A framework to study twisted bilayer graphene in a tight binding model

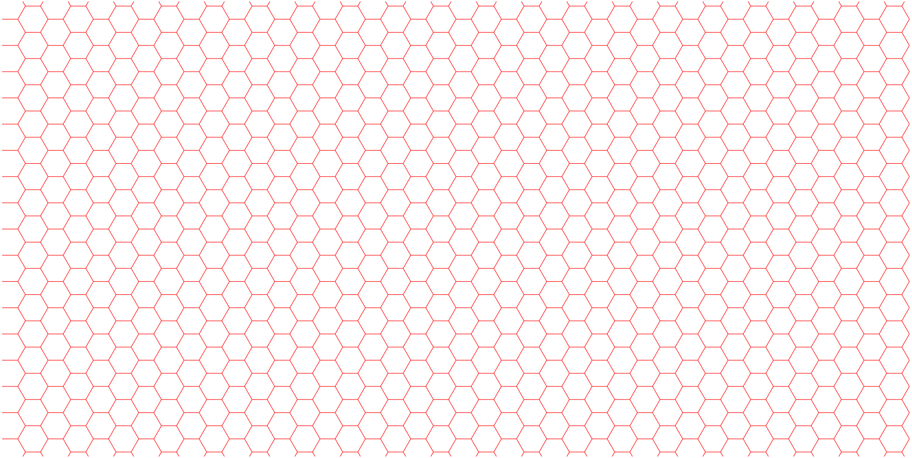
Ian Jauslin

joint with **Vieri Mastropietro**

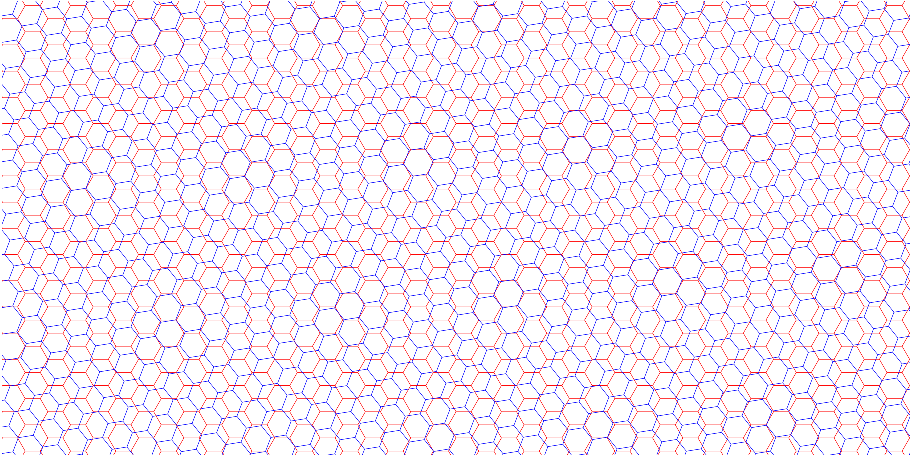
arXiv: 2510.12918

http://ian.jauslin.org

Graphene



Twisted Bilayer Graphene



Twisted Bilayer Graphene

- Two graphene sheets at an angle θ.
- Studied Theoretically [Bistritzer, MacDonald, 2011]
- Experimental realization: [Cao, Fatemi, Fang, Watanabe, Taniguchi, Kaxiras, Jarillo-Herrero, 2018]
- At certain specific angles ("magic angles"): flat bands, leading to unconventional superconductivity. [Oh, Nuckolls, Wong, Lee, Liu, Watanabe, Taniguchi, Yazdani, 2021]
- First (largest) Magic Angle: $\approx 1.05^\circ$ [Song, Wang, Shi, Li, Fang, Bernevig, 2019]

Model

- Graphene lattices: $\mathcal{L}_1$ and $\mathcal{L}_2$.
- Intra-layer: for $i = 1, 2$,

$$H_i = \sum_{x \sim y \in \mathcal{L}_i} c_{i,x}^\dagger c_{i,y}$$

- Inter-layer:

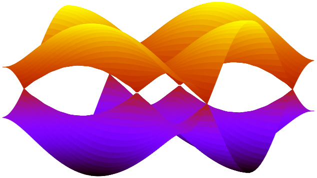
$$V = \lambda \sum_{x \in \mathcal{L}_1} \sum_{y \in \mathcal{L}_2} \phi(x - y)(c_{1,x}^\dagger c_{2,y} + c_{2,y}^\dagger c_{1,x})$$

- Total Hamiltonian

$$H = H_1 + H_2 + V.$$

Intra-layer model

- If $\lambda = 0$, $H = H_1 + H_2$: two independent graphene layers.
- Hamiltonian is diagonalizable in Fourier space: $\hat{H}(k) = \hat{H}_1(k) + \hat{H}_2(k)$
- Eigenvalues of $\hat{H}_i(k)$ as a function of k:



Intra-layer model

- Propagator for each layer ($\equiv$ correlation function):

$$g_i(k_0, k) := (ik_0 + \hat{H}_i(k))^{-1}$$

- Rotation: R_θ

$$g_1(k_0, k) \equiv g_2(k_0, R_\theta k)$$

- g_1 is singular at $p_F^\omega = (\frac{2\pi}{3}, \omega\frac{2\pi}{3\sqrt{3}})$ so g_2 is singular at $R_\theta p_F^\omega$.
- g_1 is periodic in b_1, b_2, g_2 is periodic in $R_\theta b_1, R_\theta b_2$ (notation: $R_\theta b_i =: b_i'$)

Main result

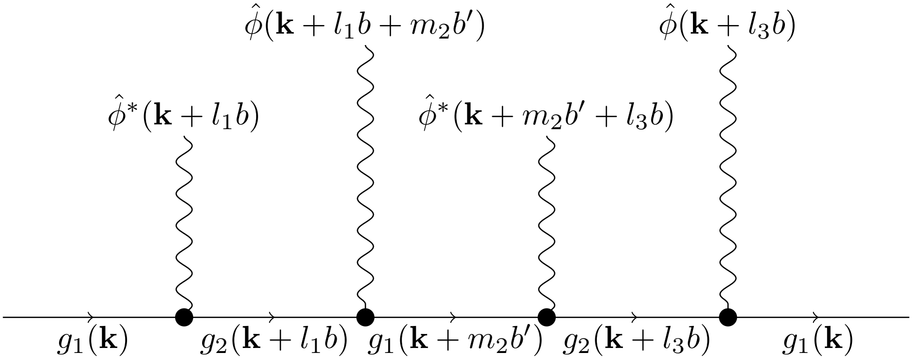
- **Theorem**: There exists a finite set $\mathcal{B}$ of pathological angles such that, if ϕ is short-ranged, and $\hat{\phi}(q) \leqslant ce^{-\kappa|q|}$ (plus a technical assumption), then, for any $\bar{\theta} \in [0, 2\pi) \setminus \mathcal{B}$, for any $\delta\theta$ small enough, for almost every $\theta \in [\bar{\theta} - \delta\theta, \bar{\theta} + \delta\theta]$, there exists λ_0 such that, for $\lambda < \lambda_0$ (and upon adding an appropriate counter-term to the Hamiltonian), the Schwinger function is close when $\lambda \ll 1$ to the intra-layer one near the Fermi points:

$$S_i(\mathbf{k} + \mathbf{p}_{F,i}) = \begin{pmatrix} -iZ_{j,\omega}k_0 & (iv_{i,\omega}k_1 - w_{i,\omega}\omega k_2) \\ (-iv^*_{i,\omega}k_1 - w^*_{i,\omega}\omega k_2) & -iZ_{j,\omega}k_0 \end{pmatrix}^{-1} (1 + O(\mathbf{k}^2))$$

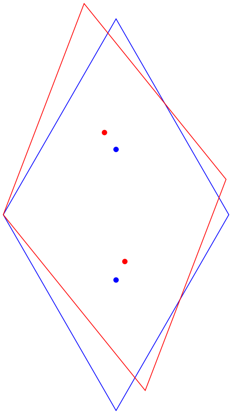
$$Z_{j,\omega} = 1 + O(\lambda) \in \mathbb{R}, \quad v_{i,\omega}, w_{i,\omega} = \frac{3}{2} + O(\lambda) \in \mathbb{C}$$

Perturbation theory

- Feynman diagram expansion for $S_{1,1}(\mathbf{k})$:



Small divisor problem (Umklapp)



Small divisor problem (Umklapp)

- Small divisor: for $l, m \in \mathbb{Z}^2$

$$|q_{i,j,\omega,\omega',l,m}| := |p_{F,i}^{\omega} - p_{F,j}^{\omega'} + l_1 b_1 + l_2 b_2 + m_1 b_1' + m_2 b_2'| \ll 1$$

  leads to a divergence in the propagators.

- However, such terms come with $\hat{\phi}(q_{i,j,\omega,\omega',l,m})$, which decays exponentially with l, m.

- Bistritzer-MacDonald model: truncate the small divisor problem: only keep 3 values of l, m. Here we keep all of them.

- Balance: we must ensure that for $|q_{i,j,\omega,\omega',l,m}|$ to be small, l, m have to be large enough to be dampened by the exponential decay of $\hat{\phi}$.

