

Exact ground state of interacting electrons in magic angle graphene

Lin Lin

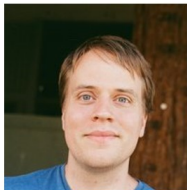
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Outline

Introduction

Main results (informal)

Main results and proof sketch

Open questions

Outline

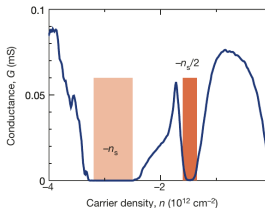
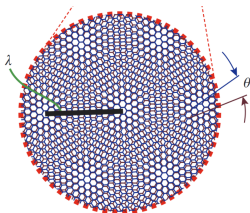
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Twisted bilayer graphene as a correlated insulator



- Flat bands predicted by Bistritzer-MacDonald in 2010, which shows a **simple metallic phase**.
- Experiments in 2018 showed a **correlated insulator phase** (at integer filling)
- Nature of electron correlation?

(Bistritzer-MacDonald PNAS 2010), (Cao et al, Nature 2018)

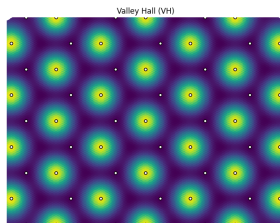
Exact ground states of FlatBand Interacting (FBI) Hamiltonian

- At chiral limit, single Slater determinants can be **exact** ground states of many-body Hamiltonian at integer-filling¹
- TBG is **strongly interacting** (beyond non-interacting) but not **strongly correlated** (beyond Hartree-Fock)?²

¹(Kang, Vafeek, PRL 2019), (Bultinck et al, PRX 2020), (Liu et al, PRR 2021), (Bernevig et al, PRB 2021)

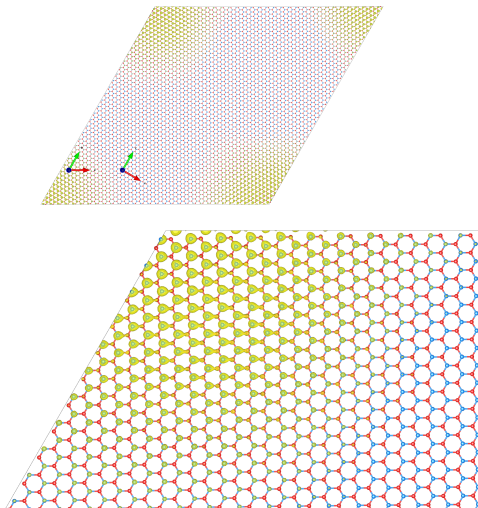
²(Soejima et al PRB 2020), (Faulstich et al PRB 2023)

Local Density of States (LDOS) of single valley ground state



- Sublattice polarized. “Valley hall” state in the two-valley model.
- “Ferromagnetic” Slater determinant.
- Flatband interacting Hamiltonian: smears out microscopic details. Only **sublattice** (σ) indices in each moire cell will matter later (defines the “ferromagnetism”)

Electron density of valley hall ground state



Acknowledgement: Raehyun Kim and Woochang Kim for ab initio simulation

Motivating questions

- Ground state is a single Slater determinant:
Very counter-intuitive viewed from Hubbard model.
- Algebraic structure underlying the exact ground state result?
- Generalization (multiple flatbands, multiple layers)?
- Unique ground states?

Chiral Hamiltonian for TBG-2

- Chiral BM Hamiltonian¹

$$H(\alpha) = \begin{bmatrix} 0 & D(\alpha)^\dagger \\ D(\alpha) & 0 \end{bmatrix}$$

$$\text{with } D(\alpha) = \begin{bmatrix} D_{x_1} + iD_{x_2} & \alpha U(\mathbf{r}) \\ \alpha U(-\mathbf{r}) & D_{x_1} + iD_{x_2} \end{bmatrix}$$

