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

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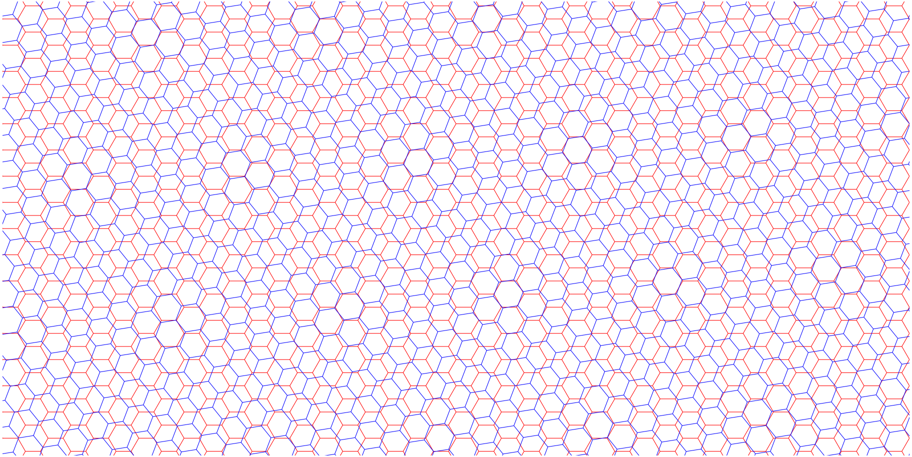
Twisted Bilayer Graphene



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: $\approx 1.05°$ [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:

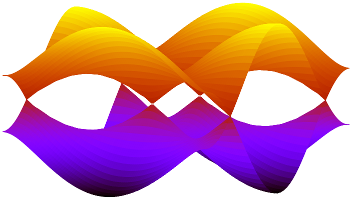
$$V = \lambda \sum_{x \in \mathcal{L}_1} \sum_{y \in \mathcal{L}_2} \phi(x-y)(c_{1,x}^\dagger c_{2,y} + c_{2,y}^\dagger c_{1,x})$$

- 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.



- Fermi points: singularities of two-point correlation.

Main result

- **Theorem**: If ϕ is short-ranged, and $\hat{\phi}(q) \leqslant ce^{-\kappa|q|}$ (plus a technical assumption), then, for any $[\theta_0, \theta_1] \subset [0, 2\pi)$ and any $C_0 > 0$, there exists a set of θ's that has large measure (its complement has measure at most $O(C_0/(\theta_0 - \theta_1)^2)$) for which (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:

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

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

Fourier space

- Fourier transform

$$\hat{c}_{1,k_1,\alpha} = \sum_{x \in \mathcal{L}_1 : \text{type } \alpha} e^{ik_1 x} c_{1,x}, \quad k_1 \in \hat{\mathcal{L}}_1 \equiv \text{span}\{b_1, b_2\}$$

$$\hat{c}_{2,k_2,\alpha} = \sum_{x \in \mathcal{L}_2 : \text{type } \alpha} e^{ik_2 x} c_{2,x}, \quad k_2 \in \hat{\mathcal{L}}_2 := R_\theta \hat{\mathcal{L}}_1$$

$$\hat{\phi}(q) = \sum_{x_1 \in \mathcal{L}_1,\ x_2 \in \mathcal{L}_2} e^{iq(x_1 - x_2)} \phi(x_1 - x_2), \quad q \in \mathbb{R}^2$$

Intra-layer term in Fourier space

- H_1, H_2 are diagonal in Fourier space:

$$H_1 = \frac{3\sqrt{3}}{8\pi^3} \int_{\hat{\mathcal{L}}_1} dk \ (\Omega(k)\hat{c}^\dagger_{1,k,\mathrm{a}}\hat{c}_{1,k,\mathrm{b}} + \Omega^*(k)\hat{c}^\dagger_{1,k,\mathrm{b}}\hat{c}_{1,k,\mathrm{a}})$$

$$H_2 = \frac{3\sqrt{3}}{8\pi^3} \int_{\hat{\mathcal{L}}_2} dk \ (\Omega(R_\theta^T k)\hat{c}^\dagger_{2,k,\mathrm{a}}\hat{c}_{2,k,\mathrm{b}} + \Omega^*(R_\theta^T k)\hat{c}^\dagger_{2,k,\mathrm{b}}\hat{c}_{2,k,\mathrm{a}})$$

