

Mathematics of magic angles for bilayer graphene

Lisbon IST QM3

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Joint work with

Mark Embree



Jens Wittsten



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The spectrum close to the Dirac points in twisted bilayer graphene is described by the following Hamiltonian acting on $L^2(\mathbb{C}; \mathbb{C}^4)$

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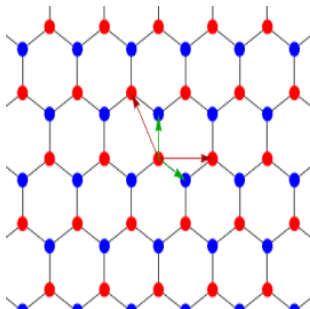
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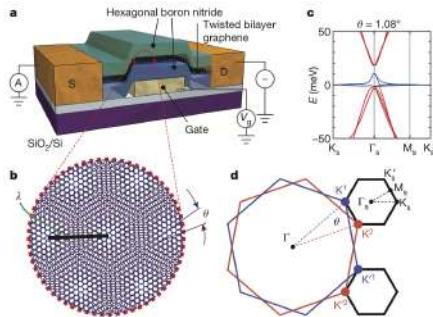
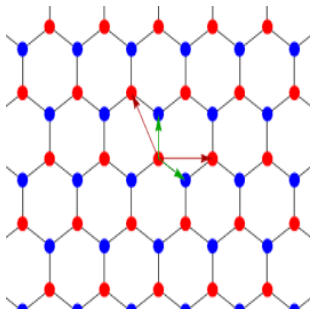
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Cao et al '18, Yankovitz et al '18: superconductivity at $\theta \simeq 1.08^\circ$

The operator of today

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

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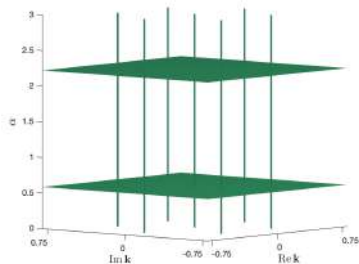
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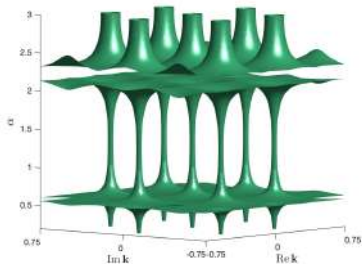
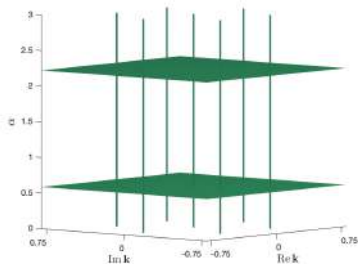
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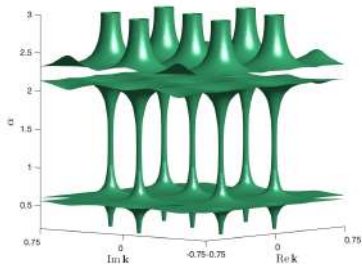
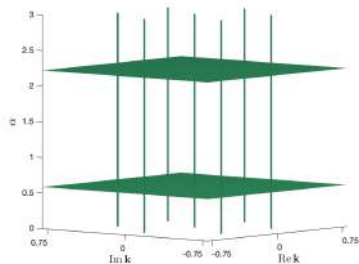
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On the right: level surface of $\mathbf{k} \mapsto \|(D(\alpha) - \mathbf{k})^{-1}\| = 10^2$ as α varies: we see that the norm of the resolvent $(D(\alpha) - \mathbf{k})^{-1}$ grows as we approach the first two magic α 's (near 0.586 and 2.221), at which it blows up for all k .