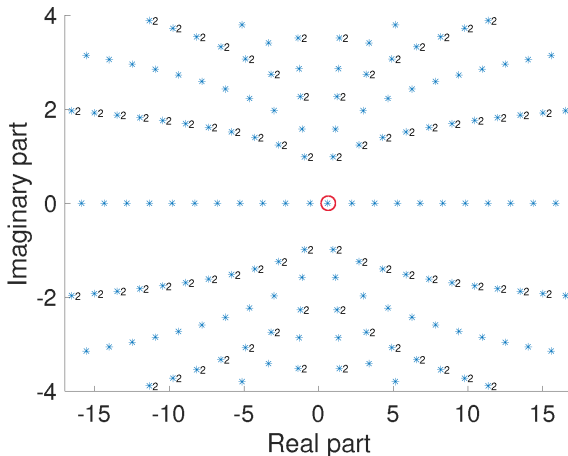
- Choice of $U(\mathbf{r})$:

$$U_0(\mathbf{r}) = \sum_{i=0}^2 \omega^i e^{-i\mathbf{q}_i \cdot \mathbf{r}} \quad (\omega = e^{2\pi i/3})$$

¹(Tarnopolsky, Kruchkov, Vishwanath, PRL 2019)

Magic angle and multiplicity of TBG-2

M = multiplicity of magic angle α . * means $M = 1$. $\#\mathcal{N} = 2M$
 $\mathcal{N} = \{-1, 1\}$ flat bands indices. For $U_0(\mathbf{r})$, $\#\mathcal{N} = 2$. (TBG-2)



Chiral Hamiltonian for TBG-4

- Chiral BM Hamiltonian

$$H(\alpha) = \begin{bmatrix} 0 & D(\alpha)^\dagger \\ D(\alpha) & 0 \end{bmatrix}$$

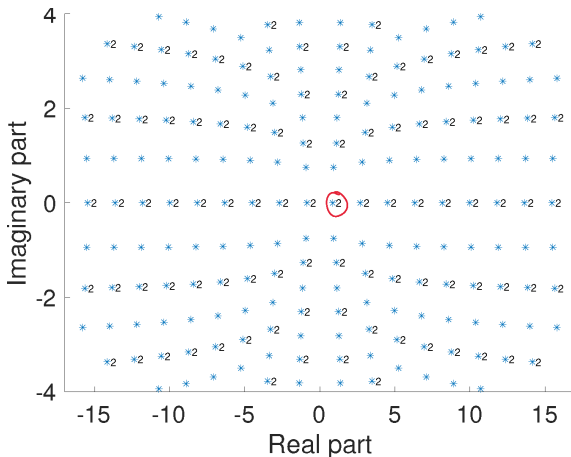
$$\text{with } D(\alpha) = \begin{bmatrix} D_{x_1} + iD_{x_2} & \alpha U(\mathbf{r}) \\ \alpha U(-\mathbf{r}) & D_{x_1} + iD_{x_2} \end{bmatrix}$$

- Alternate choice of $U(\mathbf{r})$:

$$U_{7/8}(\mathbf{r}) = \frac{1}{\sqrt{2}} \left(\sum_{i=0}^2 \omega^i e^{-i\mathbf{q}_i \cdot \mathbf{r}} - \sum_{i=0}^2 \omega^i e^{2i\mathbf{q}_i \cdot \mathbf{r}} \right)$$

Magic angle and multiplicity of TBG-4

M = multiplicity of magic angle α . * means $M = 1$. $\#\mathcal{N} = 2M$
 $\mathcal{N} = \{-2, -1, 1, 2\}$ flat bands indices. For $U_{7/8}(\mathbf{r})$, $\#\mathcal{N} = 4$
 (TBG-4).



Chiral Hamiltonian for Trilayer Graphene

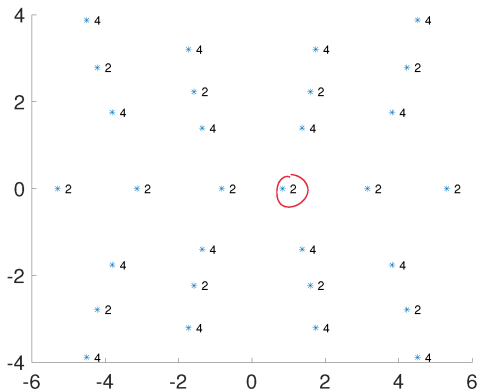
- For **equal twist angles** case same form as TBG, but $D(\alpha)$ replaced with

$$D(\alpha) = \begin{bmatrix} D_{x_1} + iD_{x_2} & \alpha U(\mathbf{r}) & 0 \\ \alpha U(-\mathbf{r}) & D_{x_1} + iD_{x_2} & \alpha U(\mathbf{r}) \\ 0 & \alpha U(-\mathbf{r}) & D_{x_1} + iD_{x_2} \end{bmatrix}$$