Diophantine condition

- For $i = j$, $\omega = \omega'$: choose θ such that

$$|l_1 b_1 + l_2 b_2 + m_1 R_\theta b_1 + m_2 R_\theta b_2| \geqslant \frac{C_0}{|l|^\tau}, \frac{C_0}{|m|^\tau}$$

- Complication: this is a two-dimensional condition, but there is only one parameter θ.
- The set of such θ's has arbitrarily high measure (at the price of decreasing C_0).
- This gives a constraint on how big l, m need to be for $|q|$ to be small. This, in turn, gives a lower bound on the rate of decay of diagrams due to the decay of $\hat{\phi}$.

Main result

- **Theorem**: There exists a finite set $\mathcal{B}$ of pathological angles such that, if ϕ is short-ranged, and $\hat{\phi}(q) \leqslant ce^{-\kappa|q|}$ (plus a technical assumption), then, for any $\bar{\theta} \in [0, 2\pi) \setminus \mathcal{B}$, for any $\delta\theta$ small enough, for almost every $\theta \in [\bar{\theta} - \delta\theta, \bar{\theta} + \delta\theta]$, there exists λ_0 such that, for $\lambda < \lambda_0$ (and upon adding an appropriate counter-term to the Hamiltonian), the Schwinger function is close when $\lambda \ll 1$ to the intra-layer one near the Fermi points:

$$S_i(\mathbf{k} + \mathbf{p}_{F,i}) = \begin{pmatrix} -iZ_{j,\omega}k_0 & (iv_{i,\omega}k_1 - w_{i,\omega}\omega k_2) \\ (-iv_{i,\omega}^* k_1 - w_{i,\omega}^* \omega k_2) & -iZ_{j,\omega}k_0 \end{pmatrix}^{-1} (1 + O(\mathbf{k}^2))$$

$$Z_{j,\omega} = 1 + O(\lambda) \in \mathbb{R}, \quad v_{i,\omega}, w_{i,\omega} = \frac{3}{2} + O(\lambda) \in \mathbb{C}$$

Fractal nature

- The dependence of λ_0 on θ is extremely rough (discontinuous almost everywhere).
- Reformulate the result from the point of view of fixing λ_0 and varying θ.

Main result

- **Theorem**: There exists a finite set $\mathcal{B}$ of pathological angles and an integer $\alpha \in \mathbb{N}$ such that, if ϕ is short-ranged, and $\hat{\phi}(q) \leqslant ce^{-\kappa|q|}$ (plus a technical assumption), then, for any $\bar{\theta} \in [0, 2\pi) \setminus \mathcal{B}$, for any $\delta\theta$ small enough, for any λ_0 there exists a subset of $[\bar{\theta} - \delta\theta, \bar{\theta} + \delta\theta]$ of measure $(1 - O(\lambda_0^\alpha))2\delta\theta$ such that, for $\lambda < \lambda_0$ (and upon adding an appropriate counter-term to the Hamiltonian), the Schwinger function is close when $\lambda \ll 1$ to the intra-layer one near the Fermi points:

$$S_i(\mathbf{k} + \mathbf{p}_{F,i}) = \begin{pmatrix} -iZ_{j,\omega}k_0 & (iv_{i,\omega}k_1 - w_{i,\omega}\omega k_2) \\ (-iv^*_{i,\omega}k_1 - w^*_{i,\omega}\omega k_2) & -iZ_{j,\omega}k_0 \end{pmatrix}^{-1} (1 + O(\mathbf{k}^2))$$

$$Z_{j,\omega} = 1 + O(\lambda) \in \mathbb{R}, \quad v_{i,\omega}, w_{i,\omega} = \frac{3}{2} + O(\lambda) \in \mathbb{C}$$

Fractal nature

- The set of θ's is a Cantor set, and depends very roughly on λ_0.
- In particular, this set of θ's certainly does not contain rational multiples of 2π.

(Counter term)

- The counter-term fixes the Fermi points. Without it, they would be shifted in momentum space.
- Form

$$\begin{pmatrix} 0 & \nu_{i,\omega} \\ \nu_{i,\omega}^* & 0 \end{pmatrix}$$

  with

$$\nu = O(\lambda) \in \mathbb{C}.$$

Renormalization group analysis

- Renormalization group: multiscale perturbation theory.
- Similar to RG for quasi-periodic potentials:
  - [Benfatto, Gentile, Mastropietro, 1997]
  - [Mastropietro, 2017]
  - [Gallone, Mastropietro, 2024].

Conclusion

- Our construction yields a framework to study twisted bilayers using absolutely convergent series.
- Can be extended fairly easily to interacting models.
- Main novelty: control of the Umklapp phenomenon.
- Next step: compute observables and study the flow of the beta function. Is there a signature of the magic angles in the perturbative regime $\lambda \ll 1$?