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Origin of Magic Angles in Twisted Bilayer Graphene

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

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

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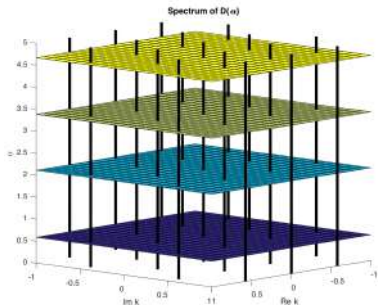
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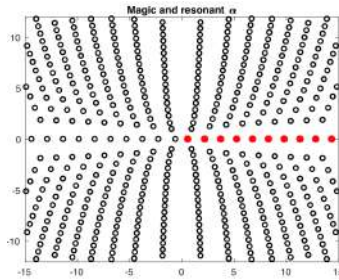
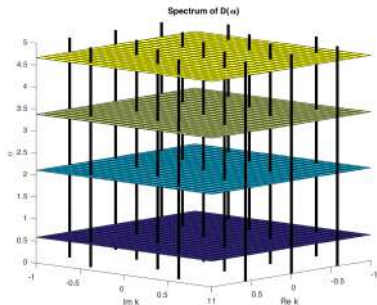
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Movie: level sets of $\lambda \mapsto \|(D(\alpha) - \lambda)^{-1}\|$

Protected state from Heisenberg group over \mathbb{Z}_3

Symmetries of $D = \begin{pmatrix} 2D_{\bar{z}} & \alpha U(z) \\ \alpha U(-z) & 2D_{\bar{z}} \end{pmatrix}$ and $H = \begin{pmatrix} 0 & D^* \\ D & 0 \end{pmatrix}$.

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

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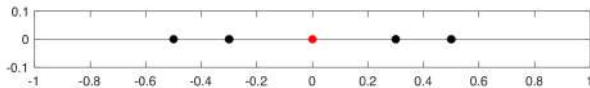
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That is because the spectrum of $H(\alpha)|_{L^2_{\rho_{1,0}}}$ is even...



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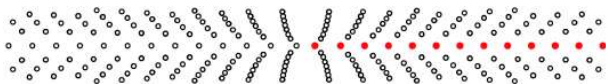
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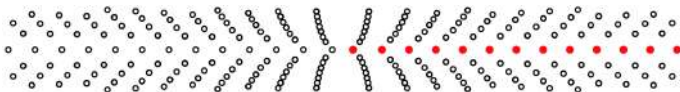
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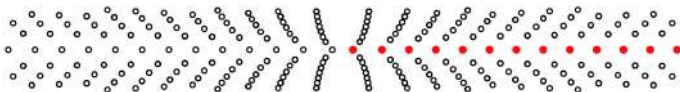
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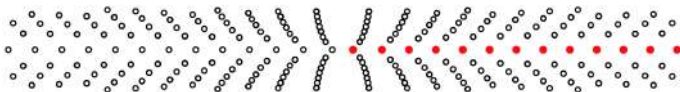


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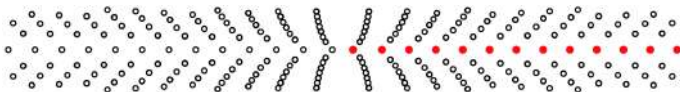
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Also, the spectral characterization allows more efficient calculation of α 's

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Flat bands

The bands are eigenvalues of $H_{\mathbf{k}} = \begin{pmatrix} 0 & D^* - \bar{\mathbf{k}} \\ D - \mathbf{k} & 0 \end{pmatrix}$ as function of $\mathbf{k} \in \mathbb{C}/\Gamma^* \simeq \mathbb{R}^2/\mathbb{Z}^2$:

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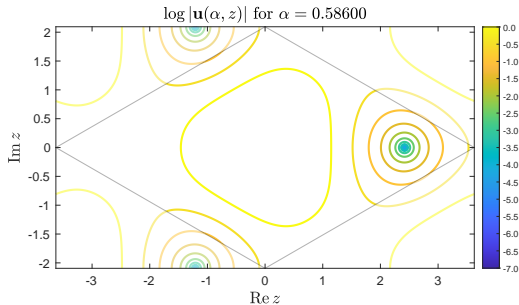
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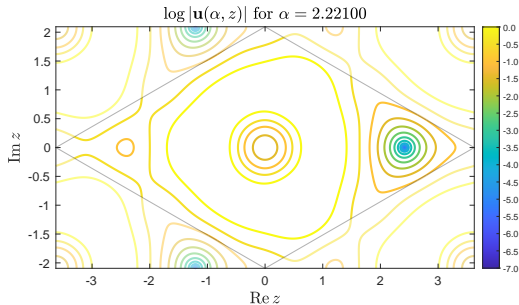
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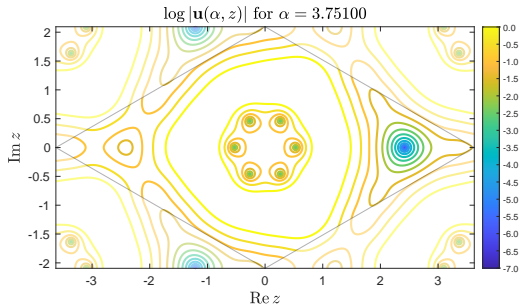
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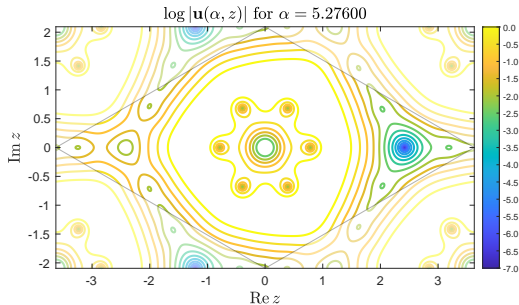
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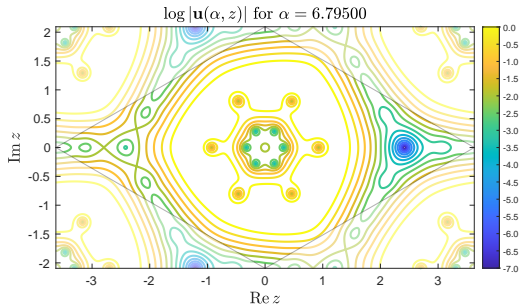
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Flat bands from theta functions

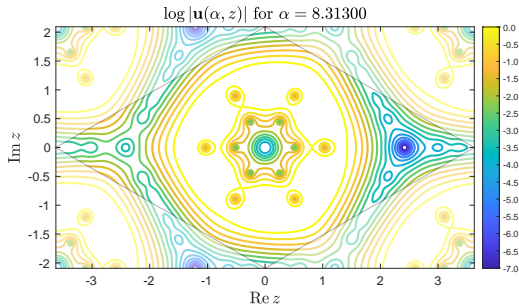
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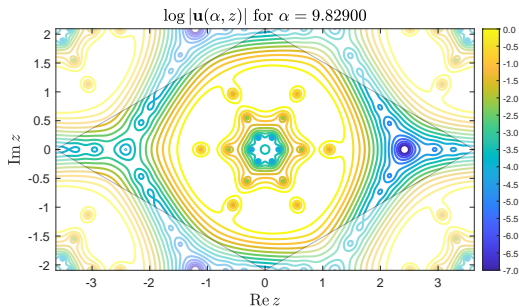
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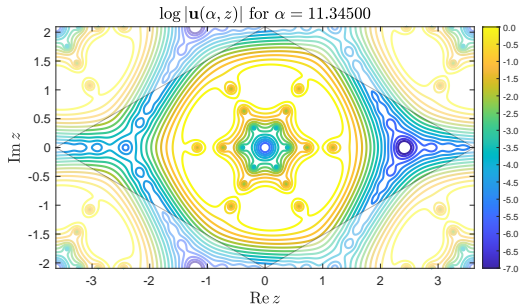
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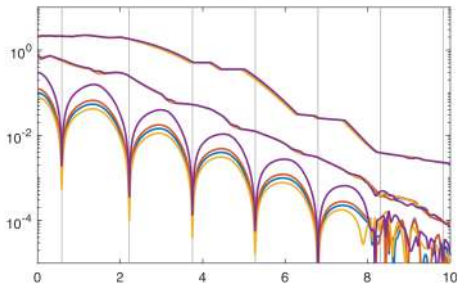
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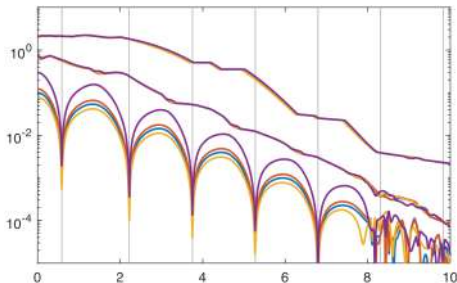
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Every **small** angle $\theta \sim 1/\alpha$ wants to be **magical**...