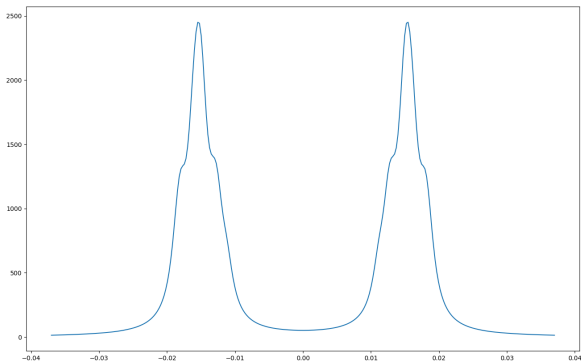
- Can have either 4 or 8 flat bands (we focus on $U = U_0(\mathbf{r})$, $\#\mathcal{N} = 4$).

Magic angle and multiplicity of eTTG-4

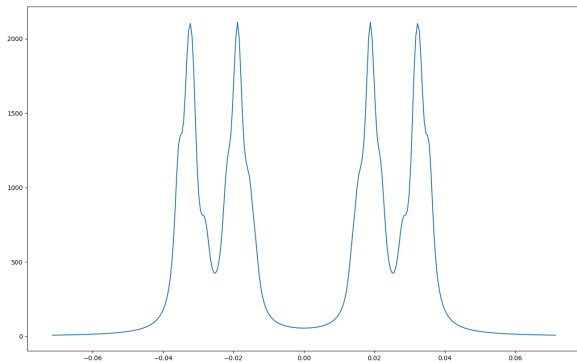
M = multiplicity of magic angle α . * means $M = 1$. $\#\mathcal{N} = 2M$
 $\mathcal{N} = \{-2, -1, 1, 2\}$ flat bands indices. For $U_0(\mathbf{r})$, $\#\mathcal{N} = 4$ (eTTG-4).



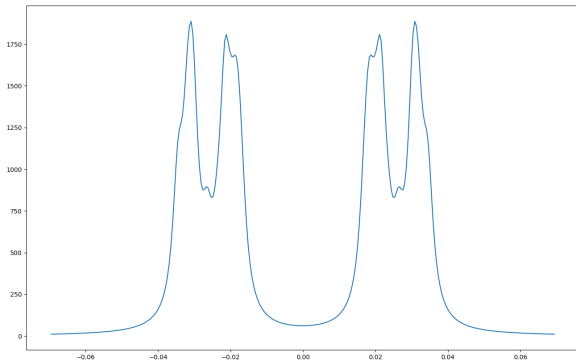
Total Density of States for Hartree-Fock ground state in TBG-2



Total Density of States for Hartree-Fock ground state in TBG-4



Total Density of States for Hartree-Fock ground state in eTTG-4



Outline

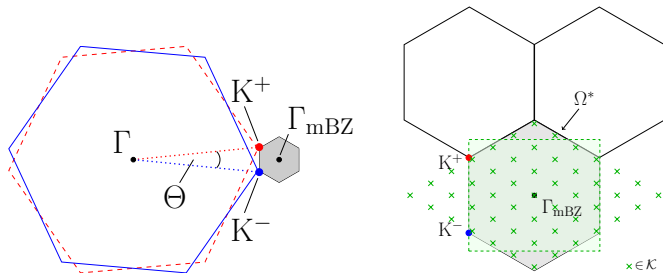
Introduction

Main results (informal)

Main results and proof sketch

Open questions

Second quantization



- Ω^* : moiré Brillouin zone. \mathcal{K} : discretization of Ω^* . **Single valley**
- At each $\mathbf{k} \in \mathcal{K}$, diagonalize BM Hamiltonian $H_{\text{BM}}(\mathbf{k})$, obtain flatbands $\{u_{n\mathbf{k}}\}$, $n \in \mathcal{N} = \{\pm 1, \dots, \pm M\}$.
- $\hat{f}_{n\mathbf{k}}^\dagger, \hat{f}_{n\mathbf{k}}$: creation, annihilation operators associated with $u_{n\mathbf{k}}$.

