Handle with care: Gapping fragile topological bands by interactions

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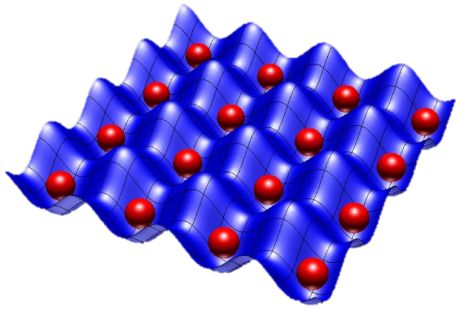
Ashvin Vishwanath (Harvard), Jong Yeon Lee (KITP)

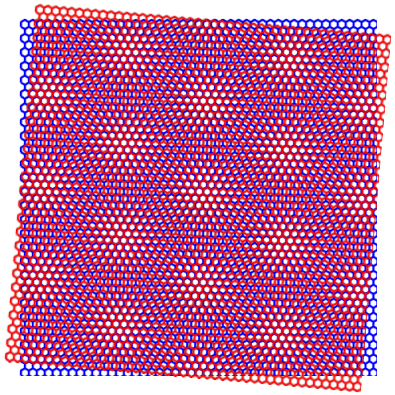
Creating flat bands

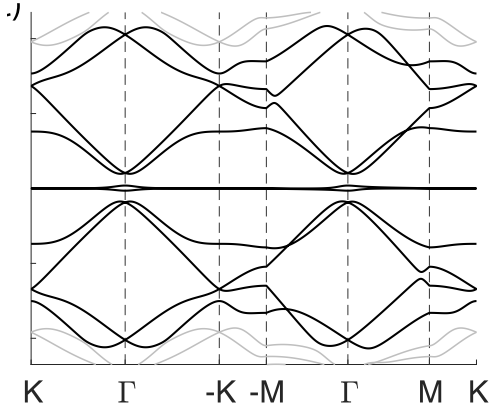
Electrons on a Lattice

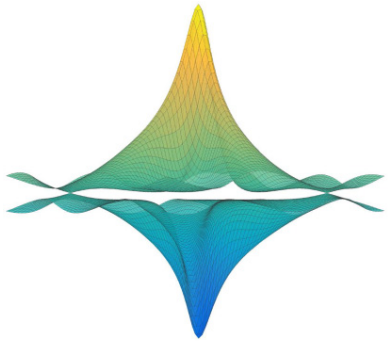


Localized

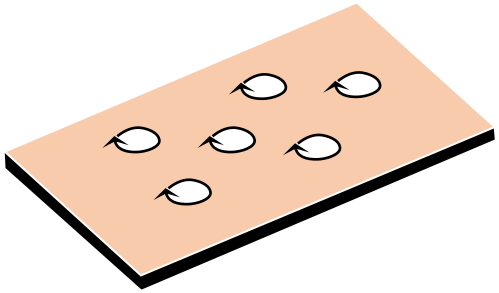
Magic angle graphene







Landau levels



Extended

topological

Po, Zou, Senthil, Vishwanath (2019)

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

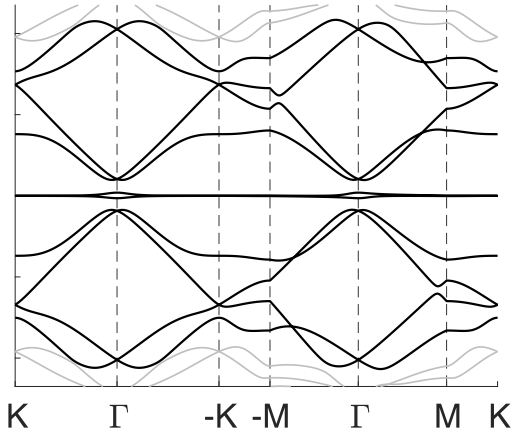
Twisted bilayer graphene at charge neutrality

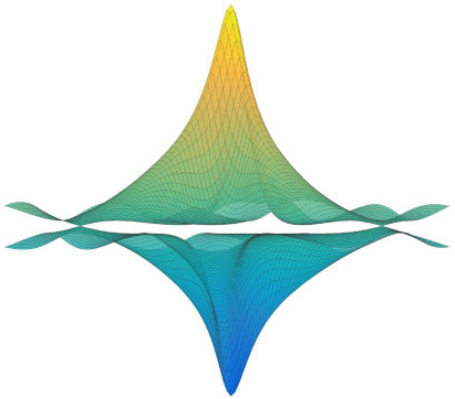
- **What *could* happen?**
  Constraints on interaction-driven insulators by topology
  Ari Turner, EB, Ady Stern, arXiv:2104.09528

- **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?

