Moiré Superlattices at Fractional Band Fillings: Particle-hole duality and Quantum Geometry

Ahmed Abouelkomsan

AA, Zhao Liu & Emil Bergholtz, Phys. Rev. Lett. **124**, 106803 (2020)

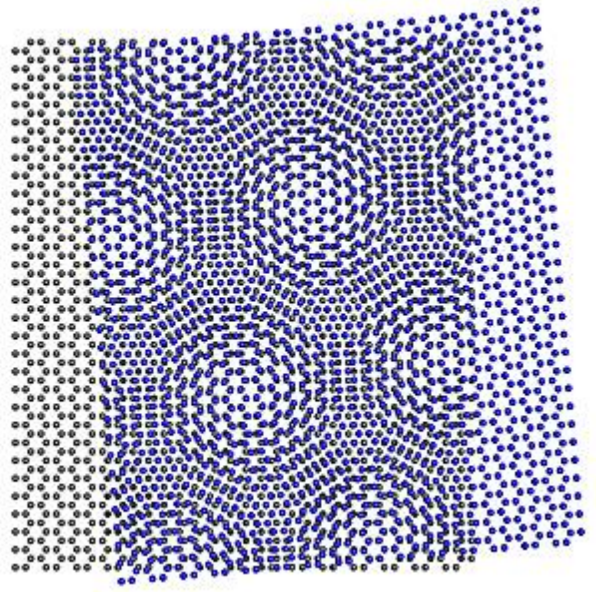
Zhao Liu, **AA** & Emil Bergholtz, Phys. Rev. Lett. **126**, 026801 (2021)

AA, Kang Yang & Emil Bergholtz, arXiv:2202.10467

Moiré systems

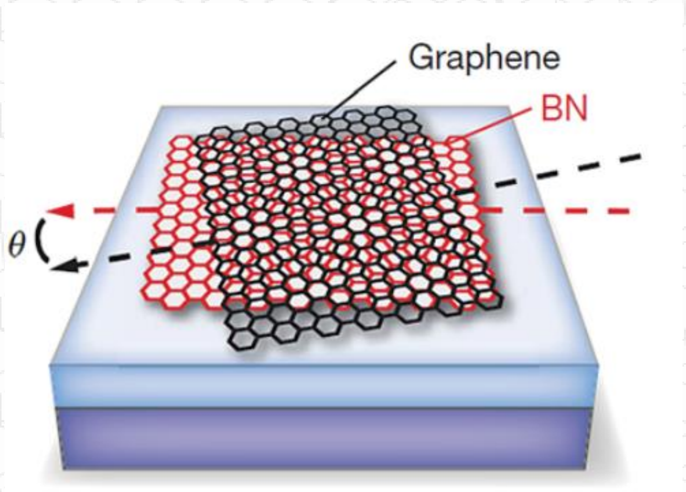
- Layered 2d materials that show Moiré patterns (long distance modulations!)
- A slight lattice mismatch or a tiny relative twist

Twisted Bilayer Graphene



Credit : NIST

Graphene on Boron Nitride



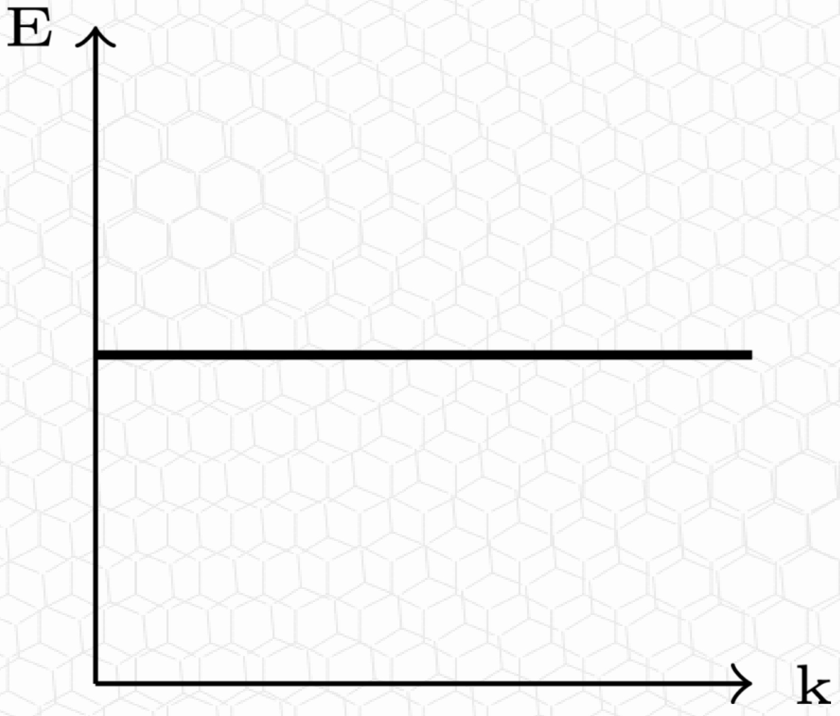
RSC Adv., 2017,**7**, 16801-16822

Moiré systems

- Moiré systems realize very flat bands!

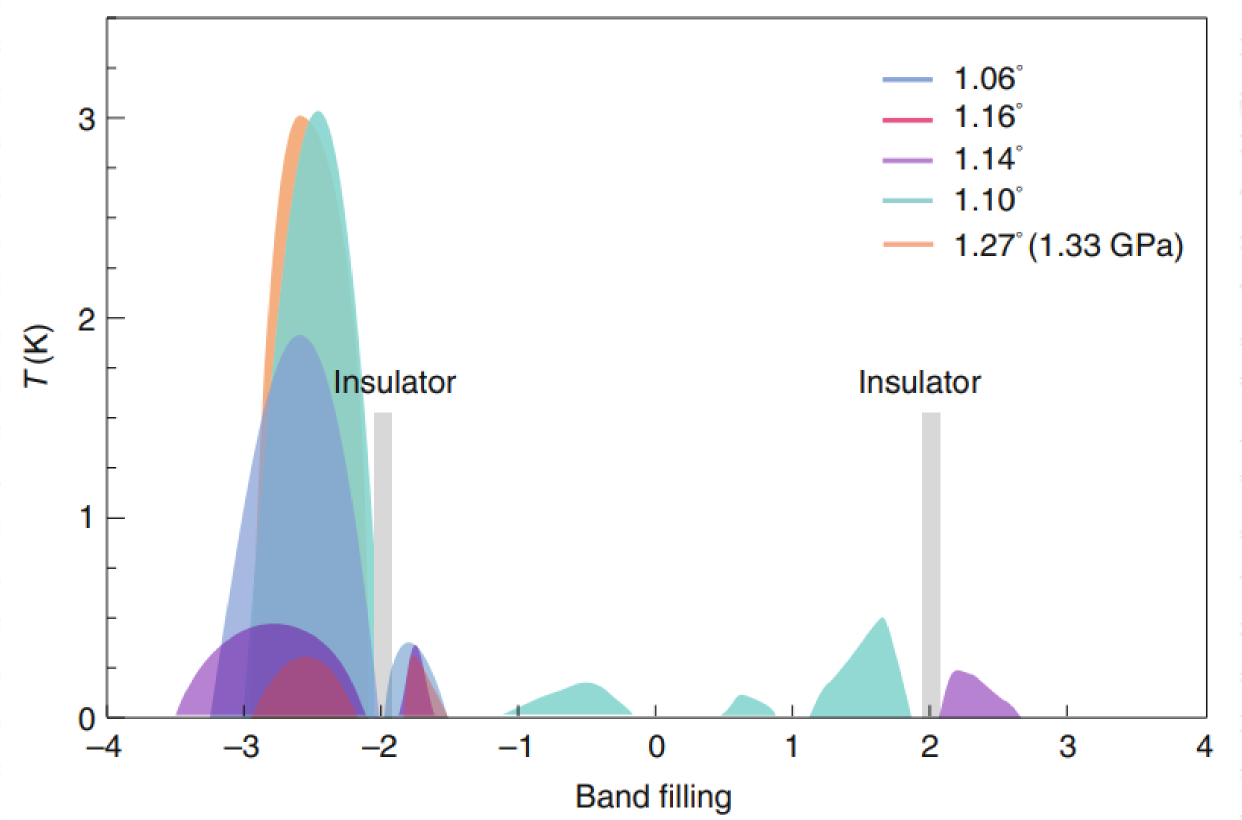
- Kinetic energy is quenched -> interactions are enhanced!

