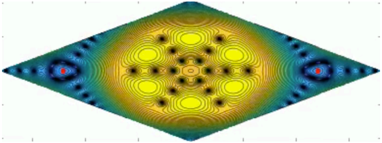

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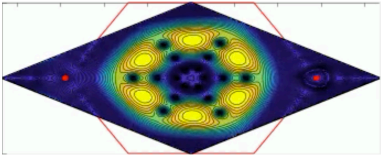
Galkowski '23: C^∞ theory of Egorov and Hörmander does not give

$$|u(\alpha,z)|\leq C_N\alpha^{-N} \quad \forall N, \quad z \text{ near } \pm z_S$$

Application to the chiral model of TBG



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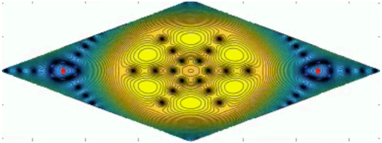

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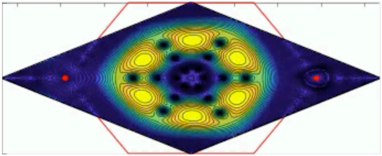
What about the center of the hexagon?

Application to the chiral model of TBG



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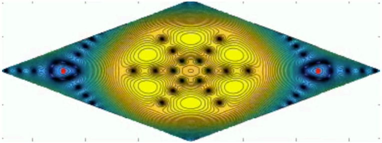

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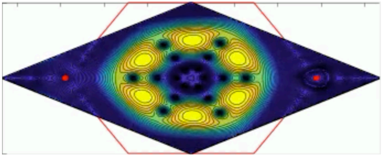
At $(x,\xi)=(0,0)$ (the center of the hexagon) the operator is not of principal type:

$$q(0,0)=0, \quad \nabla q(0,0)=0$$

Application to the chiral model of TBG



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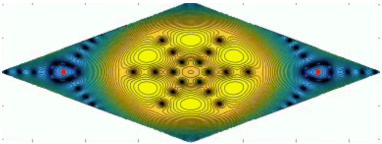

scalar model

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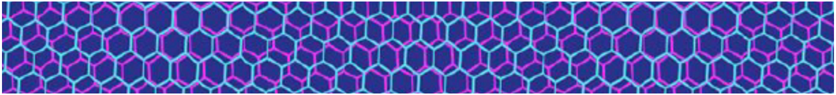
Lower order terms matter as we see in the figure above!



Anonymous '23 (communicated by Simon Becker)

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Happy Birthday!