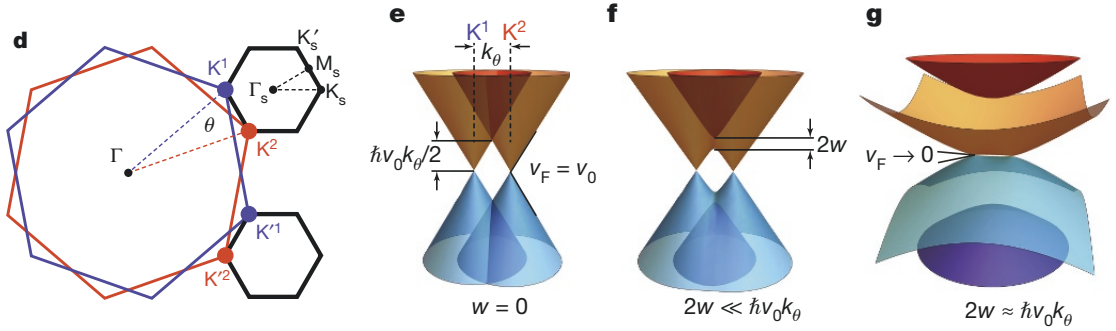
- Dirac points protected by product of $\mathcal{C}_\pi^z$ and $\mathcal{T}$





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 $\quad \mathcal{C}_\pi^z\mathcal{T} = \sigma^z\tau^x\mathcal{K}$

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

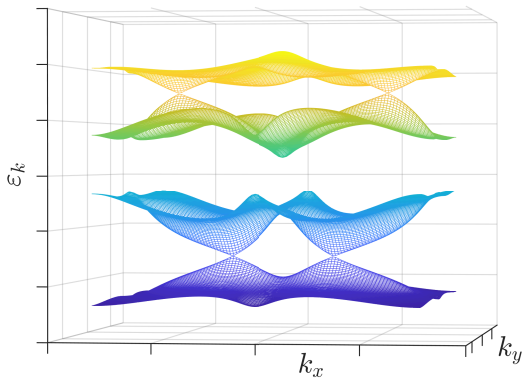
Smooth, real basis for lower bands:

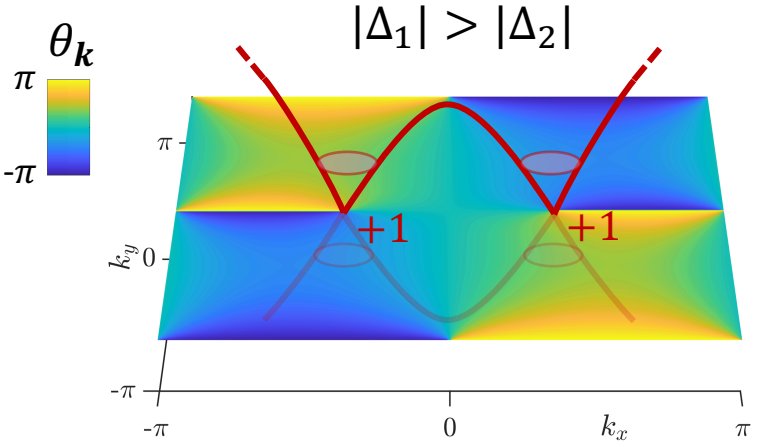
$|u_{1,2}(\boldsymbol{k})\rangle,\ \eta^z|u_{1,2}(\boldsymbol{k})\rangle = \pm|u_{1,2}(\boldsymbol{k})\rangle$

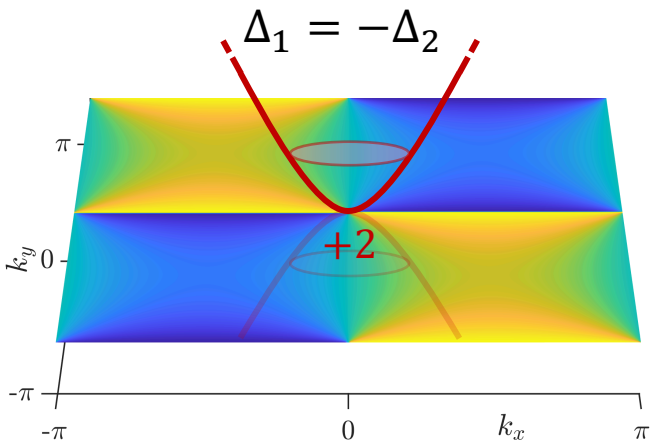
Projected Hamiltonian:

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

$-1 < m < 0$





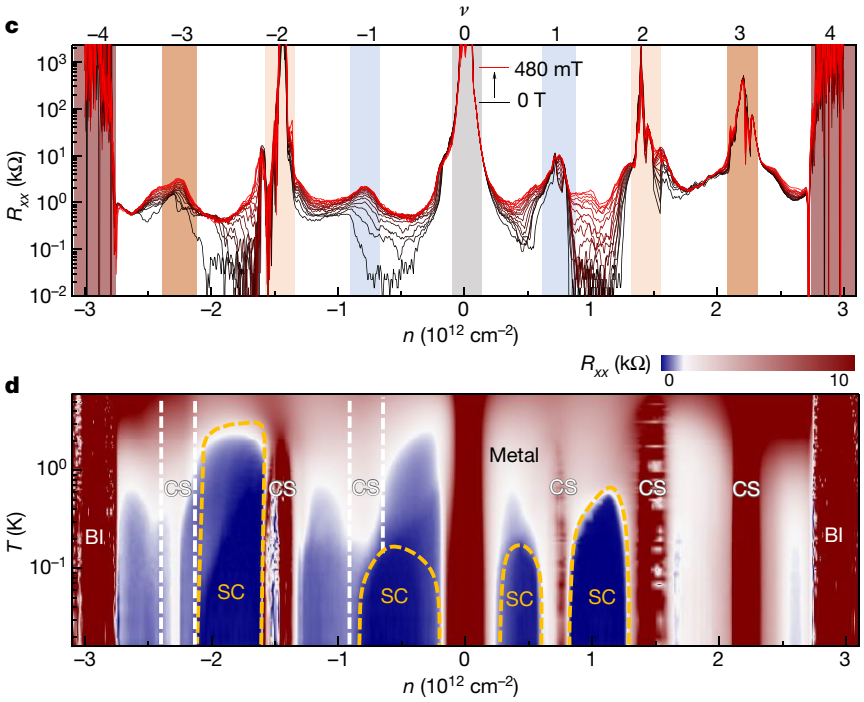


Gap at charge neutrality?

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)*

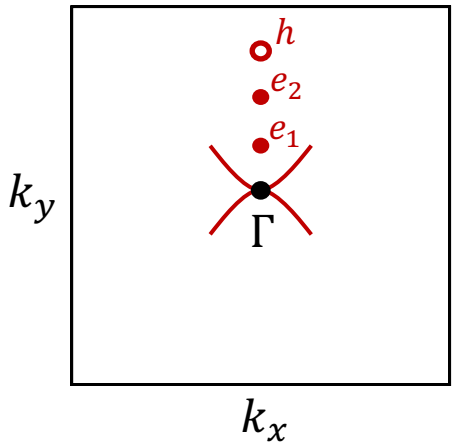
Q. With strong interactions, are there other options? Topological order? "Featureless" insulator?

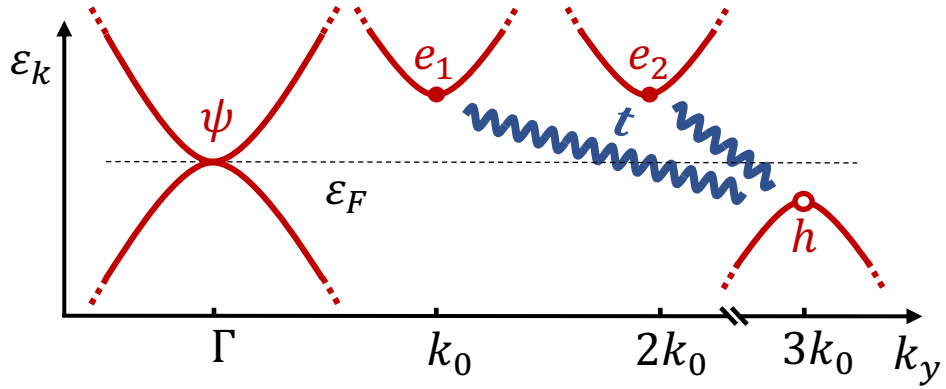


Gap at charge neutrality (theory): Xie, MacDonald (2020); Bultnik, Khalaf et al. (2020); Liao, Kang, Meng et al. (2021)