- Natural platform for strongly correlated phases of matter



• Correlated Insulators and Superconductors around integer fillings

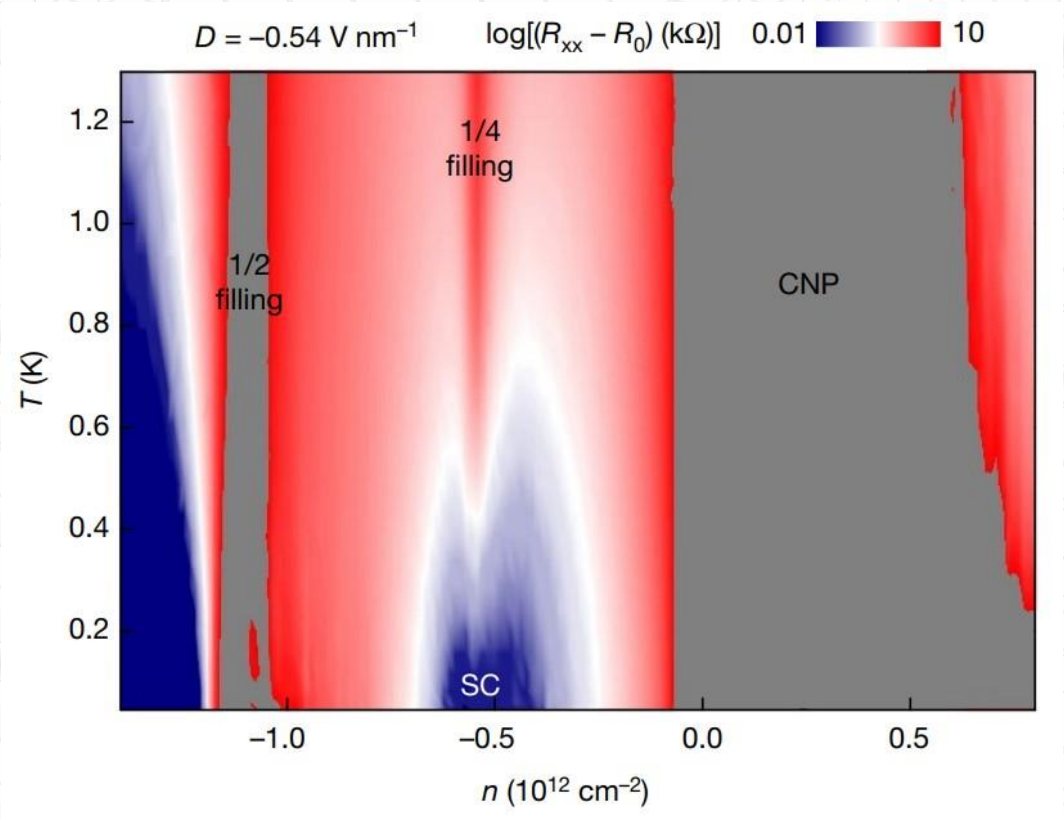
Twisted Bilayer Graphene



- Cao, Y. et al. Nature **556**, (2018).
- Yankowitz, M. et al. Science **363**, (2019).
- Lu, X. et al. Nature **574**, (2019)

Fig from : Balents et al. *Nature Physics* **16**, (2020)

ABC stacked trilayer graphene aligned with Boron Nitride

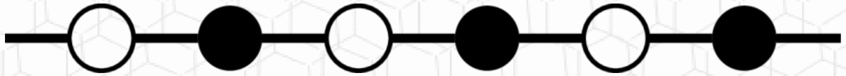


Chen et al. Nature **572**, (2019)

The Problem

A Flat Band

Fractional band filling

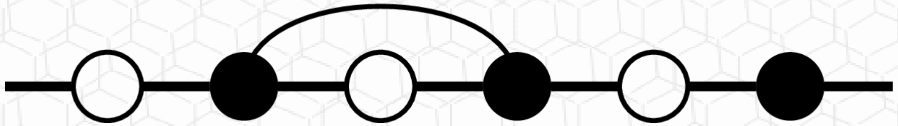


The Problem

Add interactions

A Flat Band

$$V(\mathbf{q}) \sim \frac{1}{\sqrt{\mathbf{q}^2 + \kappa^2}}$$



What is the underlying phase ?

Fractional Chern Insulators

- FCIs are lattice analogues of the fractional quantum Hall effect.

- Although theoretically predicted but never been experimentally observed at zero magnetic field!

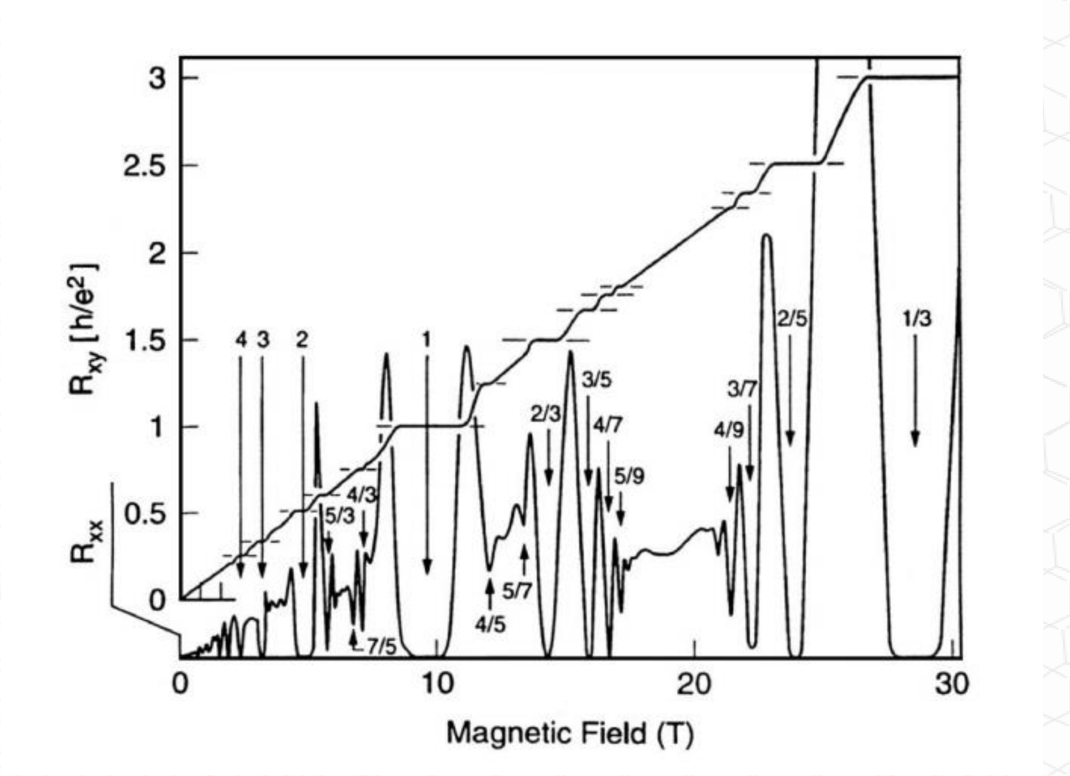


Fig from : Stormer, Physica B **177**, 1-4 (1992)

- Klitzing el at. Phys. Rev. Lett. **45**, 494 (1980)
- Tsui el at. Phys. Rev. Lett. **48**, 1559 (1982)

Fractional Chern Insulators

Break time reversal symmetry

↓

	No interactions	Strong Interactions
Continuum	IQHE (external B field) →	FQHE
Lattice	Chern Insulator →	FCI

Haldane, Phys. Rev. Lett. **61**, 2015 (1988)

FCI reviews : E.J.B, Z.L., International Journal of Modern Physics B, **27**, 24, 1330017 (2013) & S. A. P., R.R., S.L.S, Comptes Rendus Physique, **14**, 9-10 (2013)

FCIs, why bother?

- Overcomes challenges with the conventional FQHE experimental setup!

Very strong magnetic fields

$$|\mathbf{B}| \sim 10 - 30 \text{ Tesla}$$

Extremely low temperatures

$$T \lesssim 1 \text{ Kelvin}$$

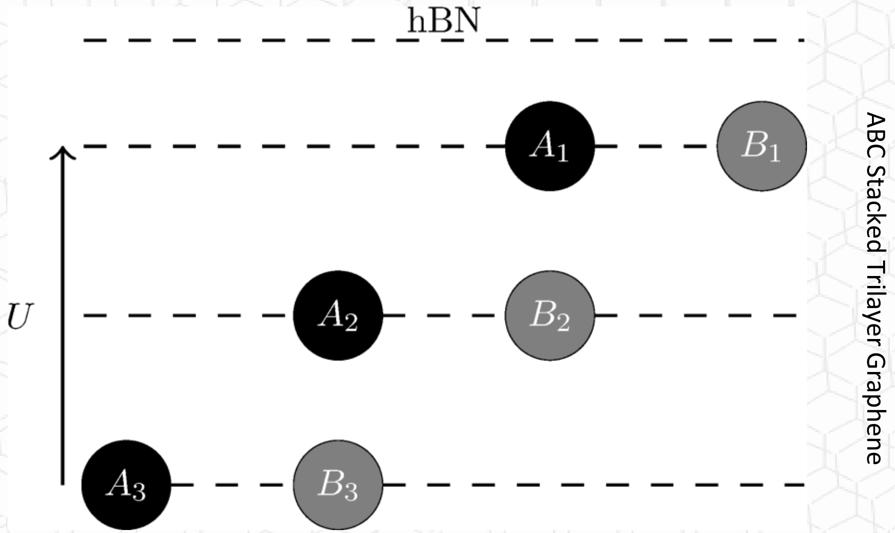
FCIs, why bother?

