

New Physics in Moiré Flat Bands

Erez Berg

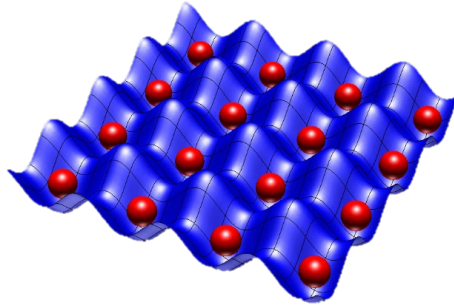
**Ari Turner (Technion), Ady Stern (WIS),
Johannes Hofmann (WIS), Eslam Khalaf (Harvard),
Ashvin Vishwanath (Harvard), Jong Yeon Lee (KITP)**



Creating flat bands

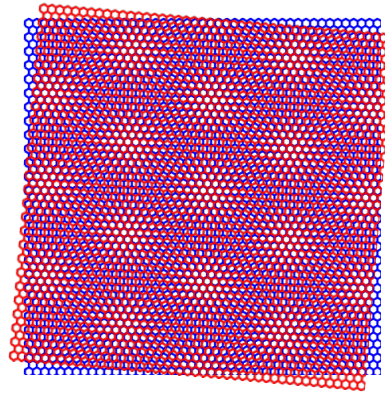
Moiré is different. -G. Baskaran

Electrons on a Lattice

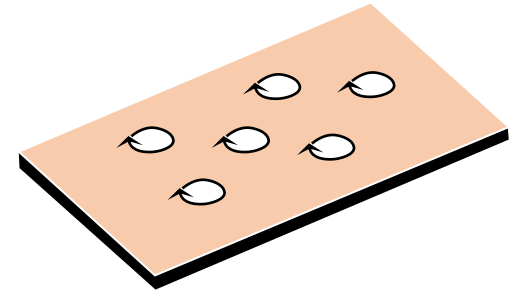


Localized

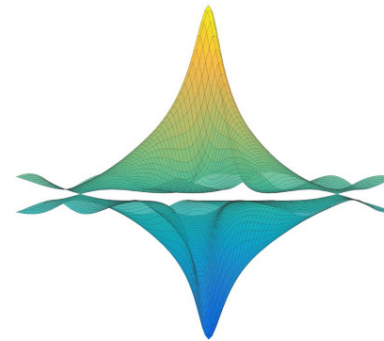
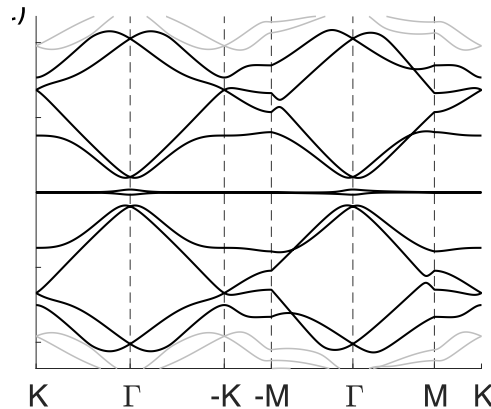
Magic angle graphene



Landau levels



Extended
topological



Po, Zou, Senthil, Vishwanath (2019)

R. Bistritzer and A. MacDonald (2011); Y. Cao, P. Jarillo-Herrero et al. (2018);...

Twisted bilayer graphene at charge neutrality

- **What *could* happen?**

Constraints on interaction-driven insulators by topology

Ari Turner, EB, Ady Stern, arXiv:2104.09528

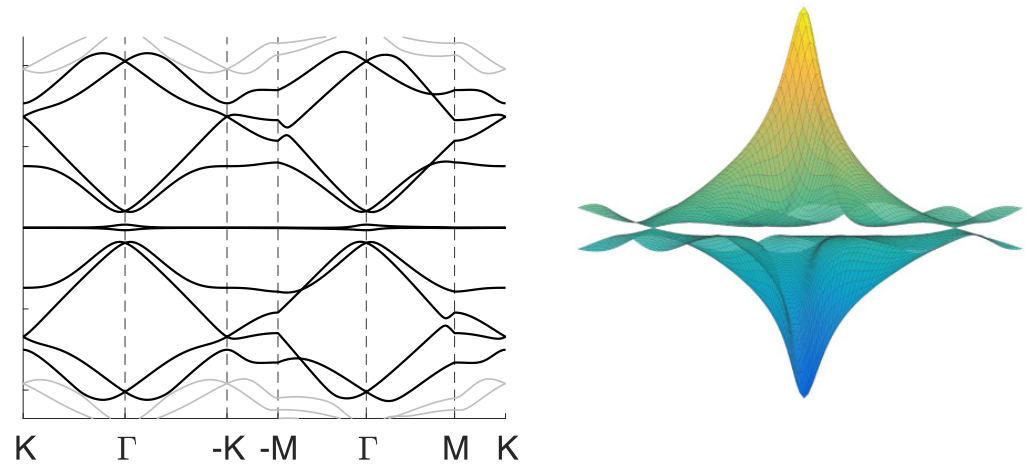
- **What *does* happen?**

Sign-free QMC simulations of TBG at charge neutrality

Johannes Hofmann, Eslam Khalaf, Ashvin Vishwanath, EB, Jong-Yeon Lee, arXiv:2105.12112