Flatband interacting (FBI) Hamiltonian

$$\hat{H}_{FBI} := \frac{1}{N_{\mathbf{k}}|\Omega|} \sum_{\mathbf{q}' \in \mathcal{K} + \Gamma^*} \hat{V}(\mathbf{q}') \hat{\rho}(\mathbf{q}') \hat{\rho}(-\mathbf{q}')$$

$$\hat{\rho}(\mathbf{q}') := \sum_{\mathbf{k} \in \mathcal{K}} \sum_{m, n \in \mathcal{N}} [\Lambda_{\mathbf{k}}(\mathbf{q}')]_{mn} \left(\hat{f}_{m\mathbf{k}}^\dagger \hat{f}_{n(\mathbf{k} + \mathbf{q}')} - \frac{1}{2} \delta_{mn} \sum_{\mathbf{G}} \delta_{\mathbf{q}', \mathbf{G}} \right).$$

- $\hat{V}(\mathbf{q}')$: Fourier transform of the (screened) Coulomb kernel.
- $\hat{V}(\mathbf{q}') \geq 0, \forall \mathbf{q}' \in \mathbb{R}^2$.
- Can show $\hat{\rho}(-\mathbf{q}') = \hat{\rho}(\mathbf{q}')^\dagger \Rightarrow \hat{H}_{FBI}$ is **positive semidefinite**.

Form Factor

- Normalization of $u_{n\mathbf{k}}(\mathbf{r}; \sigma, j)$, sublattice (σ) and layer (j)

$$\int_{\Omega} \sum_{\sigma, j} |u_{n\mathbf{k}}(\mathbf{r}; \sigma, j)|^2 d\mathbf{r} = 1.$$

- $\hat{u}_{n\mathbf{k}}(\mathbf{G}; \sigma, j)$: Fourier coefficients, $\mathbf{G} \in \Gamma^*$ reciprocal lattice vector

$$\hat{u}_{n\mathbf{k}}(\mathbf{G}; \sigma, j) := \int_{\Omega} e^{-i\mathbf{G}\cdot\mathbf{r}} u_{n\mathbf{k}}(\mathbf{r}; \sigma, j) d\mathbf{r}.$$

- **Form factor**: for $\mathbf{k} \in \mathcal{K}$, $\mathbf{q}' \in \mathbb{R}^2$

$$[\Lambda_{\mathbf{k}}(\mathbf{q}')]_{mn} := \frac{1}{|\Omega|} \sum_{\mathbf{G}' \in \Gamma^*} \sum_{\sigma, j} \overline{\hat{u}_{m\mathbf{k}}(\mathbf{G}'; \sigma, j)} \hat{u}_{n(\mathbf{k}+\mathbf{q}')}(\mathbf{G}'; \sigma, j).$$

Symmetries

- Sublattice symmetry \mathcal{Z}

$$\mathcal{Z}u(\mathbf{r}; \sigma, j) = \sigma u(\mathbf{r}; \sigma, j)$$

- $C_{2z}\mathcal{T}$ symmetry \mathcal{Q}

$$\mathcal{Q}u(\mathbf{r}; \sigma, j) = \overline{u(-\mathbf{r}; -\sigma, j)}$$

- Layer symmetry \mathcal{L}

$$\mathcal{L}u(\mathbf{r}; \sigma, j) = (-1)^j u(-\mathbf{r}; \sigma, N - j)$$

Symmetries and gauge fixing

- $Q (C_{2z} \mathcal{T})$ symmetry: gauge fixing (rotate $u_{n\mathbf{k}}$)

$$u_{(-n)\mathbf{k}}(\mathbf{r}; \sigma, j) = Q u_{n\mathbf{k}}(\mathbf{r}; \sigma, j) = \overline{u_{n\mathbf{k}}(-\mathbf{r}; -\sigma, j)}, \quad n \in \mathcal{N}.$$