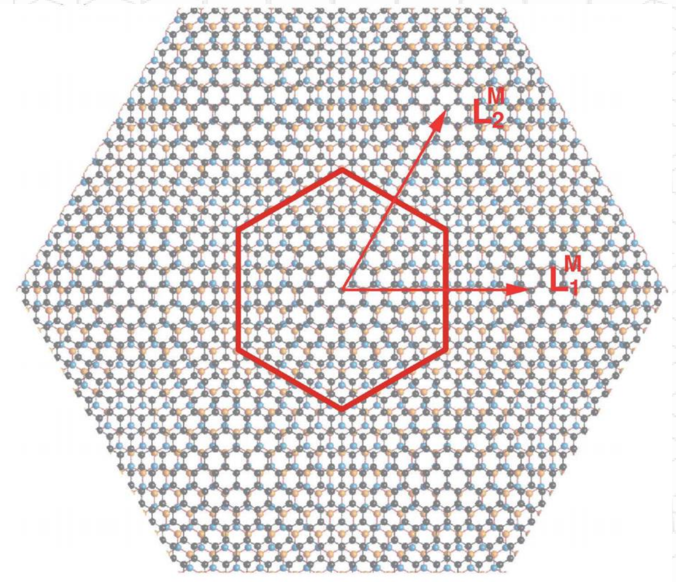
- No magnetic field required!

- Interactions on the lattice scale are greater than the magnetic length scale -> Higher energy gap!
- A step towards high temperature topological phases.

- More than FQHE!
- Higher Chern number FCIs are possible -> no mapping to decoupled Landau levels! , PRL, **109**, 186805 (2012)

Trilayer Graphene aligned with Boron Nitride

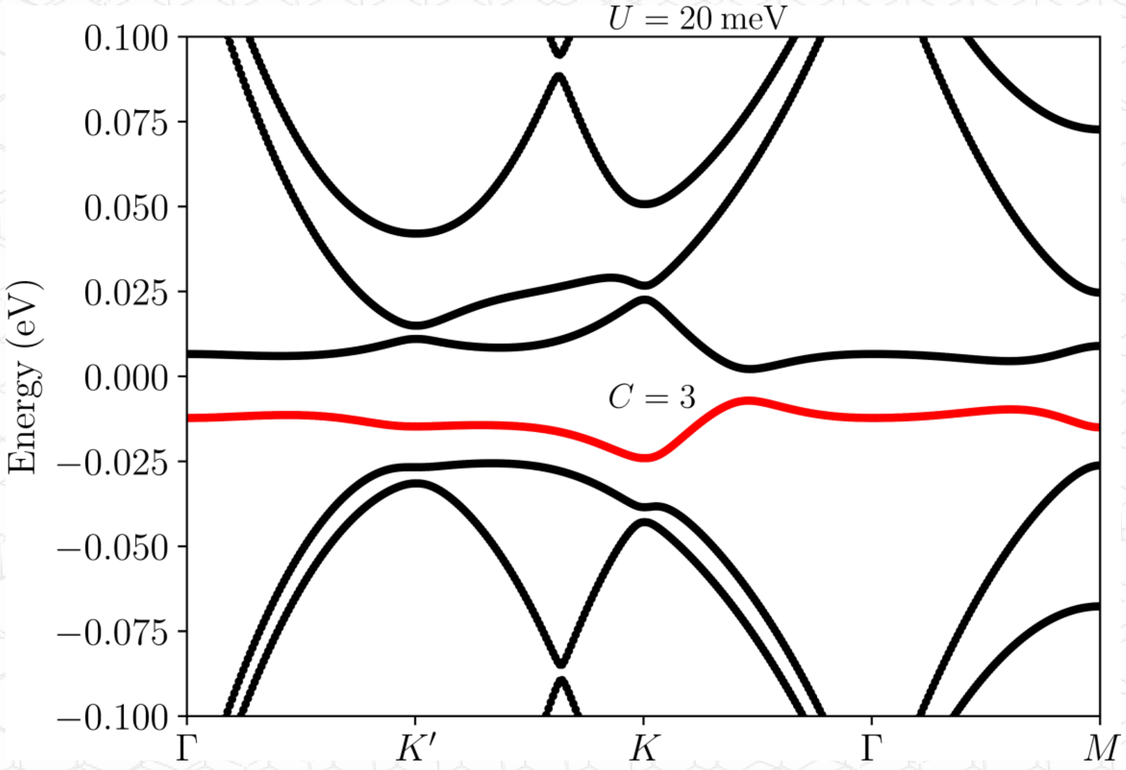




Phys. Rev. B **90**, 155406 (2014)

- Tiny lattice mismatch (1.7 %) between hBN and the top graphene layer generates a Moiré pattern.
- New lattice constant is 60 times larger!

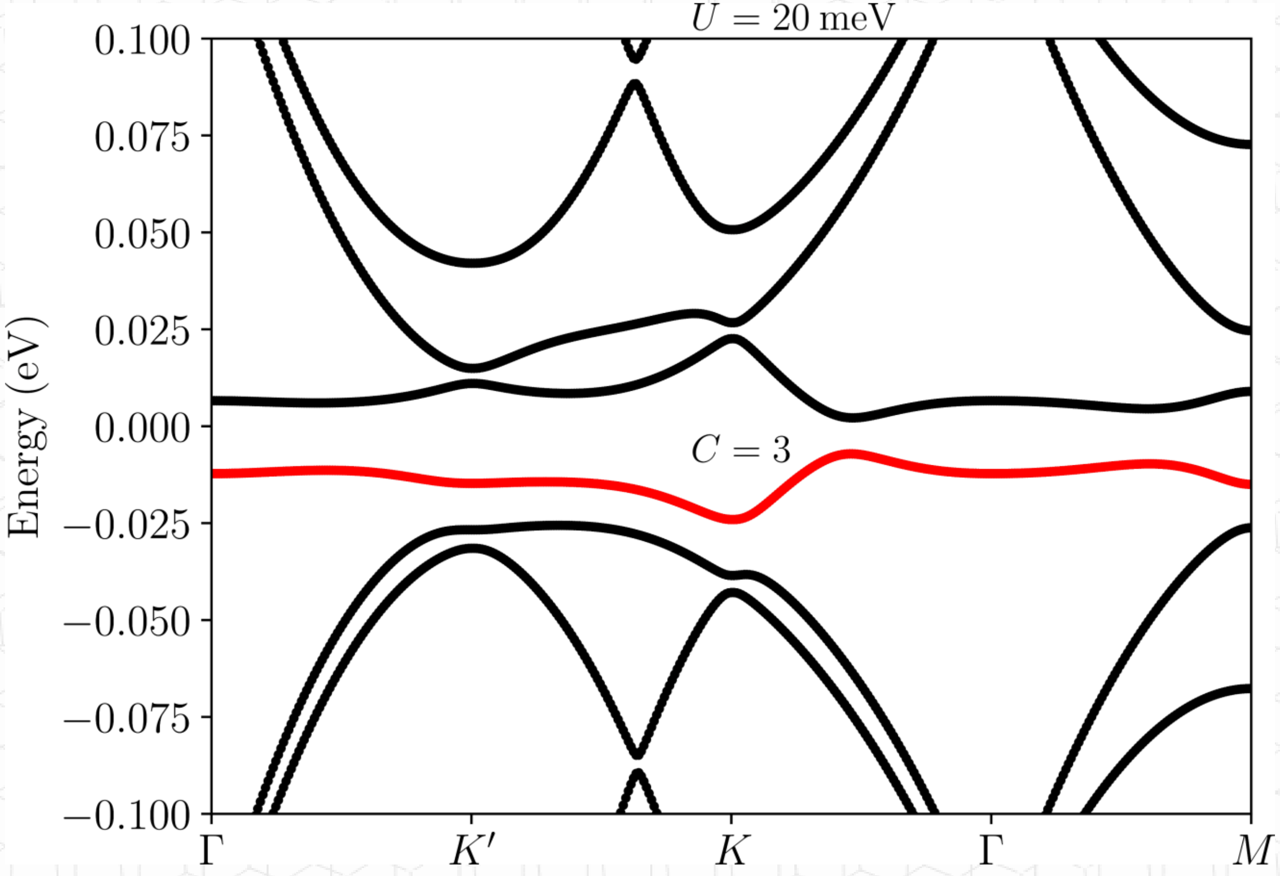
Trilayer Graphene aligned with Boron Nitride



What happens when the red band is fractionally filled?

TLG-hBN

- Are FCI states possible?
- No numerical evidence!
- Why?



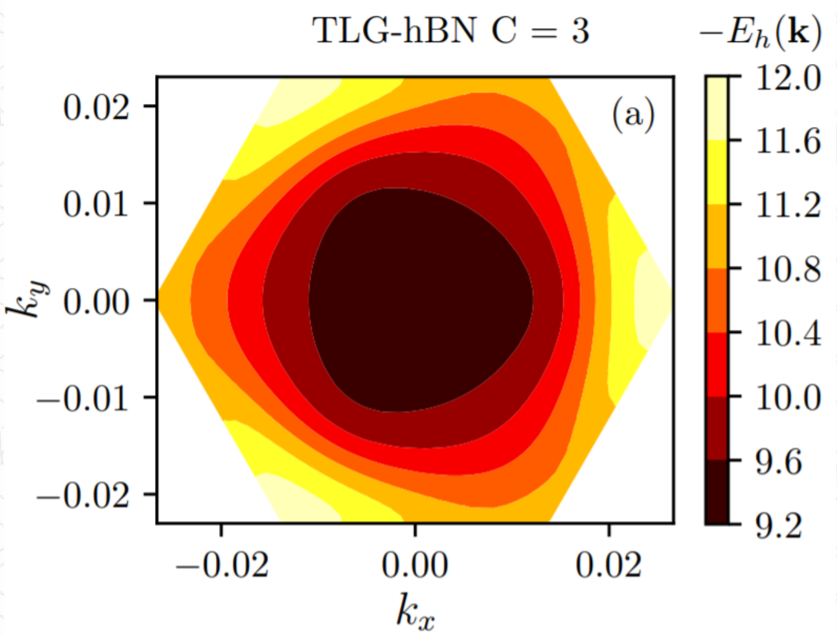
Another perspective

$$H_{\mathrm{proj}} = \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} V_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} c^\dagger_{\mathbf{k}_1} c^\dagger_{\mathbf{k}_2} c_{\mathbf{k}_3} c_{\mathbf{k}_4}$$

$\{c_{\mathbf{k}_i}\}$ are band operators!