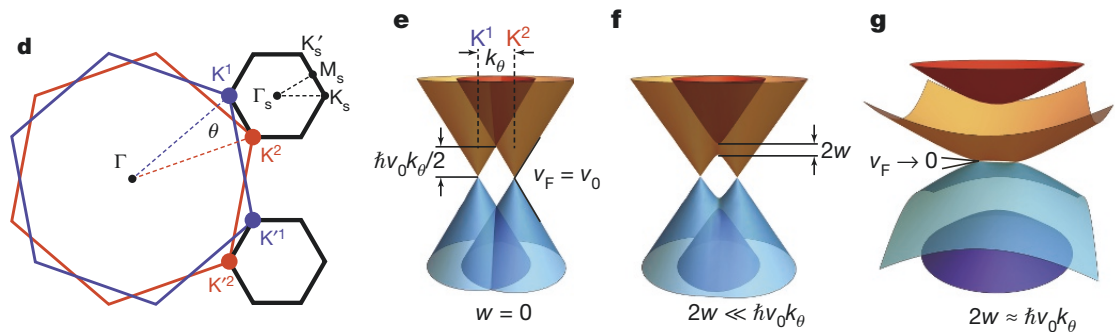
What's topological in MATBG?

- Dirac points protected by product of \mathcal{C}_π^Z and \mathcal{T}



*Po, Zou, Senthil, Vishwanath (2019);
Calculation for Bistritzer-MacDonald model*

- “Chirality” of the two Dirac points is the same!



Cao, Jarillo-Herrero et al. (2018)

Fragile topology

Po, Vishwanath, et al. (2017)

A toy 4-band model with $\mathcal{C}_\pi^z \mathcal{T}$ symmetry $\mathcal{C}_\pi^z \mathcal{T} = \sigma^z \tau^x \mathcal{K}$

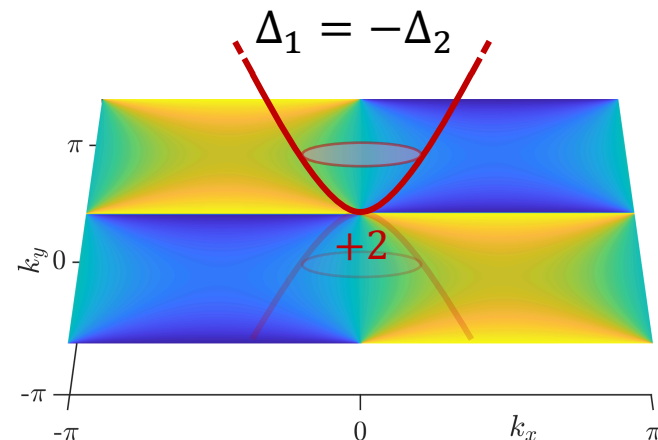
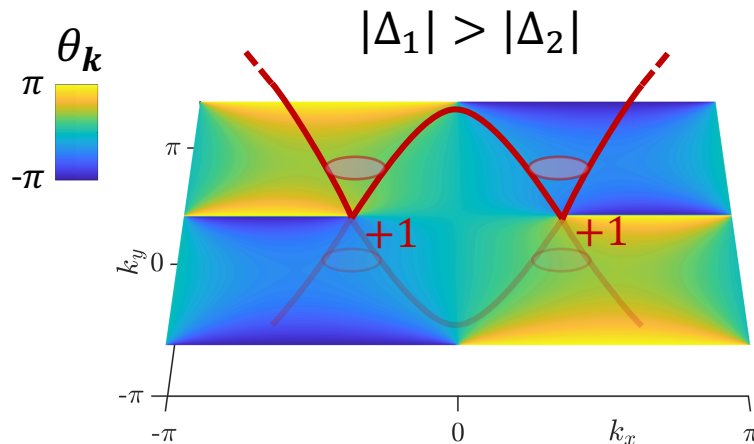
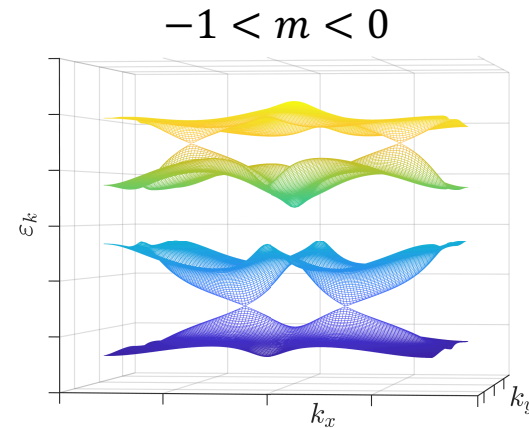
$$H_{\mathbf{k}} = \left(m + \sin^2 \frac{k_x}{2} + \sin^2 \frac{k_y}{2} \right) \sigma^z + \tau^z \sigma^x \sin k_x + \sigma^y \sin k_y + \Delta_1 \tau^x + \Delta_2 \sigma^z \tau^x$$

Smooth, real basis for lower bands:

$$|u_{1,2}(\mathbf{k})\rangle, \eta^z |u_{1,2}(\mathbf{k})\rangle = \pm |u_{1,2}(\mathbf{k})\rangle$$

Projected Hamiltonian:

$$H_{\text{eff}}(\mathbf{k}) = h_{\mathbf{k}} (\cos \theta_{\mathbf{k}} \eta^z + \sin \theta_{\mathbf{k}} \eta^x)$$