- From \mathcal{Z} (sublattice) and $Q (C_{2z} \mathcal{T})$ symmetries

$$\Lambda_{\mathbf{k}}(\mathbf{q}') = \begin{bmatrix} A_{\mathbf{k}}(\mathbf{q}') & \\ & \overline{A_{\mathbf{k}}(\mathbf{q}')} \end{bmatrix}$$

Ferromagnetic Slater Determinants

Ferromagnetic Slater determinant (FSD) states fully fill one of the two chiral sectors (half filling)

$$|\Psi_+\rangle = \prod_{\mathbf{k}} \prod_{n>0} \hat{f}_{n\mathbf{k}}^\dagger |\text{vac}\rangle \quad |\Psi_-\rangle = \prod_{\mathbf{k}} \prod_{n<0} \hat{f}_{n\mathbf{k}}^\dagger |\text{vac}\rangle$$

Theorem (Informal)

With \mathcal{Z} , \mathcal{Q} , \mathcal{L} symmetries, FSD states are many-body ground states of the FBI Hamiltonian.

There is a positive **charge gap** \Rightarrow Correlated insulator phase.

Extension of exact ground state argument (Kang, Vafeek, PRL 2019), (Bultinck et al, PRX 2020) (Liu et al, PRR 2021), (Bernevig et al, PRB 2021), and charge gap argument (Bernevig et al, PRB 2021) for TBG-2.

Main result

Theorem (Informal)

*Under additional **non-degeneracy** assumptions, the FSD states are the only **translational invariant** Slater determinant ground states at half filling.*

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Frustration-free Hamiltonian

$$\hat{H} = \sum_I \hat{H}_I, \quad \hat{H}_I \succeq 0$$

- \hat{H} is **frustration-free** if $\exists |\psi\rangle$ s.t. $\hat{H}_I |\psi\rangle = 0$ for all I .
- Determining whether \hat{H} is frustration-free is known as the quantum satisfiability (QSAT) problem.
- Usually \hat{H}_I is a local operator¹.
- \hat{H}_{ICM} is frustration-free and each \hat{H}_I is **nonlocal**.

¹(Sattah et al PNAS 2016)

FSD states are ground states

$$\hat{H}_{FBI} = \frac{1}{N_{\mathbf{k}}|\Omega|} \sum_{\mathbf{q}' \in \mathcal{K} + \Gamma^*} \hat{V}(\mathbf{q}') \hat{\rho}(\mathbf{q}') \hat{\rho}(-\mathbf{q}')$$

- \hat{H}_{FBI} positive semidefinite \Rightarrow Find $|\Psi\rangle$ so that $\forall \mathbf{q}, \hat{\rho}(-\mathbf{q}') |\Psi\rangle = 0$.
- For FSD states have

$$\hat{\rho}(-\mathbf{q}') |\Psi_{FSD}\rangle = \frac{1}{2} \left(\sum_{\mathbf{G}' \in \Gamma^*} \delta_{\mathbf{q}', \mathbf{G}'} \right) \left(\sum_{\mathbf{k} \in \mathcal{K}} \text{Im}(\text{Tr}(A_{\mathbf{k}}(\mathbf{q}')))) \right) |\Psi_{FSD}\rangle$$

- \mathcal{L} (layer) symmetry gives **sum rule**

$$\sum_{\mathbf{k} \in \mathcal{K}} \text{Im}(\text{Tr}(A_{\mathbf{k}}(\mathbf{G}))) = 0, \quad \forall \mathbf{G} \in \Gamma^*.$$

Translational invariance

- 1-RDM $[P(\mathbf{k}, \mathbf{k}')]_{nm} = \langle \Psi | \hat{f}_{m\mathbf{k}'}^\dagger \hat{f}_{n\mathbf{k}} | \Psi \rangle$.

$$P = \begin{pmatrix} P(\mathbf{k}_1, \mathbf{k}_1) & P(\mathbf{k}_1, \mathbf{k}_2) & \cdots & P(\mathbf{k}_1, \mathbf{k}_{N_k}) \\ P(\mathbf{k}_2, \mathbf{k}_2) & P(\mathbf{k}_2, \mathbf{k}_2) & \cdots & P(\mathbf{k}_2, \mathbf{k}_{N_k}) \\ \vdots & \vdots & \ddots & \vdots \\ P(\mathbf{k}_{N_k}, \mathbf{k}_{N_k}) & P(\mathbf{k}_{N_k}, \mathbf{k}_2) & \cdots & P(\mathbf{k}_{N_k}, \mathbf{k}_{N_k}) \end{pmatrix}$$