Particle-Hole Transformation, $c_{\mathbf{k}} \to d^\dagger_{\mathbf{k}}$

$$H_{\mathrm{proj}} \to \sum_{\mathbf{k}} E_h(\mathbf{k}) d^\dagger_{\mathbf{k}} d_{\mathbf{k}} + \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} V^*_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} d^\dagger_{\mathbf{k}_1} d^\dagger_{\mathbf{k}_2} d_{\mathbf{k}_3} d_{\mathbf{k}_4}$$



$$E_h(\mathbf{k}) = \sum_{\mathbf{k}'} \left(V_{\mathbf{k}'\mathbf{k}\mathbf{k}'\mathbf{k}} + V_{\mathbf{k}\mathbf{k}'\mathbf{k}\mathbf{k}'} - V_{\mathbf{k}\mathbf{k}'\mathbf{k}'\mathbf{k}} - V_{\mathbf{k}'\mathbf{k}\mathbf{k}\mathbf{k}'}\right)$$

Dispersive!
for projected interactions

Unlike Landau levels!

Another perspective

$$H_{\text{proj}} = \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} V_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} c^\dagger_{\mathbf{k}_1} c^\dagger_{\mathbf{k}_2} c_{\mathbf{k}_3} c_{\mathbf{k}_4}$$

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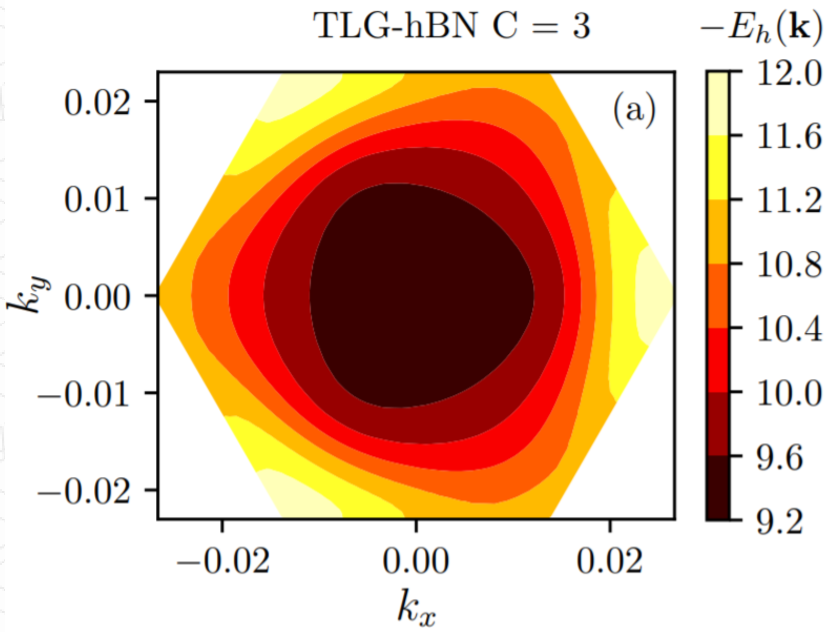
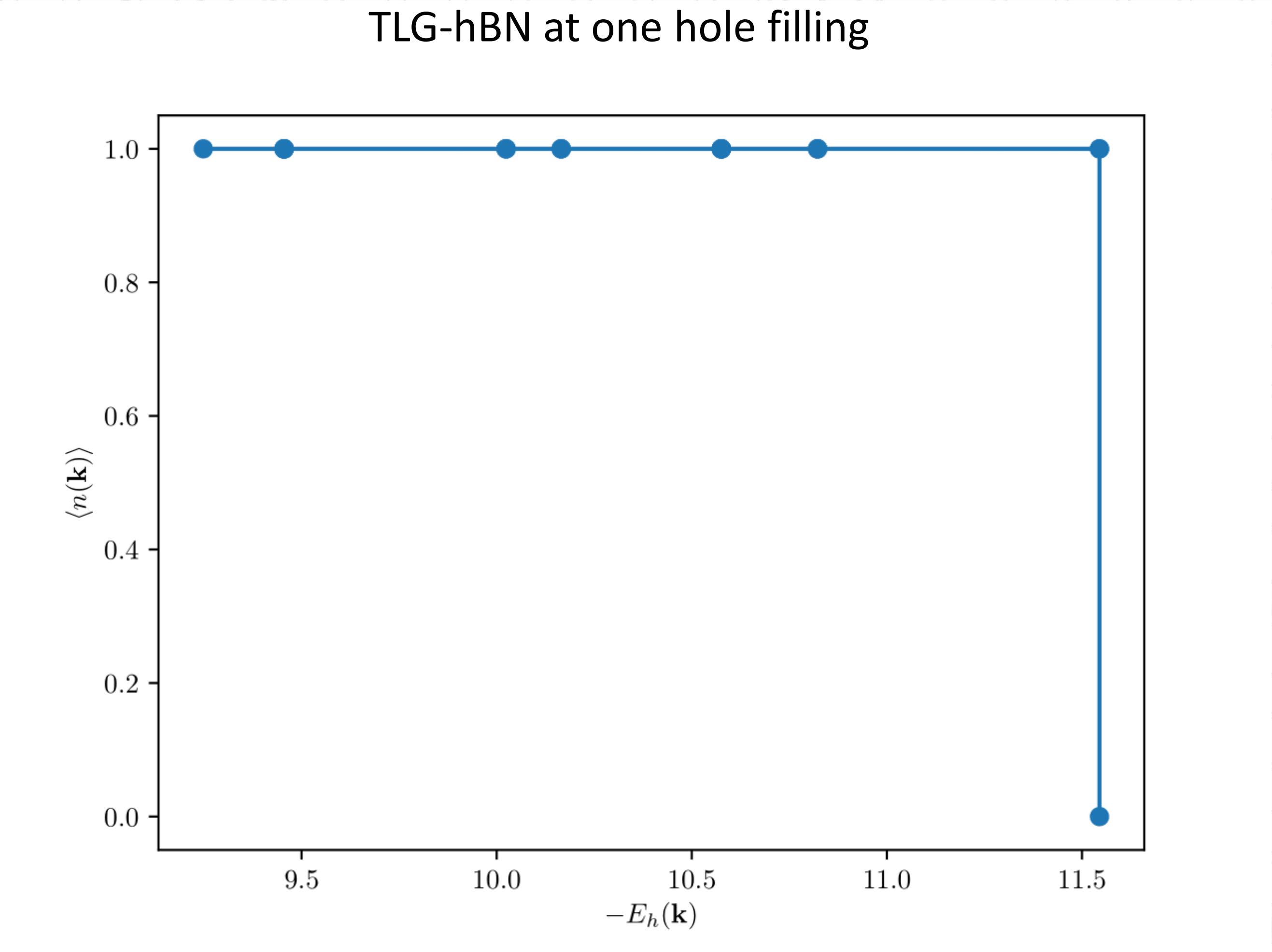


$$\frac{W_h(\text{Hole dispersion bandwidth})}{W(\text{Flatband bandwidth})} \sim 5$$

Emergent Fermi Liquids in TLG-hBN



$\langle n(\mathbf{k}) \rangle = \langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}} \rangle$ is electron occupation in the many-body ground state

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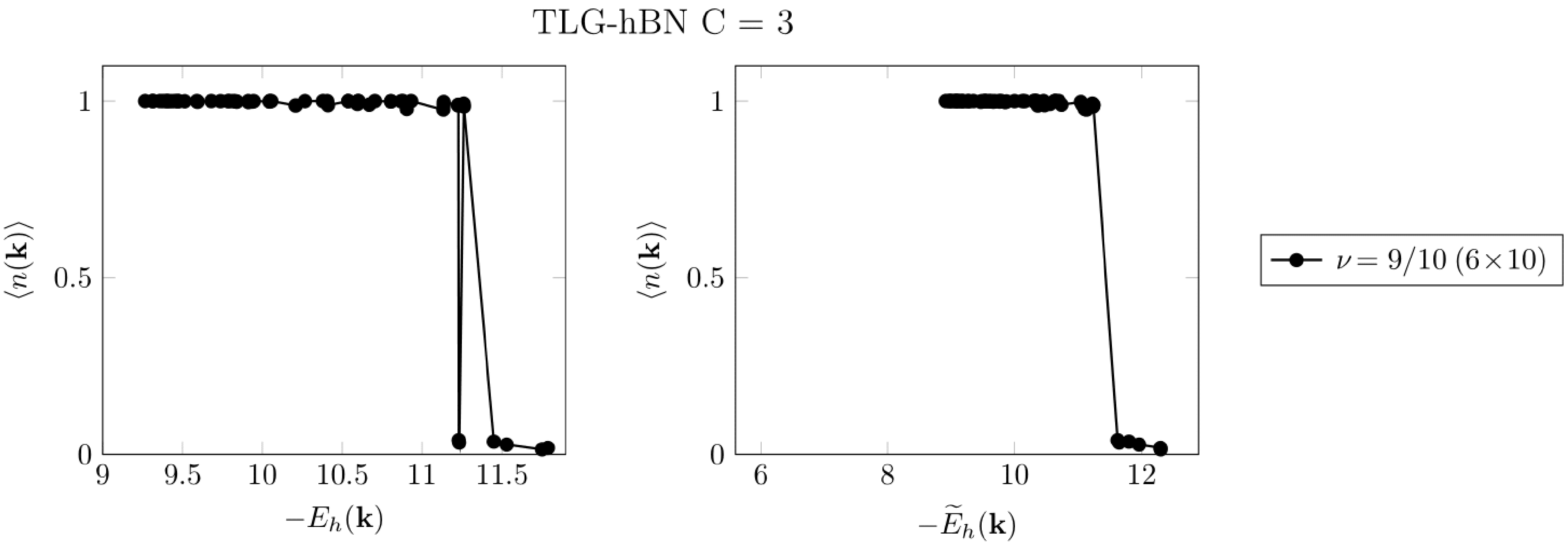