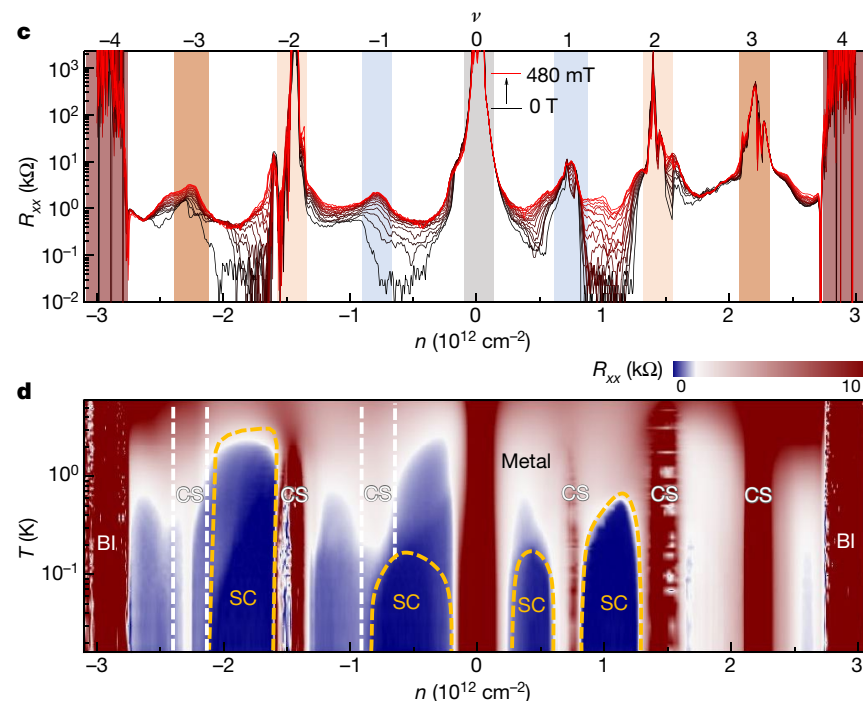
Gap at charge neutrality?

Without interactions: at **charge neutrality**, if the active bands are **separated** from the rest of the spectrum, the system is metallic unless a symmetry (e.g. $\mathcal{C}_\pi^Z \mathcal{T}$) is broken.*

* *Translation symmetry breaking can also open a gap: Kang, Vafek (2019)*

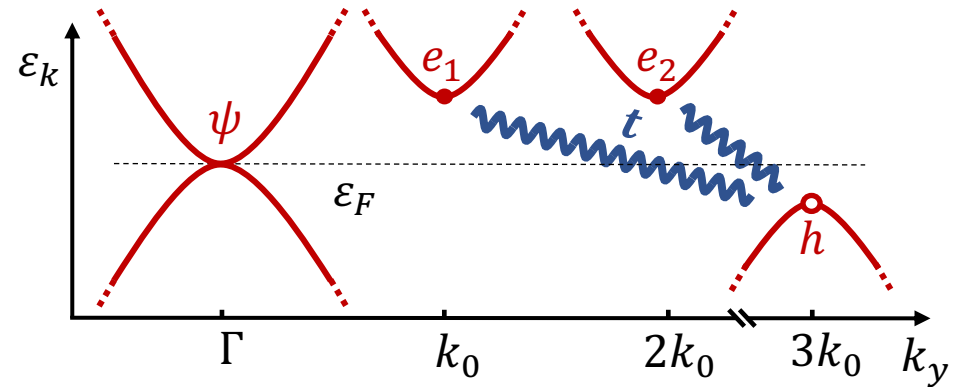
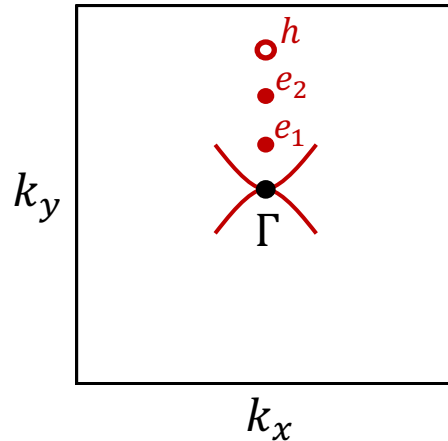
**Q. With strong interactions,
are there other options?
Topological order?
“Featureless” insulator?**

*Gap at charge neutrality (theory):
Xie, MacDonald (2020); Bultnik, Khalaf et al. (2020); Liao, Kang, Meng et al. (2021)*



*Gap at charge neutrality in MATBG
Lu, Efetov et al. (2018)*

Gap opening by interactions



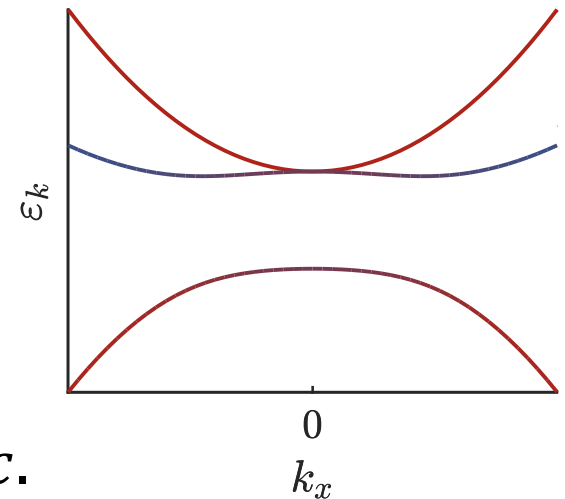
1. Turn on interaction:

$$H_{int,1} = -|V_1|(e_1^\dagger e_1 + e_2^\dagger e_2)h^\dagger h$$

\Rightarrow “Trion” $t^\dagger = e_1^\dagger e_2^\dagger h^\dagger$ bound state near Γ