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

Gap opening by interactions

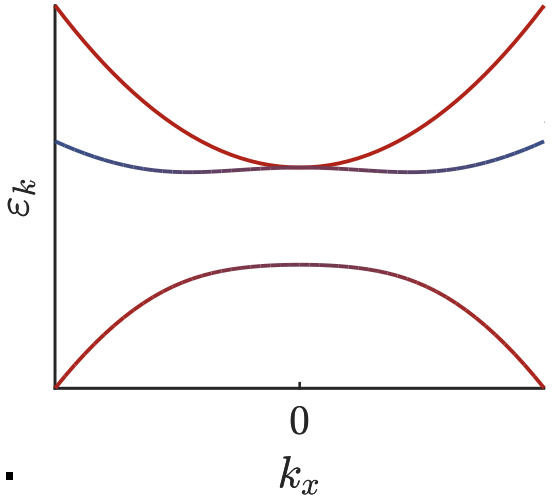




1. Turn on interaction:

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

⇒ "Trion" $t^\dagger = e_1^\dagger e_2^\dagger h^\dagger$ bound state near Γ



2. Turn on trion-electron hybridization:

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

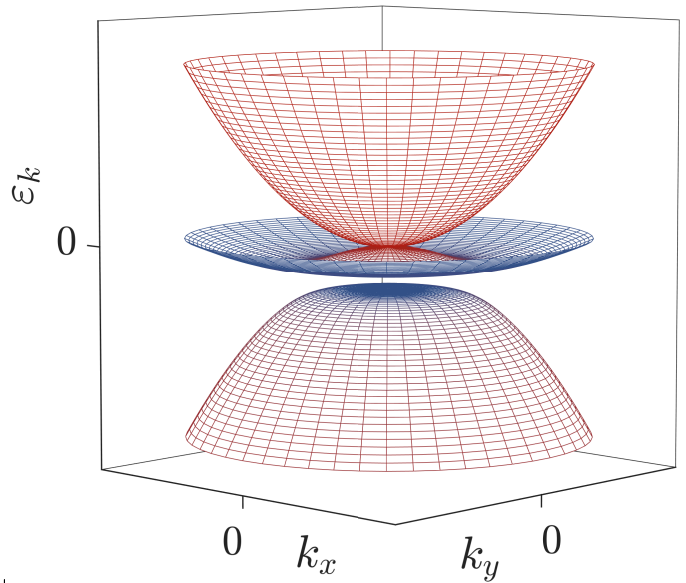
Turner, EB, Stern, arXiv:2104.09528

Gap opening by interactions

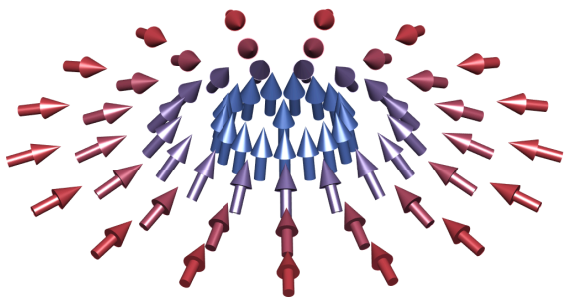
Near $\boldsymbol{k} = 0$, 3×3 effective real Hamiltonian:

electrons trions

$$H_{\text{eff}} = \begin{pmatrix} k_y^2 - k_x^2 & -2k_xk_y & \alpha k_x \\ -2k_xk_y & k_x^2 - k_y^2 & \alpha k_y \\ \alpha k_x & \alpha k_y & \dfrac{k^2}{2m_t} - E_0 \end{pmatrix}$$



Wavefunction of lowest band:



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

Turner, EB, Stern, arXiv:2104.09528

Twisted bilayer graphene at charge neutrality

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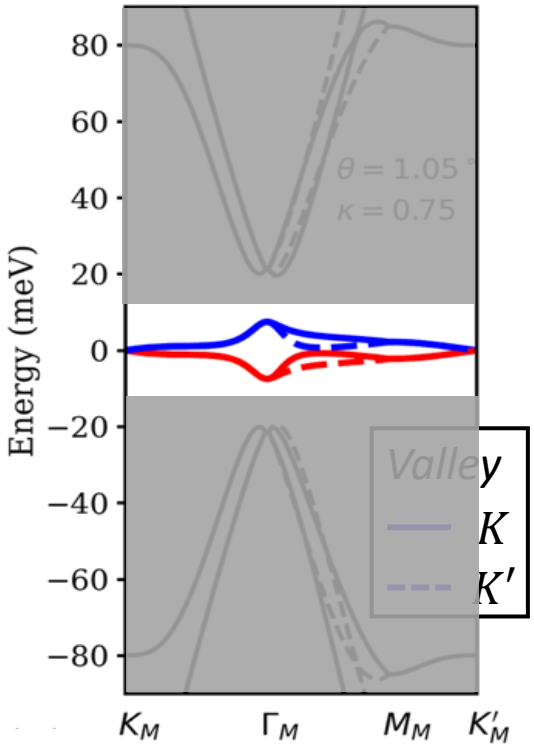
Johannes Hofmann (WIS)