with

$$\Omega(k_x, k_y) = 1 + 2e^{-i\frac{3}{2}k_x}\cos(\tfrac{\sqrt{3}}{2}k_y)$$

Inter-layer term in Fourier space

- Essentially,

$$V \approx \lambda \frac{3\sqrt{3}}{32\pi^4} \sum_{\alpha} \left(\sum_{l \in \mathbb{Z}^2} \int_{\hat{\mathcal{L}}_1} dk \; \hat{\phi}^*(k + lb) \hat{c}^\dagger_{1,k,\alpha} \hat{c}_{2,k+lb,\alpha} + \right.$$

$$\left. + \sum_{m \in \mathbb{Z}^2} \int_{\hat{\mathcal{L}}_2} dk \; \hat{\phi}(k + mb') \hat{c}^\dagger_{2,k,\alpha} \hat{c}_{1,k+mb',\alpha} \right)$$

where $lb \equiv l_1 b_1 + l_2 b_2$, $mb' \equiv m_1 b'_1 + m_2 b'_2$.

Perturbation theory

- Propagator for each layer

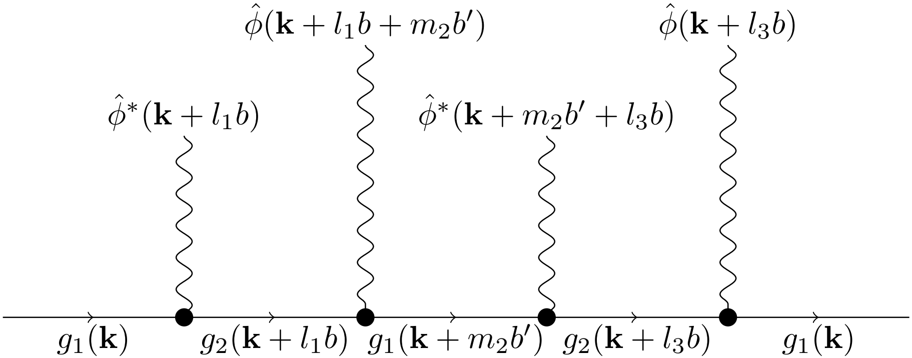
$$g_1(\mathbf{k}) := \begin{pmatrix} ik_0 & \Omega(k) \\ \Omega^*(k) & ik_0 \end{pmatrix}^{-1}, \quad g_2(\mathbf{k}) := \begin{pmatrix} ik_0 & \Omega(R_\theta^T k) \\ \Omega^*(R_\theta^T k) & ik_0 \end{pmatrix}^{-1}$$

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

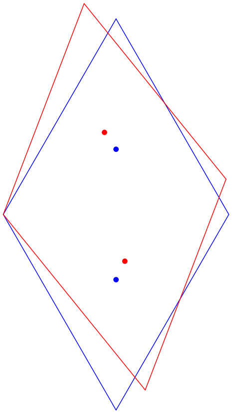
$$g_1(\mathbf{k} + p_F^\omega) \sim \frac{1}{|\mathbf{k}|}, \quad g_2(\mathbf{k} + R_\theta p_F^\omega) \sim \frac{1}{|\mathbf{k}|}$$

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 $\hat{\phi}$.

Aside: Diophantine condition in KAM theory

- **Theorem**: for any $\epsilon > 0$, $\tau > 2$, $f : [0, 2\pi)^2 \to \mathbb{R}^2$, f continuously differentiable, invertible, $|\det Df| > \beta > 0$,

$$\mu\left(\left\{(\theta_1, \theta_2) : \ \forall n \in \mathbb{Z}^2, \ |n \cdot f(\theta_1, \theta_2)| \geqslant \frac{\epsilon}{|n|^\tau}\right\}\right) \geqslant 4\pi^2 - O(\epsilon)$$

  where μ is the Lebesgue measure

- For almost all θ_1, θ_2, in order for $n \cdot f(\theta)$ to be small, $|n|$ must be large.

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**: If ϕ is short-ranged, and $\hat{\phi}(q) \leqslant ce^{-\kappa|q|}$ (plus a technical assumption), then, for any $[\theta_0, \theta_1] \subset [0, 2\pi)$ and any $C_0 > 0$, there exists a set of θ's that has large measure (its complement has measure at most $O(C_0/(\theta_0 - \theta_1)^2)$) for which (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:

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

(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 $\lambda \ll 1$?