2. Turn on trion-electron hybridization:

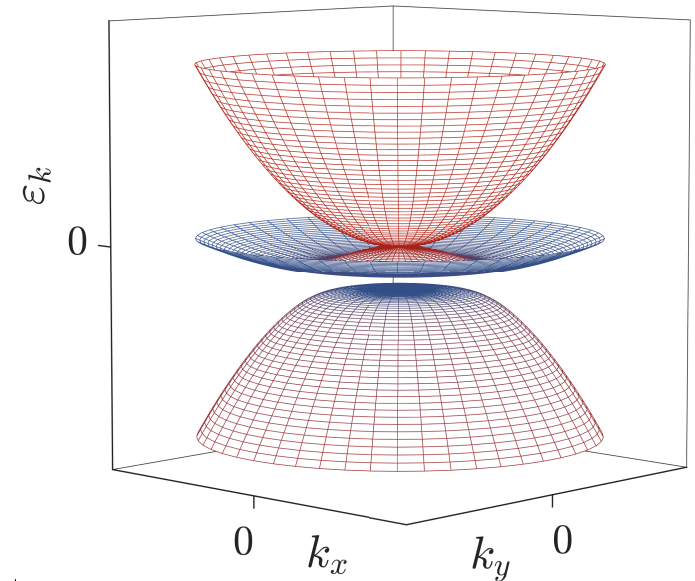
$$H_{int,2} = V_2(h^\dagger e_1^\dagger e_2^\dagger \psi + h.c.) \sim t^\dagger \psi + h.c.$$



Gap opening by interactions

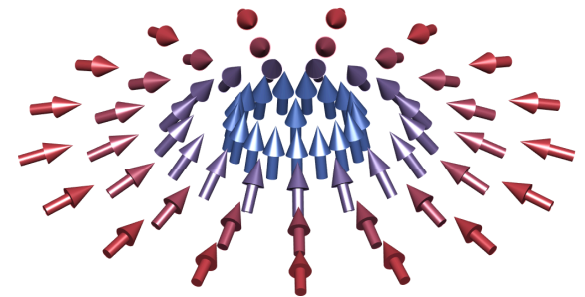
Near $\mathbf{k} = 0$, 3×3 effective real Hamiltonian:

$$H_{\text{eff}} = \begin{pmatrix} \overbrace{\begin{matrix} k_y^2 - k_x^2 & -2k_x k_y \\ -2k_x k_y & k_x^2 - k_y^2 \end{matrix}}^{\text{electrons}} & \overbrace{\begin{matrix} \alpha k_x \\ \alpha k_y \\ \frac{k^2}{2m_t} - E_0 \end{matrix}}^{\text{trions}} \end{pmatrix}$$



Wavefunction of lowest band:

Note: not possible with a single Dirac point (π Berry phase)



Twisted bilayer graphene at charge neutrality

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Ari Turner, EB, Ady Stern, arXiv:2104.09528

- **What *does* happen?**

Sign-free QMC simulations of TBG at charge neutrality

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Johannes Hofmann (WIS)



Eslam Khalaf (Harvard)



Jong Yeon Lee (KITP)

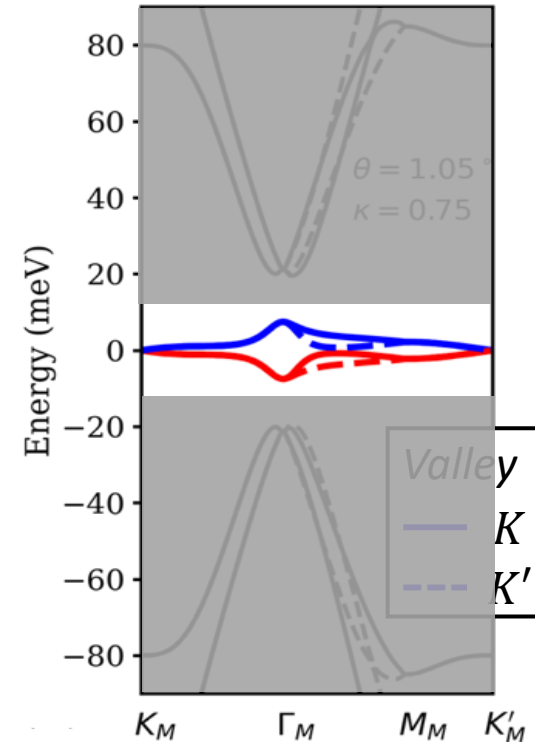
Many-body simulations of twisted bilayer graphene

- No localized Wannier description of narrow bands: k-space description required
- 2 bands, 2 valleys, 2 spins = 8 degrees of freedom per unit cell
- Long-range Coulomb interactions

T = 0 simulations of TBLG:

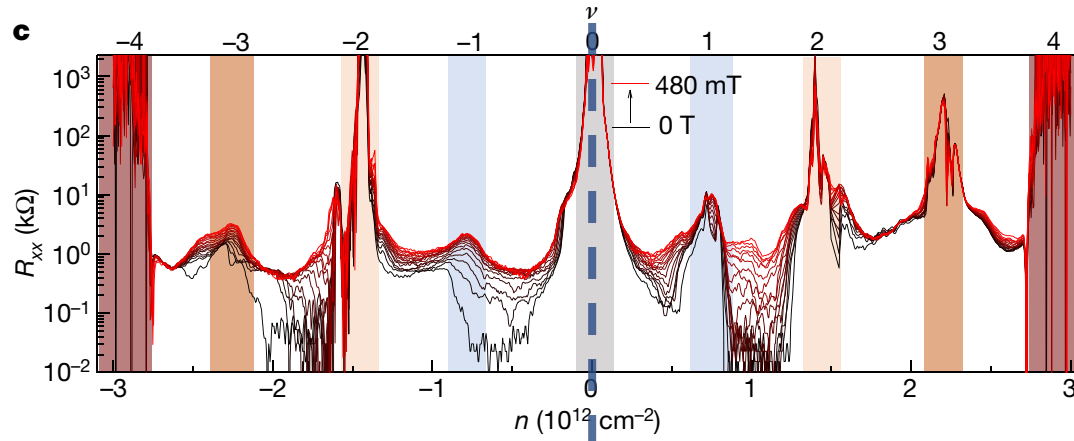
ED: *Repellin, Senthil et al. (2020); Xie, Regnault et al. (2021); Potasz, MacDonald et al (2021),...*

DMRG: *Kang, Vafek (2020); Soejima, Zaletel et al. (2020); Chatterjee, Zaletel (2020)*

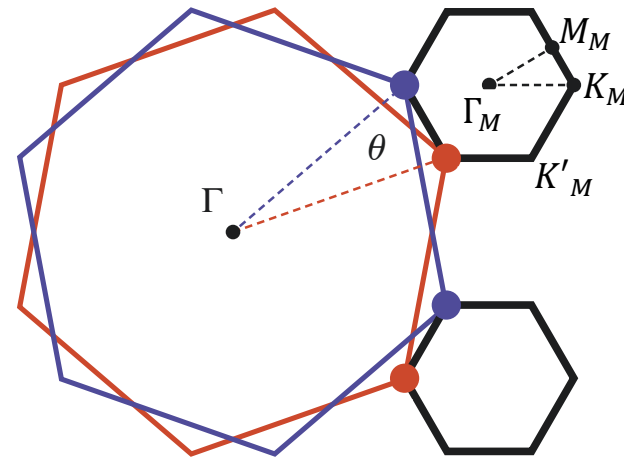
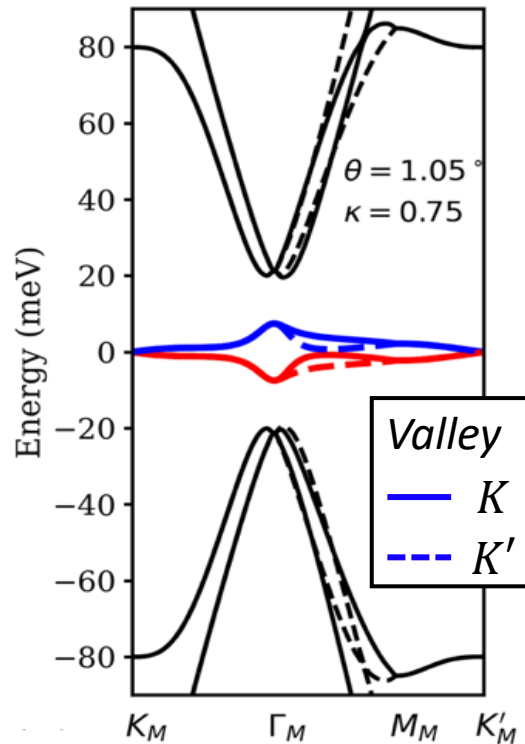


This work: sign-free momentum space quantum Monte Carlo simulations at $\nu = 0$, enabled by particle-hole symmetry

Particle-hole symmetry at $\nu = 0$?



Lu, Efetov et al. (2018)



Many-body Hamiltonian

“Standard model” of TBLG:

$$H = \hat{H}_{BM} + \hat{V}$$

$$\hat{H}_{BM} = \int d^2r c^\dagger (H_g + H_T) c \quad \hat{V} = \frac{1}{2} \sum_{\mathbf{q}} V_{\mathbf{q}} \delta\rho_{\mathbf{q}} \delta\rho_{-\mathbf{q}}$$

$$c^\dagger = (c^\dagger_{\sigma, \mu, s, \tau})$$

σ : sublattice, μ : layer, s : spin, τ : valley

Isolated
graphene

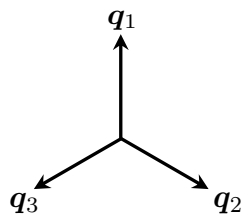
$$H_g = -v e^{-i \frac{\theta}{4} \cancel{\mu^z} \cancel{\sigma^z} \tau^z} \left(\tau^z \sigma^x \frac{1}{i} \partial_x + \sigma^y \frac{1}{i} \partial_y \right) e^{i \frac{\theta}{4} \cancel{\mu^z} \cancel{\sigma^z} \tau^z}$$

$\theta \approx 1.1^\circ \approx 0.02$

Inter-layer
tunneling

$$H_T = \sum_{m=1}^3 \mu^+ \left[w_0 + w_1 \left(e^{(\frac{2\pi i m}{3} + i \mathbf{q}_m \cdot \mathbf{r}) \tau^z} \sigma^+ + h.c. \right) \right] + h.c.$$