Eslam Khalaf (Harvard)

Jong Yeon Lee (KITP)

Many-body simulations of twisted bilayer graphene

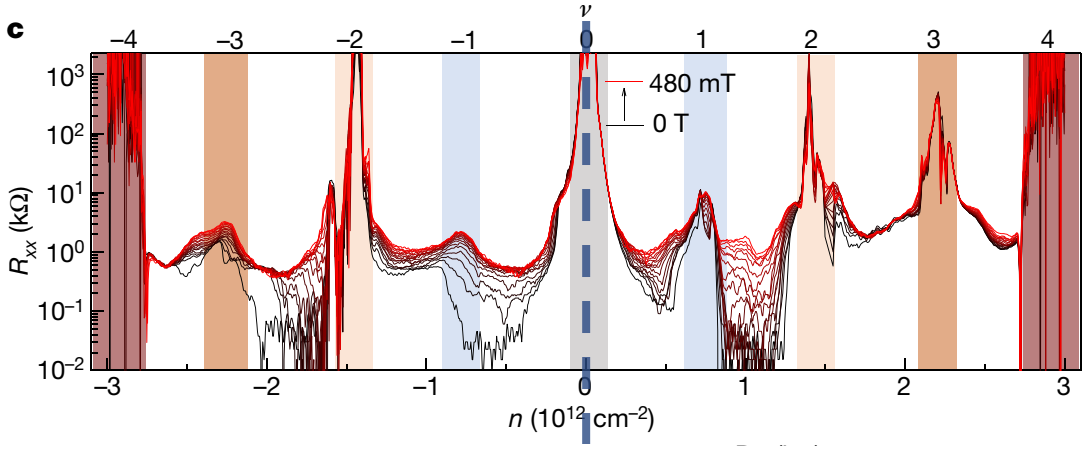
- No localized Wannier description of narrow bands: k-space description required
- 2 bands, 2 valleys, 2 spins = 8 degrees of freedom per unit cell
- Long-range Coulomb interactions



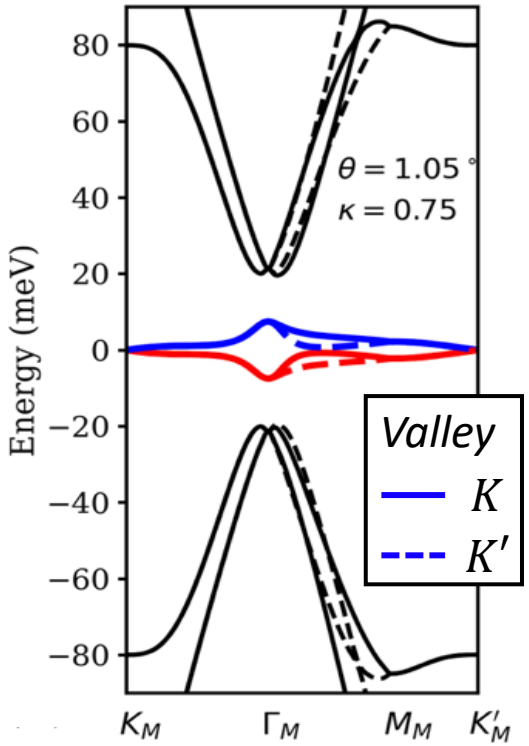
T = 0 simulations of TBLG:
ED: *Repellin, Senthil et al. (2020); Xie, Regnault et al. (2021); Potasz, MacDonald et al (2021),…*
DMRG: *Kang, Vafek (2020); Soejima, Zaletel et al. (2020); Chatterjee, Zaletel (2020)*

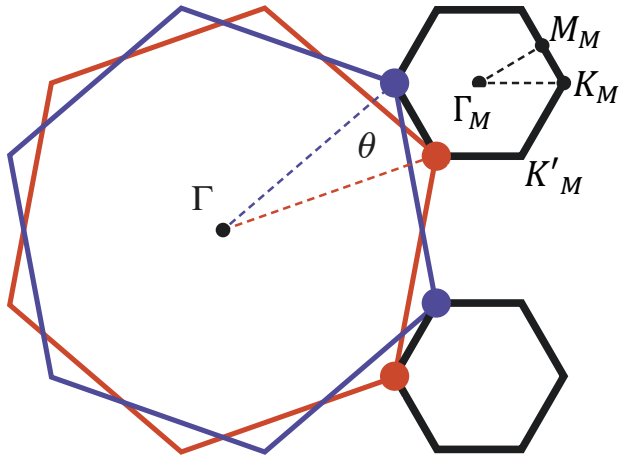
This work: sign-free momentum space quantum Monte Carlo simulations at $\nu = 0$, enabled by particle-hole symmetry