- Translational invariance

$$P = \begin{pmatrix} P(\mathbf{k}_1, \mathbf{k}_1) & 0 & \cdots & 0 \\ 0 & P(\mathbf{k}_2, \mathbf{k}_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & P(\mathbf{k}_{N_k}, \mathbf{k}_{N_k}) \end{pmatrix}$$

- If $|\Psi\rangle$ is a single Slater determinant: alternative characterization
 $P^2(\mathbf{k}, \mathbf{k}) = P(\mathbf{k}, \mathbf{k})$

Uniqueness (May, Flatiron)

Theorem (Informal)

Generically, FSD states are the only *translational invariant* Slater determinant ground states of \hat{H}_{FBI} at half filling.

Uniqueness

Theorem

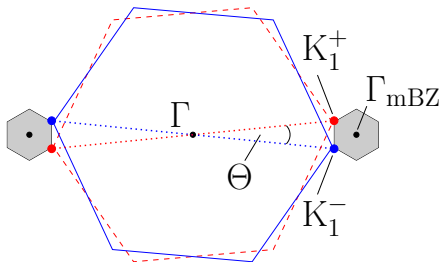
Assume \mathcal{K} is a sufficiently fine grid. If $\exists \mathbf{k} \in \mathcal{K}$,

1. (Finite energy penalty of local flip) for some $\mathbf{G} \in \Gamma^*$,
 $\text{Im Tr}(A_{\mathbf{k}}(\mathbf{G})) \neq 0$
2. (No hidden invariant subspace) for all non-trivial orthogonal projectors Π (i.e. $\Pi \neq 0, I$), there exists a $\mathbf{G} \in \Gamma^*$ so that

$$\|(I - \Pi)A_{\mathbf{k}}(\mathbf{G})\Pi\| > 0$$

then FSD states are the only *translational invariant* Slater determinant ground states of \hat{H}_{FBI} at half filling.

Why non-degeneracy conditions? Two-valley model



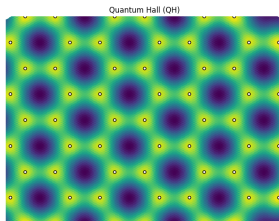
For two-valley models, for all $\mathbf{k} \in \Omega^*$ and $\mathbf{G} \in \Gamma^*$

- $\text{Im Tr}(A_{\mathbf{k}}(\mathbf{G})) = 0$ (no energy penalty)
- $A_{\mathbf{k}}(\mathbf{G})$ are simultaneously block diagonalizable (invariant subspace)

With spins, this gives $U(4) \times U(4)$ “hidden” symmetry¹

¹(Bultinck et al PRX 2020) (Bernevig et al, PRB 2021)

Local Density of States (LDOS) of other possible ground states in two valley model



- “Quantum hall” state. **Not** sublattice polarized.
- Many other competing states¹

¹(Hong, Soeijima, Zaletel, PRL 2022) (Nuckolls et al, Nature 2023)

Concrete Examples of Main Result

- **No hidden invariant subspace** condition is difficult to check ¹
- Conditions for two band and four band can be simplified.
- Explicit verification of **non-degeneracy conditions** using Jacobi θ functions and Weierstrass \wp functions for Twisted Bilayer Graphene with 2 flat bands (TBG-2), Twisted Bilayer Graphene with 4 flat bands (TBG-4), Equal Twist Angle Trilayer Graphene with 4 flat bands (eTTG-4)

¹(Al-Dweik et al, 2103.08316)

Specialization to Two and Four Bands

Corollary (Two Band Case, e.g., TBG-2)

If $|\mathcal{N}| = 2$, it is sufficient to check there exists a $\mathbf{k} \in \mathcal{K}$ so that

- For some \mathbf{q}' , $\text{Im Tr}(A_{\mathbf{k}}(\mathbf{q}')) \neq 0$.