Intra-sublattice Inter-sublattice



$$|\mathbf{q}_m| = \frac{8\pi \sin(\theta/2)}{3\sqrt{3}a}$$

Many-body Hamiltonian

Approximate anti-unitary
particle-hole symmetry ($\nu = 0$):

$$C c^\dagger C^{-1} = \tau^x \sigma^x \mu^y c$$

$$C i C^{-1} = -i$$



$$c^\dagger = (c_{\sigma, \mu, s, \tau}^\dagger)$$

σ : sublattice, μ : layer, s : spin, τ : valley

Isolated
graphene

$$H_g = -v e^{-i \frac{\theta}{4} \cancel{\mu^z} \cancel{\sigma^z} \tau^z} \left(\tau^z \sigma^x \frac{1}{i} \partial_x + \sigma^y \frac{1}{i} \partial_y \right) e^{i \frac{\theta}{4} \cancel{\mu^z} \cancel{\sigma^z} \tau^z}$$

$$\theta \approx 1.1^\circ \approx 0.02$$

Inter-layer
tunneling

$$H_T = \sum_{m=1}^3 \mu^+ \left[\underset{\text{Intra-sublattice}}{w_0} + \underset{\text{Inter-sublattice}}{w_1} \left(e^{(\frac{2\pi i m}{3} + i \mathbf{q}_m \cdot \mathbf{r}) \tau^z} \sigma^+ + h.c. \right) \right] + h.c.$$

Intra-sublattice Inter-sublattice

$$|\mathbf{q}_m| = \frac{8\pi \sin(\theta/2)}{3\sqrt{3}a}$$

Projection to the narrow bands

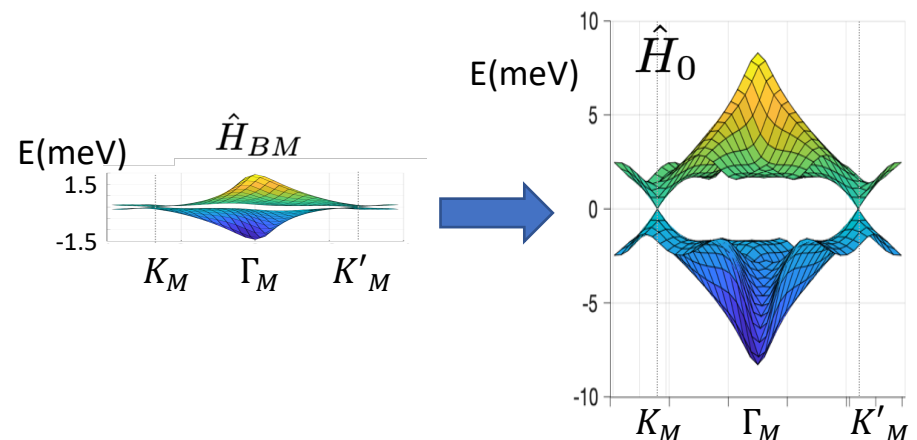
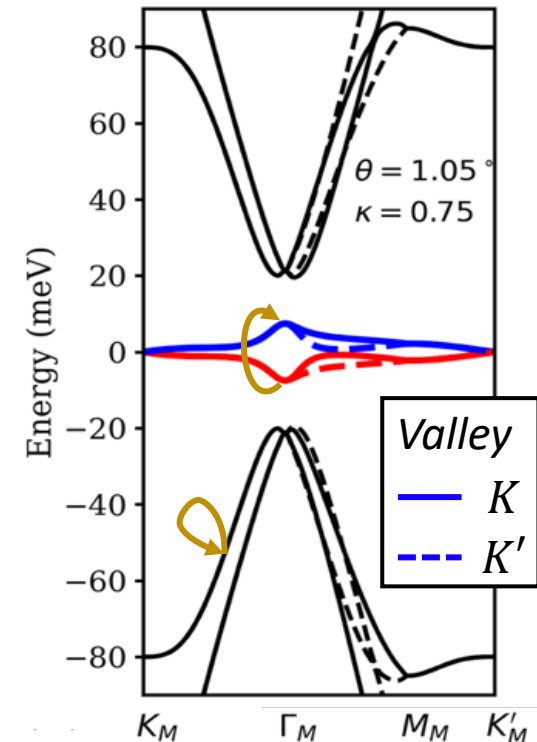
“Freeze” the remote bands,
leave only active bands: $n = +1, -1$

Interaction renormalization of single particle
Hamiltonian:

$$\hat{H}_{BM} \rightarrow \hat{H}_0 = \hat{H}_{BM} - [\hat{V}]_{\Psi_0}$$

$[\hat{V}]_{\Psi_0}$: Hatree-Fock decoupling of \hat{V}
w.r.t. to ground state of
decoupled layers

*See: Bultnick, Zaletel et al. (2020);
Liu, Vishwanath et al. (2021)*



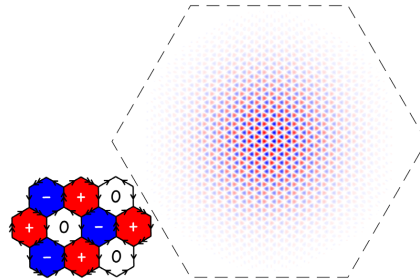
Results

$$\kappa = \frac{w_0}{w_1} = 0.75, W \approx 8 \text{ meV}$$

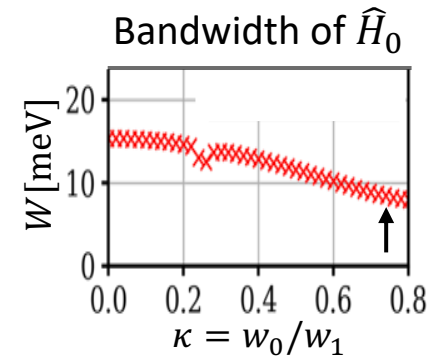
Ground state:
Kramers Inter-Valley
Coherent state (K-IVC)