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



Lu, Efetov et al. (2018)





Many-body Hamiltonian

"Standard model" of TBLG:

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

$$\hat{H}_{\mathrm{BM}} = \int d^2r\, c^\dagger \left(H_g + H_T\right) c \qquad \hat{V} = \frac{1}{2}\sum_{\boldsymbol{q}} V_{\boldsymbol{q}} \delta\rho_{\boldsymbol{q}} \delta\rho_{-\boldsymbol{q}}$$

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

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

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

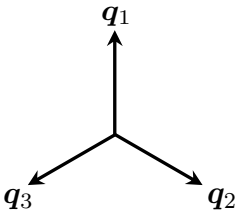
Isolated graphene

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

Inter-layer tunneling

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

Intra-sublattice Inter-sublattice



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

Many-body Hamiltonian

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

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

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

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

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

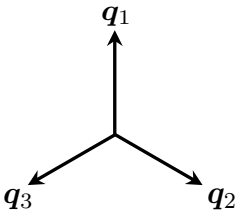
Isolated graphene

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

Inter-layer tunneling

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

Intra-sublattice Inter-sublattice



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

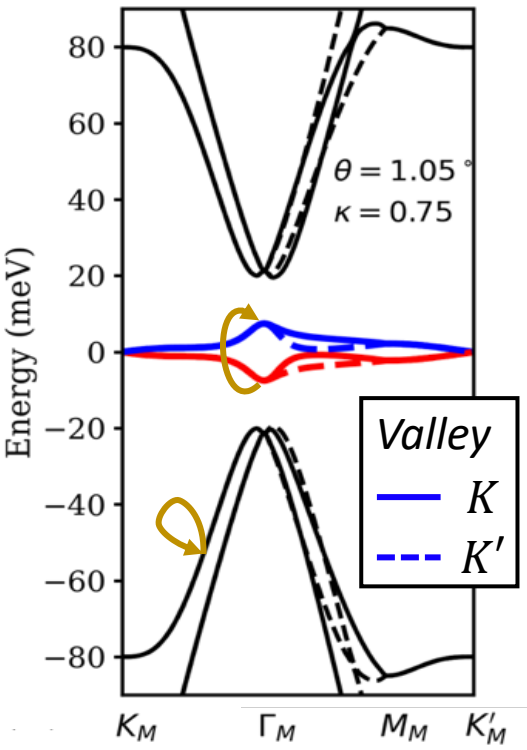
Projection to the narrow bands

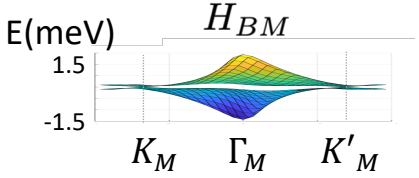
"Freeze" the remote bands,
leave only active bands: $n = +1, -1$

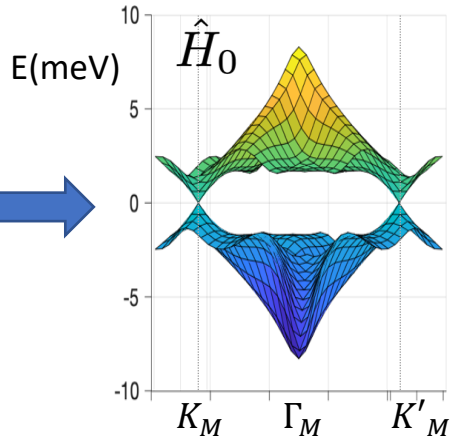
Interaction renormalization of single particle Hamiltonian:

$$\hat{H}_{BM} \to \hat{H}_0 = \hat{H}_{BM} - \left[\hat{V}\right]_{\Psi_0}$$

$\left[\hat{V}\right]_{\Psi_0}$: 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)

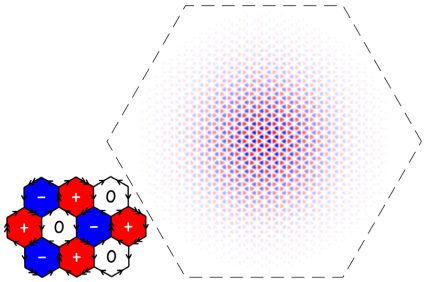
Results

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

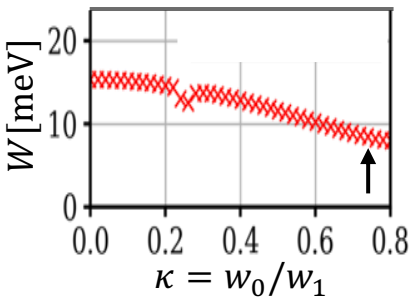
Ground state:
Kramers Inter-Valley
Coherent state (K-IVC)