$\langle n(\mathbf{k})\rangle = \langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}}\rangle$ is electron occupation in the many-body ground state

$\widetilde{E}_h(\mathbf{k})$ is the renormalized single-hole energy after Hartree-Fock mean field of the interaction

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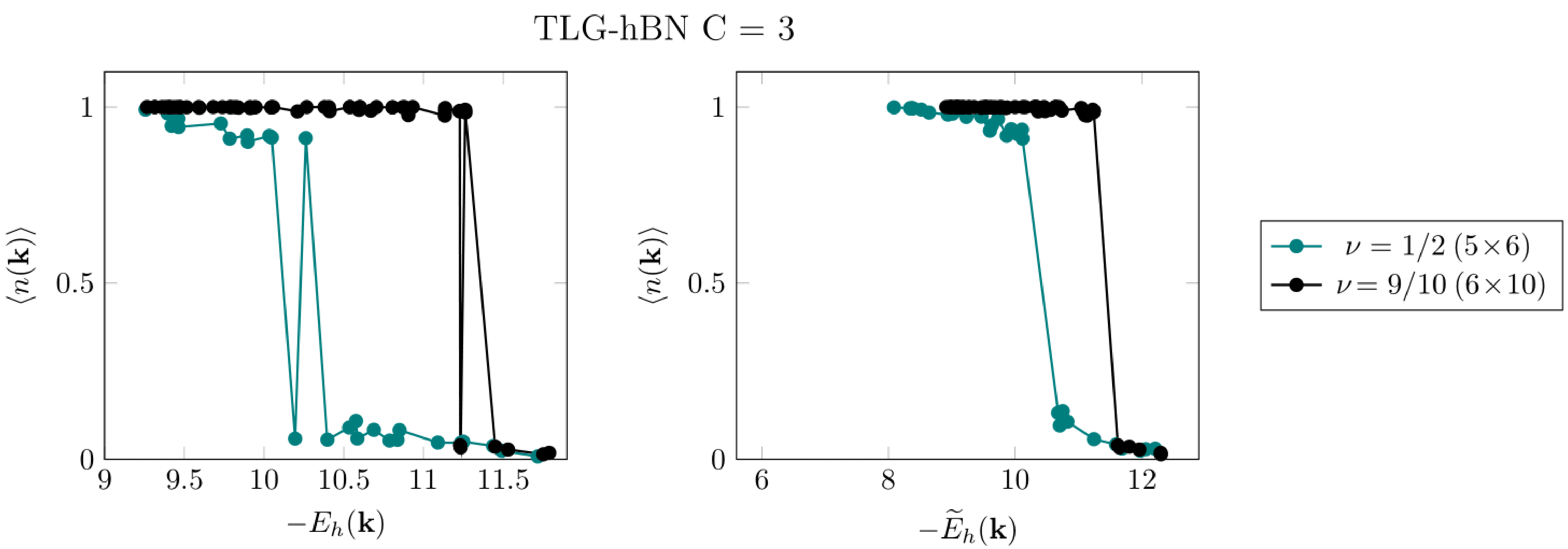

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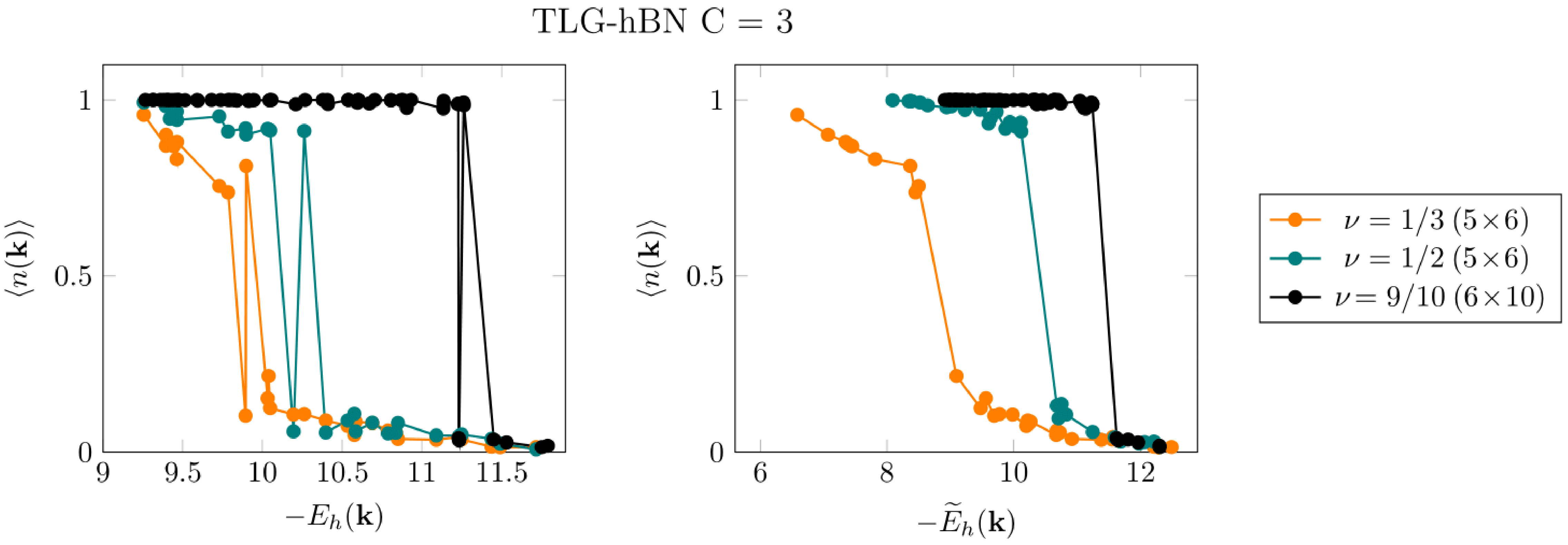

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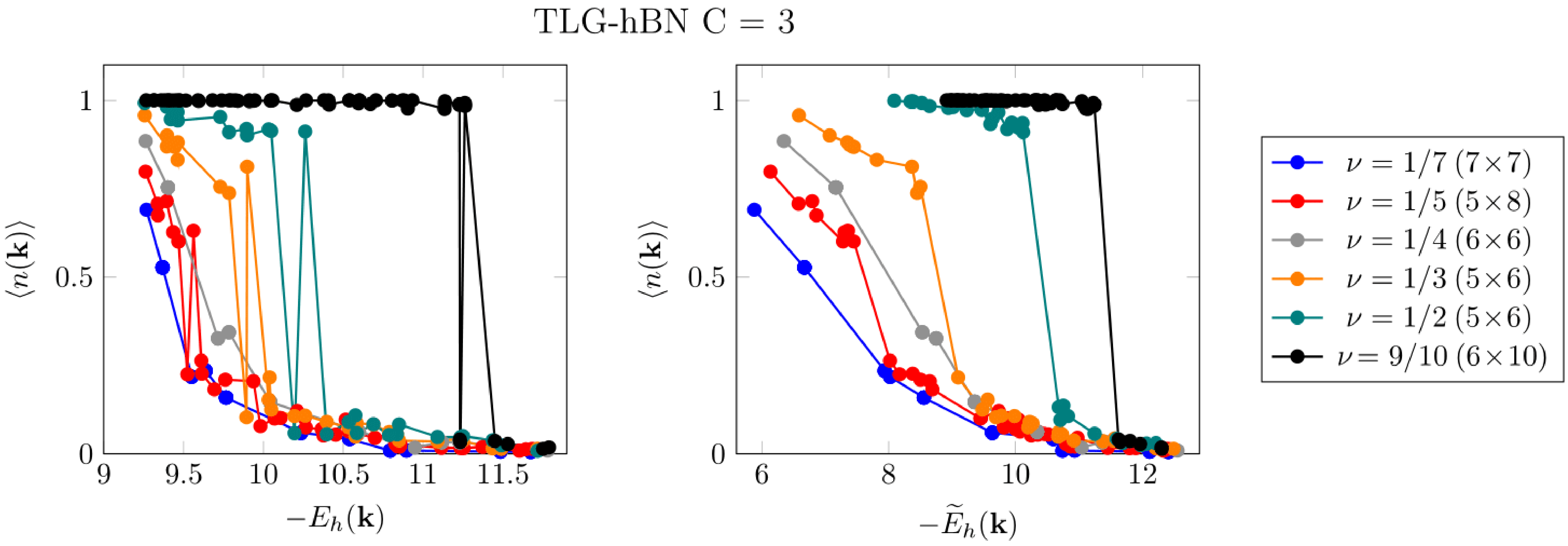