Order parameter: $\langle c^\dagger \tau^{x,y} \sigma^y c \rangle \neq 0$

$$\tilde{\mathcal{J}} = \tau^y \mathcal{K}$$

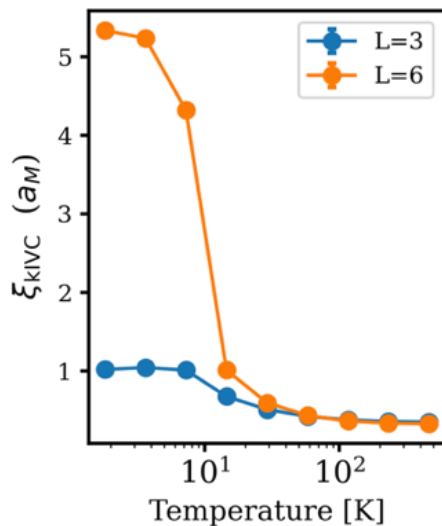


*Bultnick, Khalaf, Liu,
Chatterjee, Vishwanath,
Zaletel (2020)*

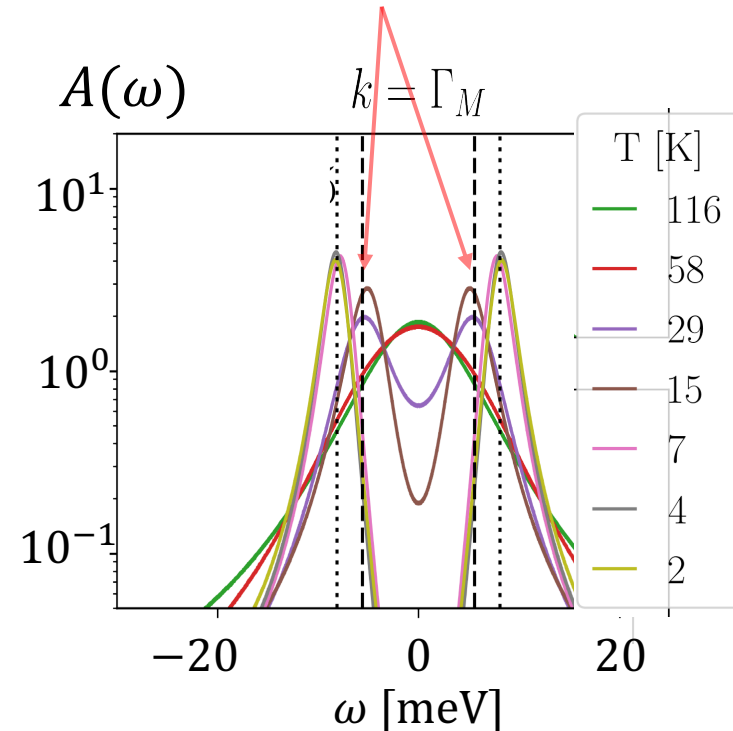
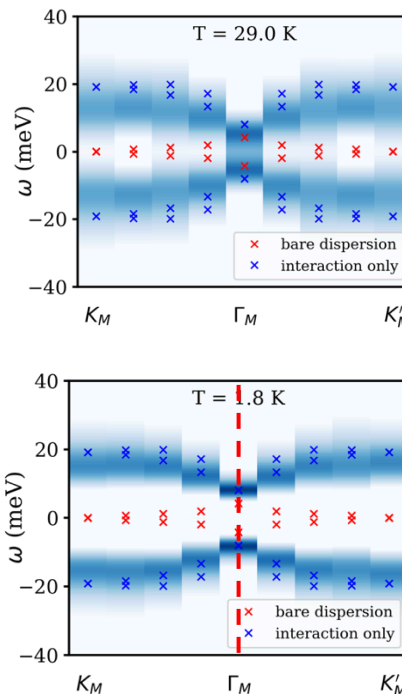


**Gap-like feature onsets
far above ordering**

K-IVC correlation length



$$\xi_a^2/a_M^2 = \frac{3}{16 \sin^2(\pi/L)} \left(\frac{S_a(\mathbf{q}=0)}{S_a(\mathbf{q}=\mathbf{q}_{nn})} - 1 \right)$$