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

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



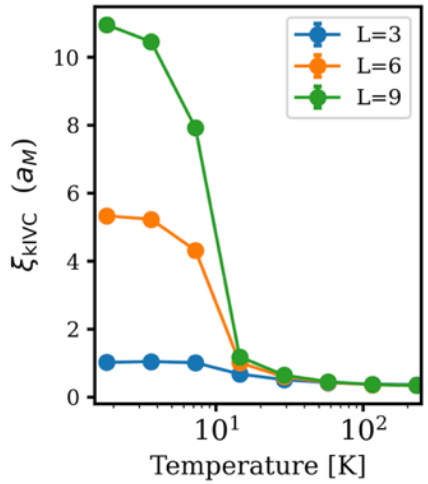
Bandwidth of $\hat{H}_0$



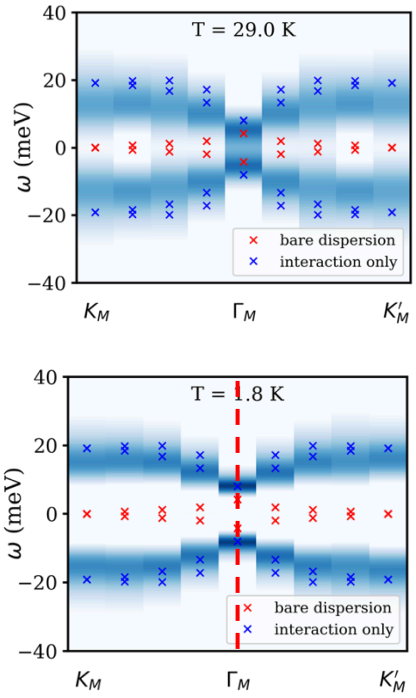
Bultnick, Khalaf, Liu, Chatterjee, Vishwanath, Zaletel (2020)

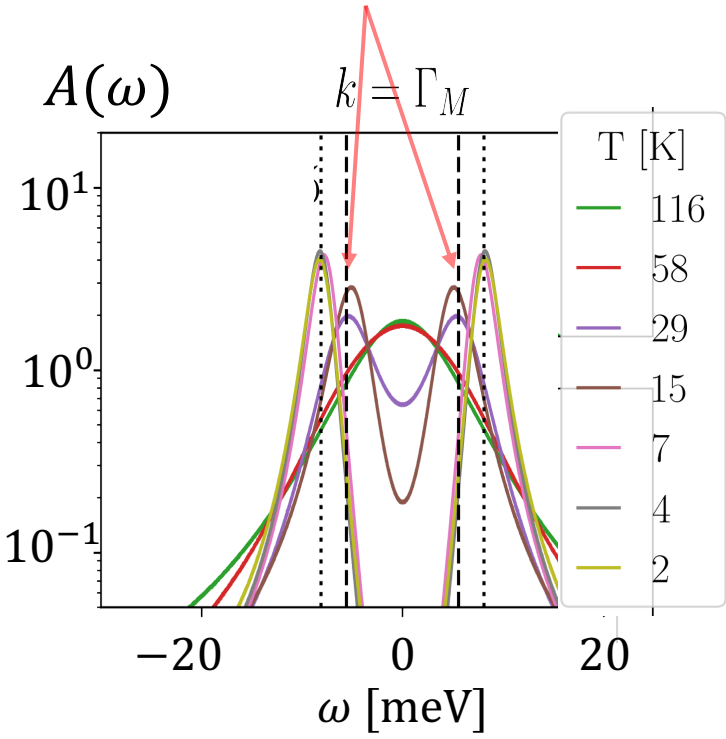
Gap-like feature onsets far above ordering