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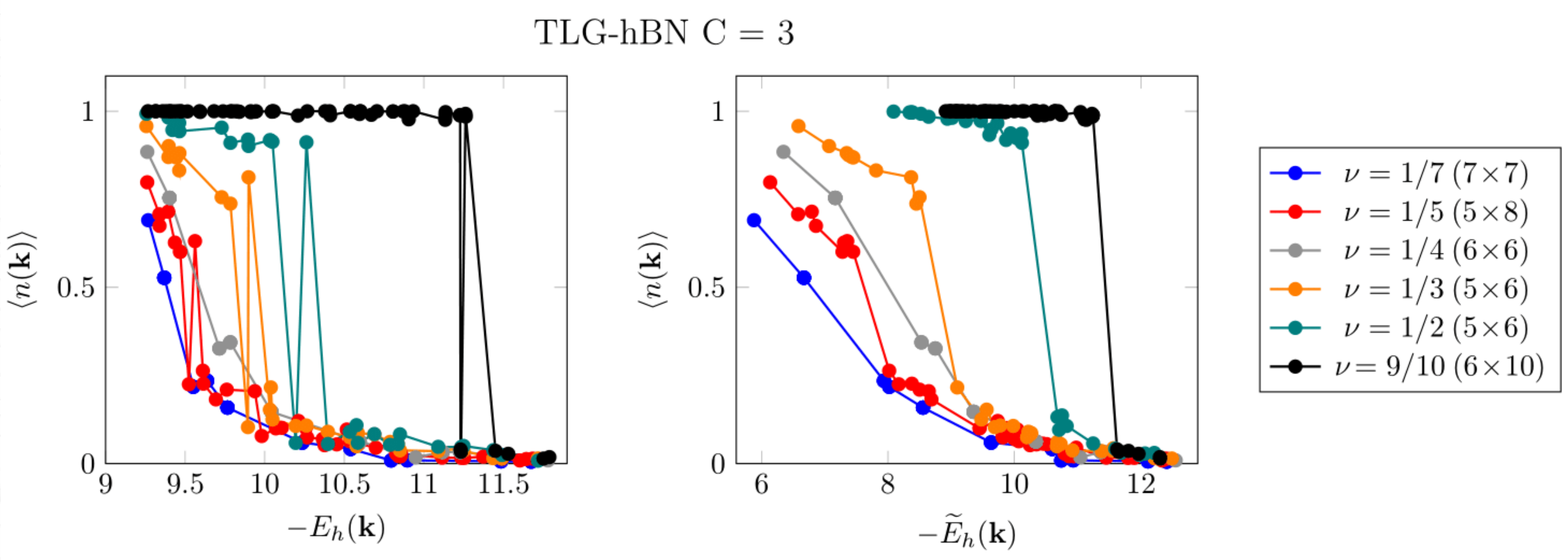
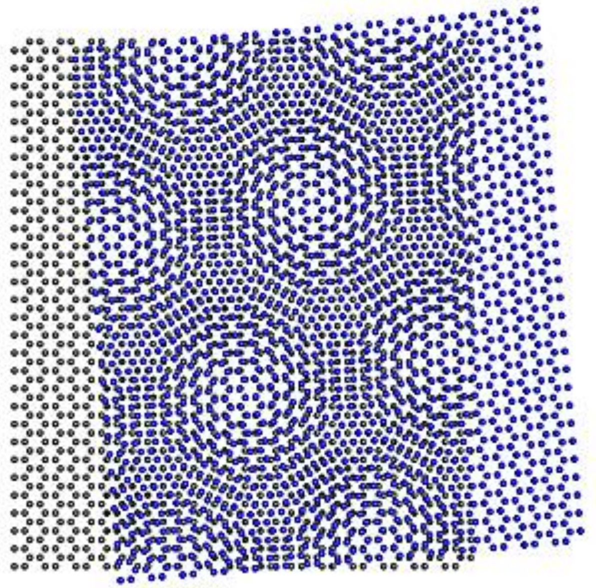
What happened here?

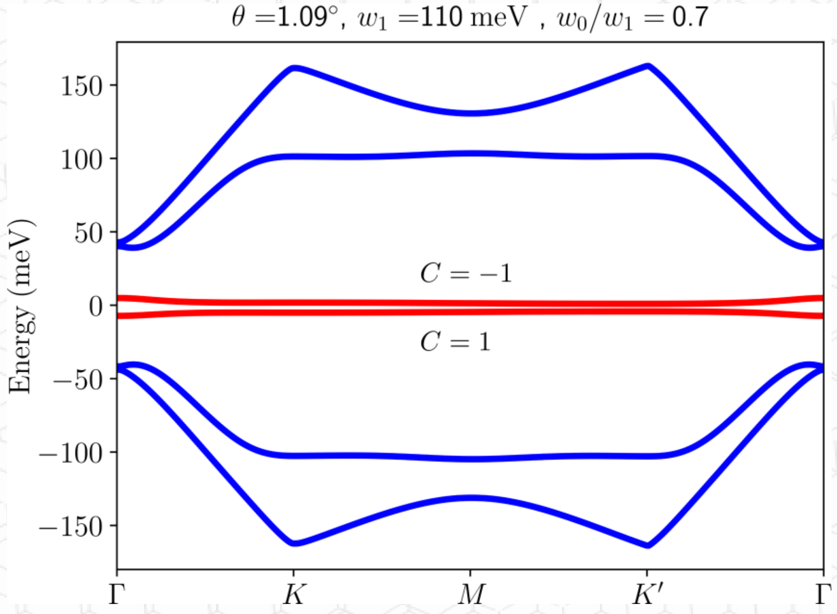


- The problem is weakly interacting in terms of holes!
- Emergent Fermi Liquids from an initial strongly interacting problem.
- The hole dispersion dictates the underlying physics.
- Guiding principle : Electrons prefer to occupy states with the lowest hole-energy.

Twisted Bilayer Graphene aligned with Boron Nitride



Credit : NIST



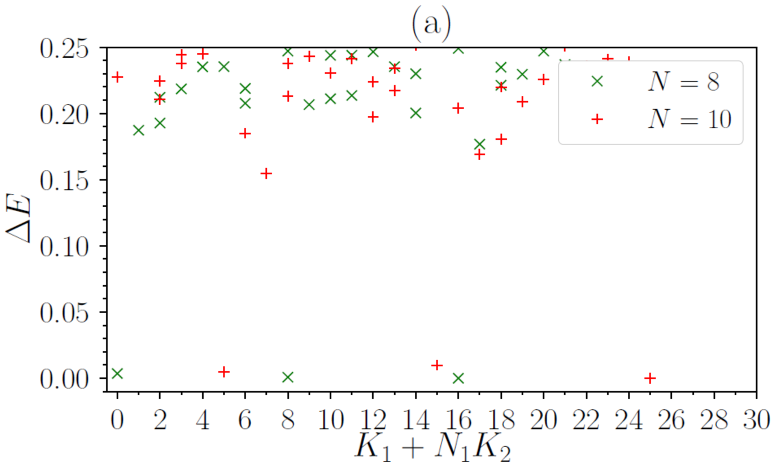
- Alignment with hBN breaks $C_2\mathcal{T}$ symmetry.
- Induces sublattice potential on one of the layers.
- The bands acquire non-zero Chern numbers.

- Could FCI states stabilized upon fractional fillings (e.g 1/3) of one of the red bands?

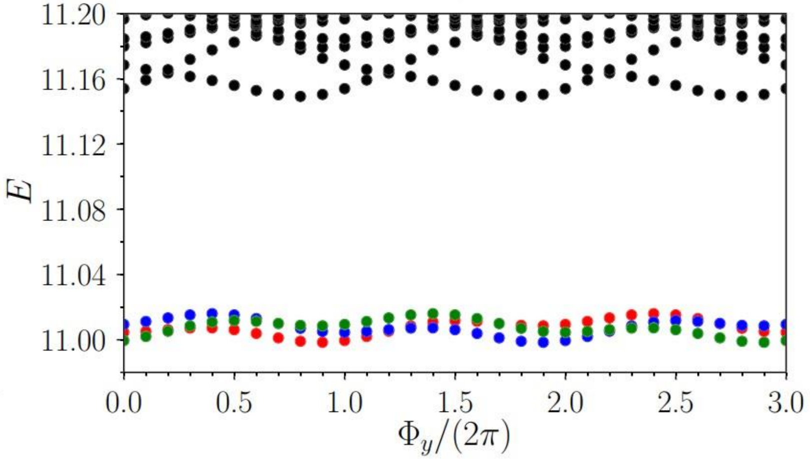
Yes, FCIs, finally!