Exponential squeezing of bands via solvability of PDE

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$$Q = \sum_{|\alpha| \leq m} a_\alpha(x) (hD)^\alpha, \quad a_\alpha \in C^\omega, \quad a_\alpha(x, h) = a_\alpha^0(x) + ha_\alpha^1(x, h),$$

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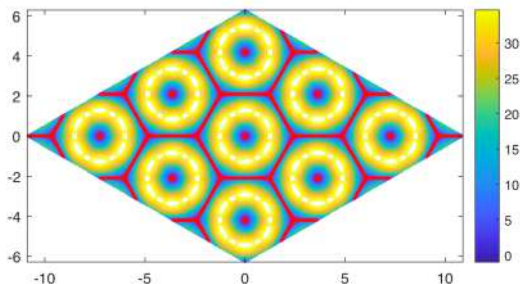
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A contour plot of

$$|\{q, \bar{q}\}|, \quad q(x, \xi) = 2\bar{\zeta} - U(z)U(-z), \quad z = x_1 + ix_2, \quad 2\zeta = \xi_1 - i\xi_2.$$

Integrated density of states To study the density of states, we introduce the regularized trace

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We then use the Helffer-Sjöstrand formula

$$f(T) = \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \widetilde{f}(z) (T - z)^{-1} \, dz$$

and find that

$$\widetilde{\mathrm{tr}}(f(P_{\mathrm{BM}}(h\mathbf{x}, D_{\mathbf{x}}))) = \sum_{j=0}^N h^j A_j(f) + \mathcal{O}(h^{N+1}).$$

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$$\widetilde{\mathrm{tr}}(f(P_{\mathrm{BM}})) = \frac{\theta^2}{4\pi^2} \int_{\mathcal{B}} \mathrm{tr}(\mathbf{1}_M f(H_{\mathrm{sem}}^{\mathbf{k}})) \, d\mathbf{k}.$$

We then use the Helffer-Sjöstrand formula

$$f(T) = \frac{1}{\pi} \int_{\mathbb{C}} \partial_{\bar{z}} \widetilde{f}(z) (T - z)^{-1} \, dz$$

and find that

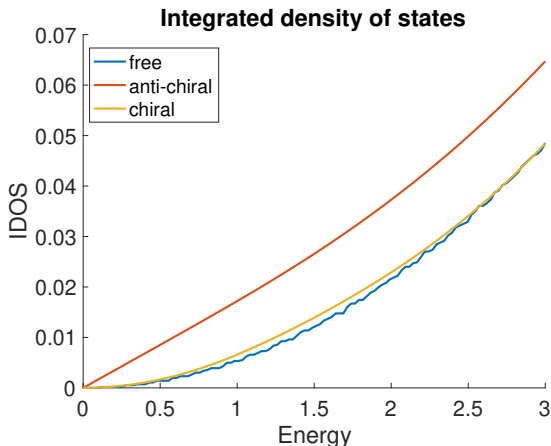
$$\widetilde{\mathrm{tr}}(f(P_{\mathrm{BM}}(h\mathbf{x}, D_{\mathbf{x}}))) = \sum_{j=0}^N h^j A_j(f) + \mathcal{O}(h^{N+1}).$$

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$$A_j(f) := \int_{\mathcal{B}} \int_{T^{\dagger}M} \int_{\mathbb{C}} \partial_{\bar{\lambda}} \widetilde{f}(\lambda) \\ \frac{\mathrm{tr}_{\mathbb{C}^2} \lambda \sigma_j \left((\lambda^2 - D^{\dagger}D)^{-1} + (\lambda^2 - DD^{\dagger})^{-1} \right) (\mu)}{16\pi^5} d\lambda d\mu d\mathbf{k}.$$

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