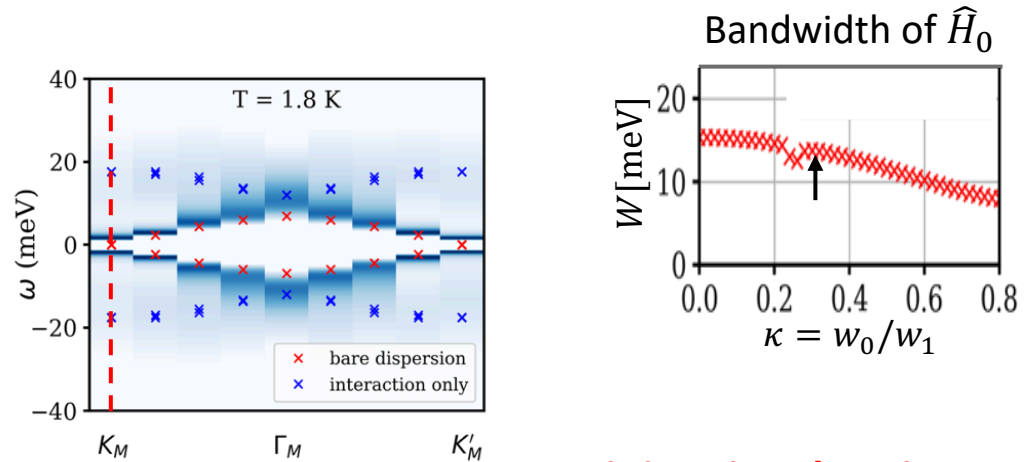


Results

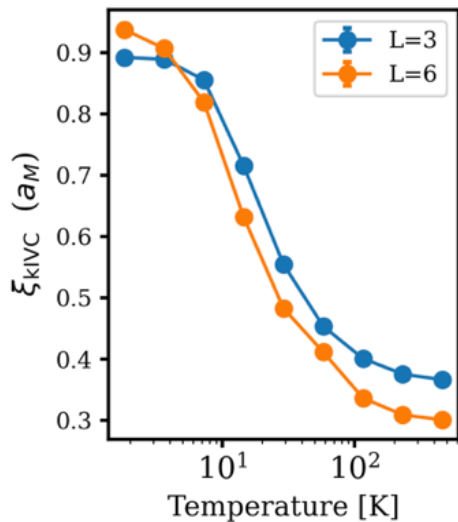
$$\kappa = \frac{w_0}{w_1} = 0.3, W \approx 14 \text{ meV}$$

Ground state:
Correlated semi-metal

HF predicts K-IVC with a
gap of $\sim 17\text{meV}$



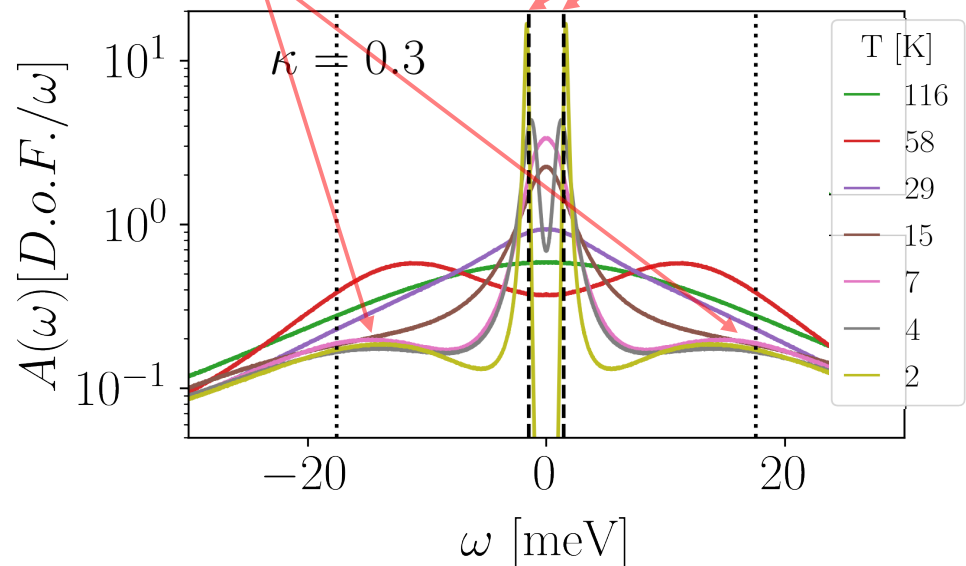
K-IVC correlation length



$$\xi_a^2/a_M^2 = \frac{3}{16 \sin^2(\pi/L)} \left(\frac{S_a(\mathbf{q} = 0)}{S_a(\mathbf{q} = \mathbf{q}_{nn})} - 1 \right)$$

**'Shoulders' at the incipient
gap (interaction scale)**

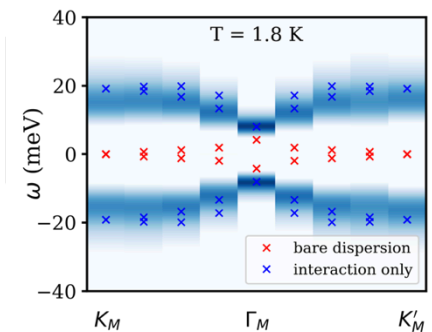
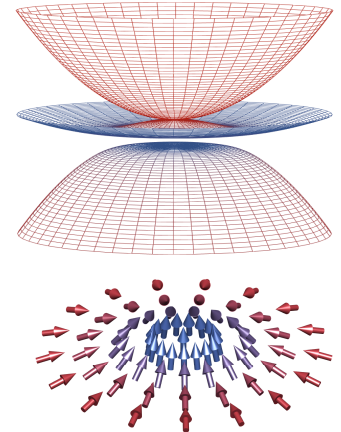
**Finite-size charging
energy $\propto 1/L^2$**



Summary

Moiré superlattices are a fascinating new playground combining topology and correlated electron physics.

- **Strongly correlated fragile topological bands: unusual gapping mechanism can lead to “featureless insulator”.**
- **TBLG at charge neutrality: no sign problem in QMC due to approximate P-H symmetry.**
- **Competition between K-IVC and semi-metal, ‘pseudo-gap’ onsets above ordering temperature.**



Thank you!