In twisted bilayer graphene aligned with boron nitride — but only **at slightly weaker inter-layer tunnelling than in current experiments**…

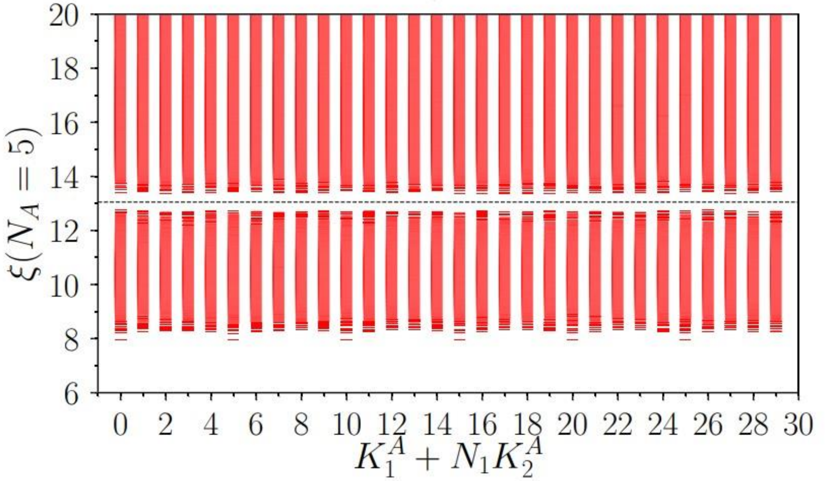
Ground state degeneracy on a torus



Spectral flow of ground states



Particle entanglement spectrum

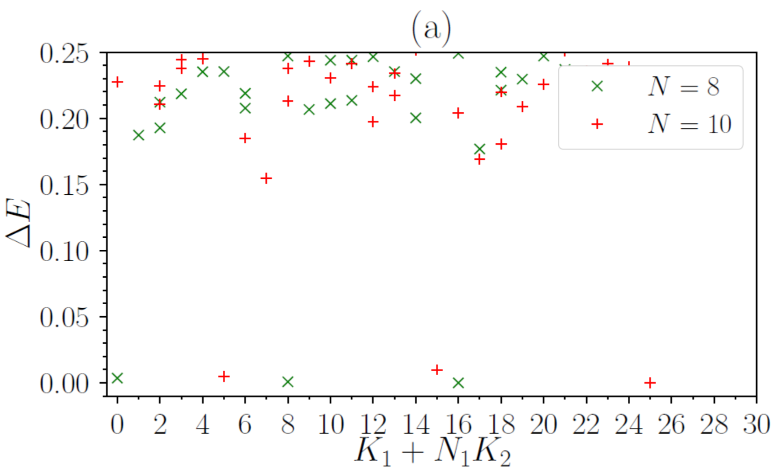


- Laughlin like state at filling $\nu = 1/3$
- Gap ~ 10 K

Yes, FCIs, finally!

In twisted bilayer graphene aligned with boron nitride — but only **at slightly weaker inter-layer tunnelling than in current experiments**…

Ground state degeneracy on a torus



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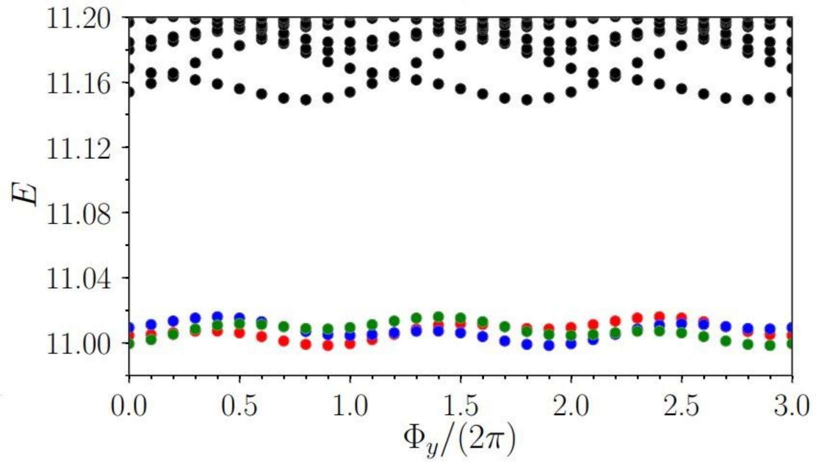
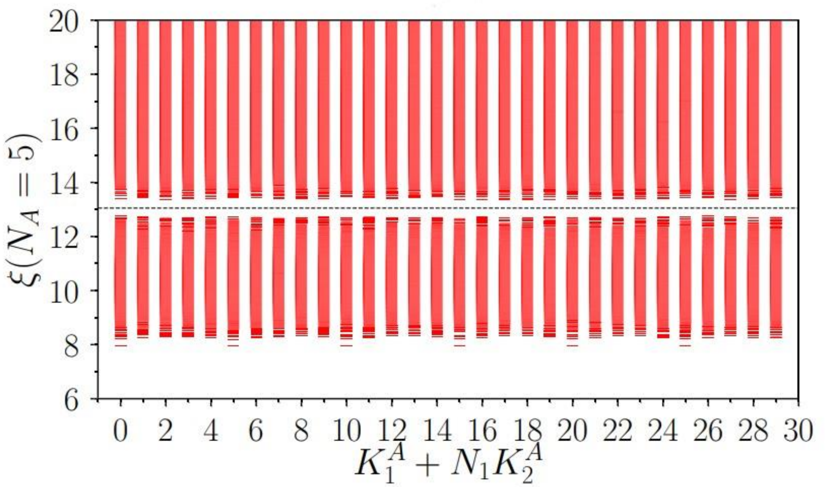


Particle entanglement spectrum



•Corroborated by subsequent works

- Spin polarization confirmed by Repellin and Senthil, Phys. Rev. Research 2, 023238 (2020)
- Solvable “chiral limit” identified by Ledwith et. al., Phys. Rev. Research 2, 023237 (2020)

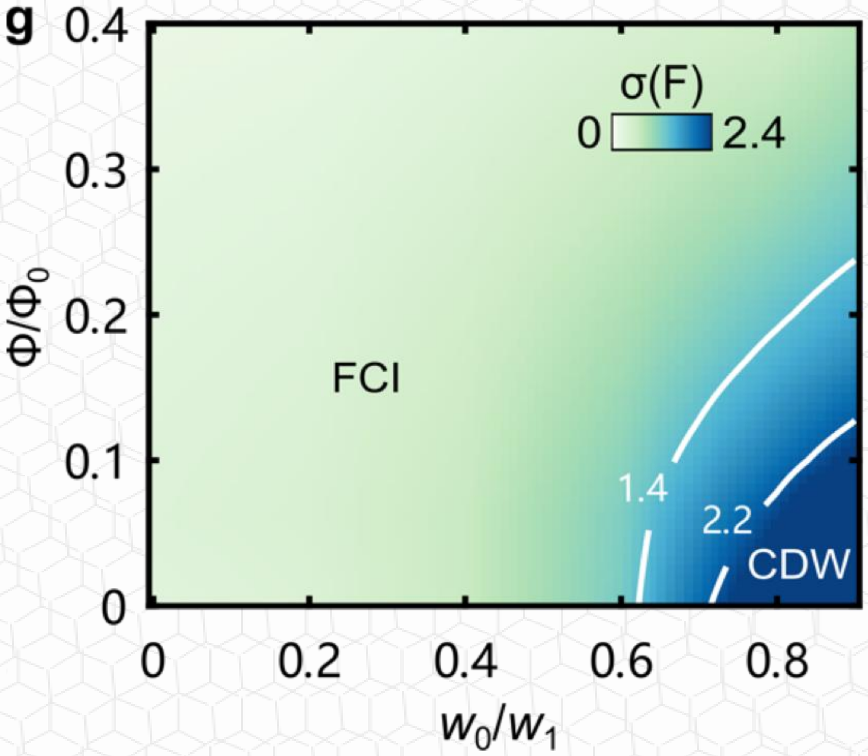
Article | Open Access | Published: 15 December 2021

Fractional Chern insulators in magic-angle twisted bilayer graphene

Yonglong Xie, Andrew T. Pierce, Jeong Min Park, Daniel E. Parker, Eslam Khalaf, Patrick Ledwith, Yuan Cao, Seung Hwan Lee, Shaowen Chen, Patrick R. Forrester, Kenji Watanabe, Takashi Taniguchi, Ashvin Vishwanath, Pablo Jarillo-Herrero & Amir Yacoby

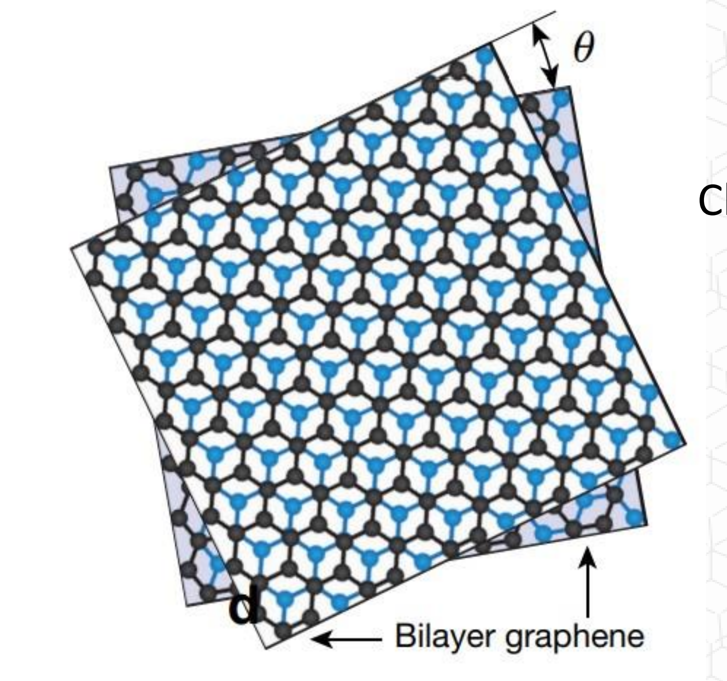
Nature **600**, 439–443 (2021) | Cite this article