Corollary (Four Band Case, e.g., TBG-4, eTTG-4)

If $|\mathcal{N}| = 4$, it is sufficient to check there exists a $\mathbf{k} \in \mathcal{K}$ so that

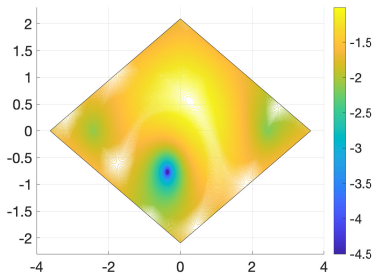
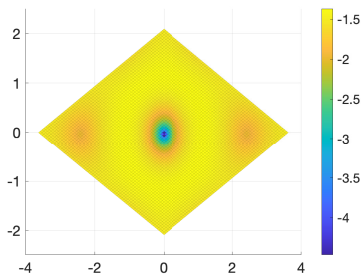
1. For some \mathbf{q}' , $\text{Im Tr}(A_{\mathbf{k}}(\mathbf{q}')) \neq 0$,
2. (No simultaneous diagonalization) For some \mathbf{q}'' , \mathbf{q}''' , $[A_{\mathbf{k}}(\mathbf{q}''), A_{\mathbf{k}}(\mathbf{q}''')] \neq 0$.

Example: TBG-2

- $\text{Im}(A_{\mathbf{k}}(\mathbf{q}')) \neq 0$ equiv. to $\|u_{\mathbf{k}}(\mathbf{r})\| \neq \|u_{\mathbf{k}}(-\mathbf{r})\|$ for some $\mathbf{r} \in \Omega$.

$$\mathbf{u}_{\mathbf{k}}(\mathbf{r}) = \mathbf{u}_0(\mathbf{r}) e^{\frac{(k_1 + ik_2)}{2}(-i(1+\omega)x_1 + (\omega-1)x_2)} \frac{\theta\left(\frac{3(x_1 + ix_2)}{4\pi i\omega} + \frac{k_1 + ik_2}{\sqrt{3}\omega}\right)}{\theta\left(\frac{3(x_1 + ix_2)}{4\pi i\omega}\right)}$$

- Below, $\log(\|u_{\mathbf{k}}(\mathbf{r})\|)$ for $\mathbf{k} = (0, 0)$ (left) and $\mathbf{k} \neq (0, 0)$ (right)



Proof strategy of main result

- Hartree-Fock energy (no **extra** quadratic term)

$$E_{HF}[P] = E_H[P] + E_F[P].$$

$$\min_P E_{HF}[P] \geq \min_P E_H[P] + \min_P E_F[P] \geq 0.$$

- P needs to simultaneously minimize Hartree and Fock.

Minimize **Fock energy** requires

- Uniform filling: $\text{Tr}[P(\mathbf{k})] = M$ for all \mathbf{k}
- No intra-band rotations for the **special** \mathbf{k} satisfying non-degeneracy condition.
- Fine \mathbf{k} mesh and continuity: no intra-band rotation for all \mathbf{k} .
- Fixes ferromagnetic ground state (which minimizes Hartree).

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Open questions

- Strengthen assumptions to rule out translational symmetry breaking? (solving a set of Sylvester equations)
- Uniqueness of many-body ground states?
- Two-valley model. Uniqueness up to $U(4) \times U(4)$ symmetry and other integer fillings?
- TTG with non-equal twisting angle, helical TTG?
- Beyond chiral limit: Importance of material details and *ab initio* modeling
- Is MATBG ever strongly correlated? (FQHE; Finite temperature; Doping)

Acknowledgment

Thank you for your attention.

We are hiring!