K-IVC correlation length



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



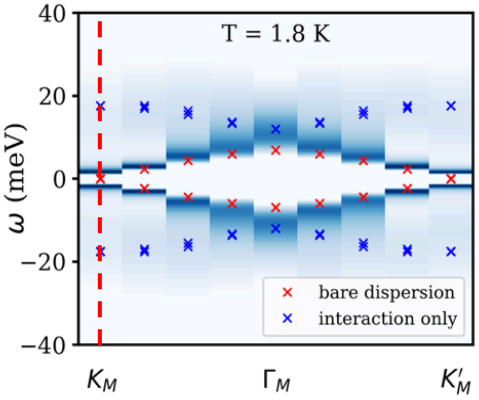


Results

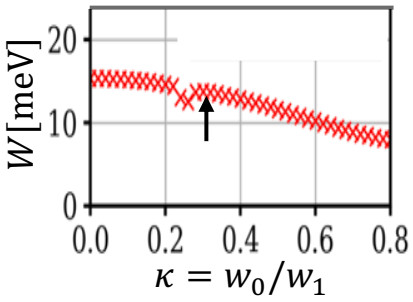
$\kappa = \frac{w_0}{w_1} = 0.3, W \approx 14$ meV

Ground state:
Correlated semi-metal

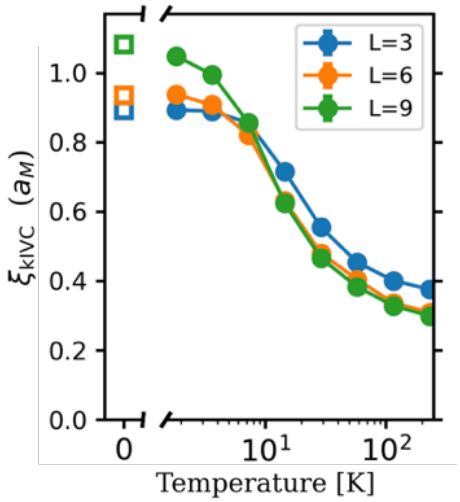
HF predicts K-IVC with a gap of ~ 17meV



Bandwidth of $\hat{H}_0$



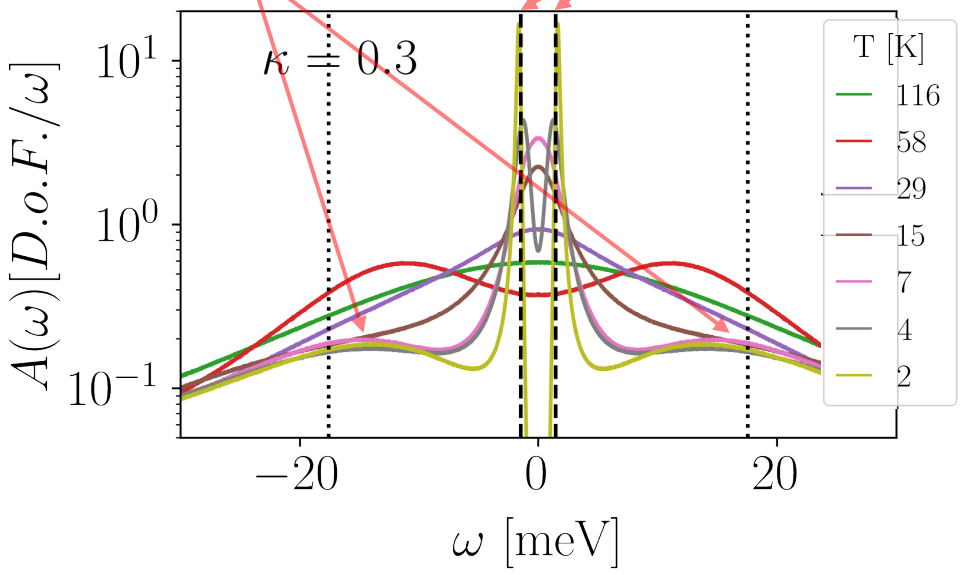
K-IVC correlation length



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

'Shoulders' at the incipient gap (interaction scale)

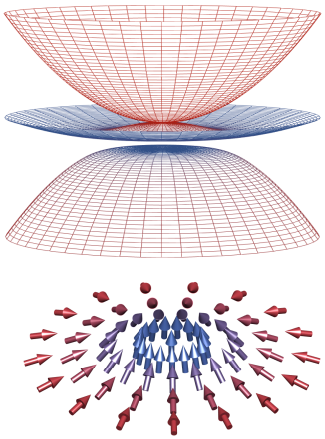
Finite-size charging energy$\propto 1/L^2$



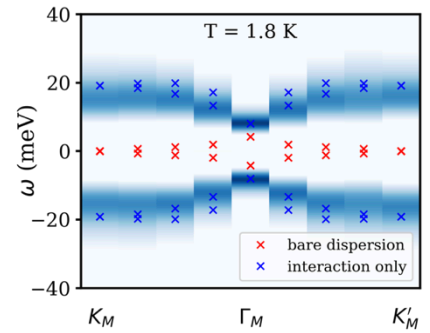
Summary

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!