Lin Lin

<https://math.berkeley.edu/~linlin/>



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Notational Setup

- N : number of layers
- \mathcal{N} : set of flat bands
- Γ^* : reciprocal moiré lattice
- Ω, Ω^* : moiré unit cell and moiré Brillouin zone
- $u_{n\mathbf{k}}$: periodic Bloch functions $u_{n\mathbf{k}} : \Omega \rightarrow \mathbb{C}^2 \times \mathbb{C}^N$
- \mathcal{K} : discrete set of momenta $\subseteq \Omega^*$
- $N_{\mathbf{k}}$: number of elements in \mathcal{K}

Discretization of the Brillouin Zone

- We discretize the Brillouin zone by fixing (n_{k_x}, n_{k_y}) odd and taking \mathcal{K} to be the set:

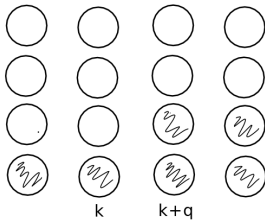
$$\left\{ \left(\frac{2i - n_{k_x} - 1}{2n_{k_x}} \right) \mathbf{g}_1 + \left(\frac{2j - n_{k_y} - 1}{2n_{k_y}} \right) \mathbf{g}_2 : i \in [n_{k_x}], j \in [n_{k_y}] \right\}$$

Under this definition $\mathbf{0} \in \mathcal{K}$ and $\mathcal{K} = -\mathcal{K}$

- For technical reasons, must choose n_{k_x}, n_{k_y} to be sufficiently large.

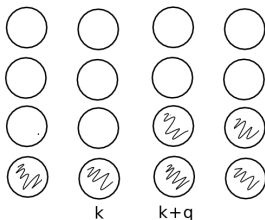
Uniformly Filled States are Optimal

- Suppose you had two neighboring points \mathbf{k} and $\mathbf{k} + \mathbf{q}$ with different fillings.



Uniformly Filled States are Optimal

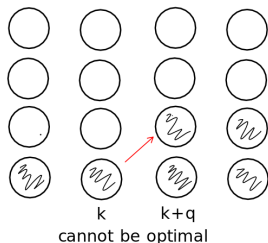
- Suppose you had two neighboring points \mathbf{k} and $\mathbf{k} + \mathbf{q}$ with different fillings.



- Since \mathbf{k} and $\mathbf{k} + \mathbf{q}$ are close, overlap between \mathbf{k} and $\mathbf{k} + \mathbf{q}$ is bounded away from zero.

Uniformly Filled States are Optimal

- Suppose you had two neighboring points \mathbf{k} and $\mathbf{k} + \mathbf{q}$ with different fillings.



- Since \mathbf{k} and $\mathbf{k} + \mathbf{q}$ are close, overlap between \mathbf{k} and $\mathbf{k} + \mathbf{q}$ is bounded away from zero.
- Non-trivial overlap + different filling implies exchange energy must be smaller than true minimizer. Contradiction.

Optimization over Local Rotations

- Proof is a fairly involved calculation, but key mechanism can be understood with 2 bands.
- Can parameterize Hartree-Fock state by 1-body reduced density matrices $P(\mathbf{k})$:

$$P(\mathbf{k}) = \frac{1}{2}I + \frac{1}{2} \begin{bmatrix} \cos(\theta(\mathbf{k})) & \sin(\theta(\mathbf{k}))e^{i\phi(\mathbf{k})} \\ \sin(\theta(\mathbf{k}))e^{-i\phi(\mathbf{k})} & -\cos(\theta(\mathbf{k})) \end{bmatrix}$$

- For simplicity, take $\phi(\mathbf{k}) = 0$ so $P(\mathbf{k})$ is purely real.

Optimization over Local Rotations

- Minimizing exchange energy leads to the expression

$$\begin{aligned}
 & -|A_{\mathbf{k}}(\mathbf{q}')|^2 \cos(\theta(\mathbf{k})) \cos(\theta(\mathbf{k} + \mathbf{q}')) \\
 & \quad - |\operatorname{Re}(A_{\mathbf{k}}(\mathbf{q}'))|^2 \sin(\theta(\mathbf{k})) \sin(\theta(\mathbf{k} + \mathbf{q}'))
 \end{aligned}$$

- Under assumptions, $A_{\mathbf{k}}(\mathbf{q}') \neq \operatorname{Re}(A_{\mathbf{k}}(\mathbf{q}'))$ for some $\mathbf{k}, \mathbf{q}' \rightarrow$ pick $\cos(\theta(\mathbf{k})) = 1$ or $\cos(\theta(\mathbf{k})) = -1$ for all \mathbf{k} .
 - This gives the FSD states.
- For $2N$ -bands, proof involves parameterizing $\operatorname{Gr}(N, 2N)$ and performing similar calculations.