- Weak field (5 Tesla), similar effect as changing inter-layer tunnelling

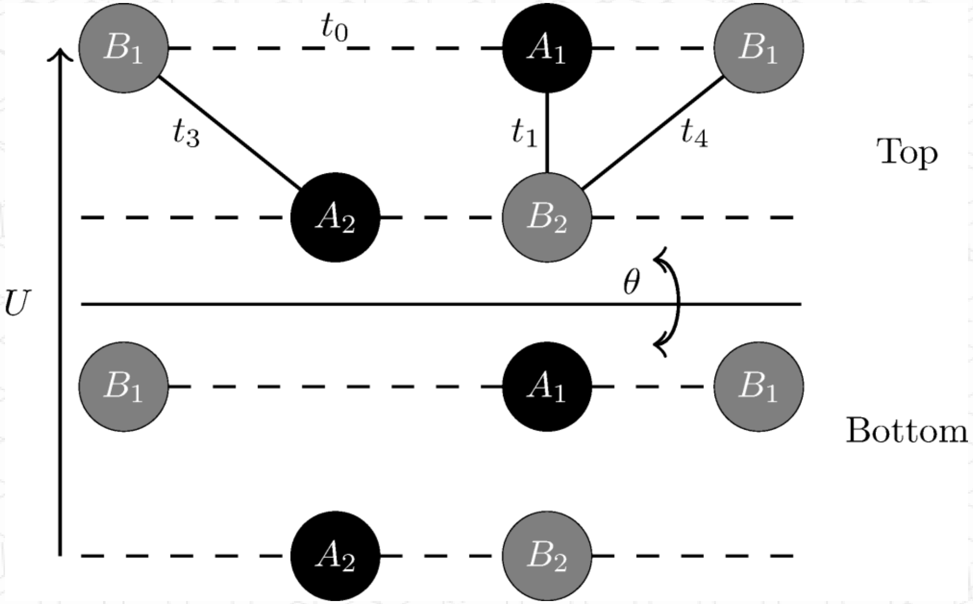


There is even a better system!

- Twisted Double Bilayer Graphene



Click to add text



Credit : Liu et al, *Nature* **583**, (2020)

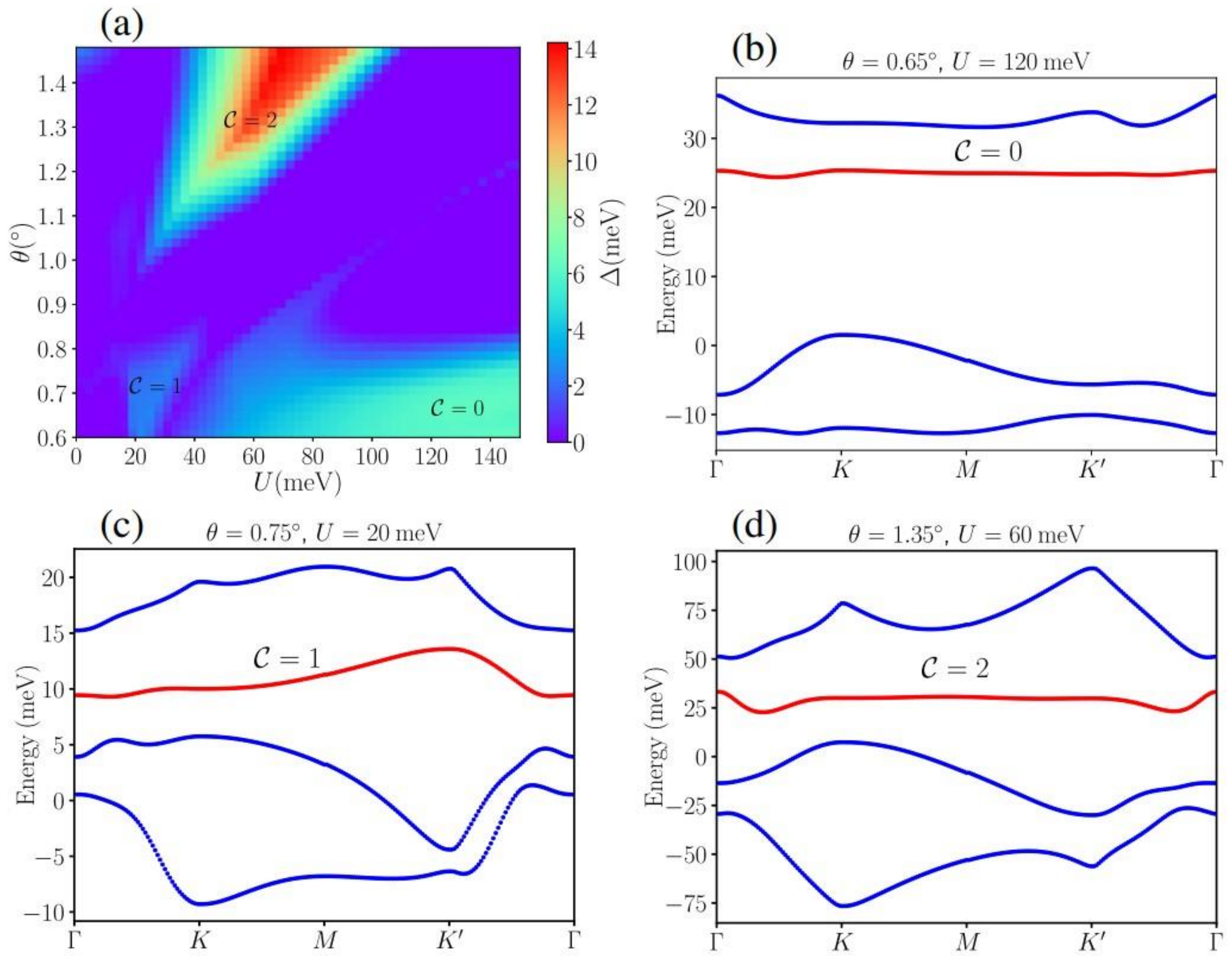
Tunability!

Nat Commun **10,** 5333 (2019).

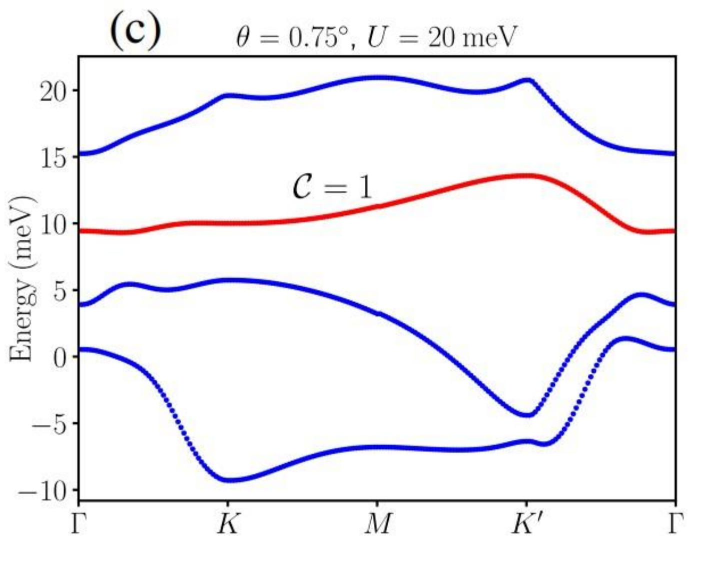
Δ is gap

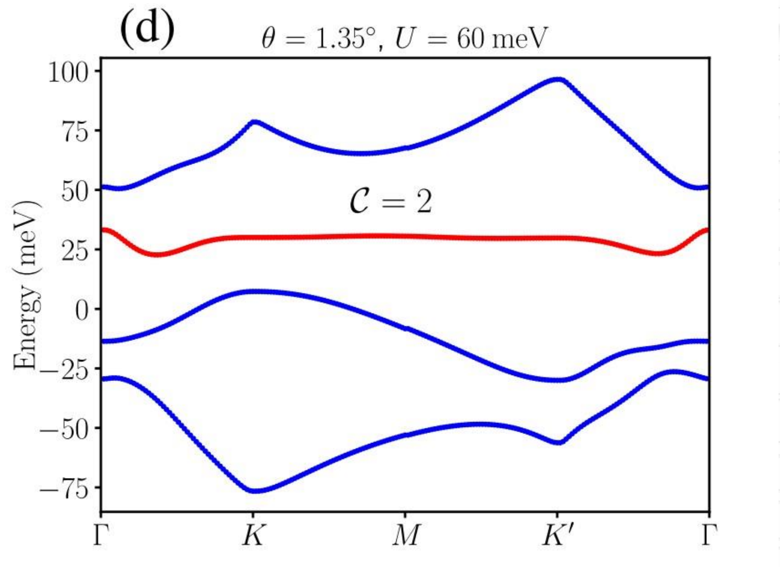
U is electric field

θ is twist angle



A series of FCIs in TDBG





- Spin-polarized Laughlin like state at $\nu = 1/3$
- Laughlin state particle-hole conjugate at $\nu = 2/3$
- Spin-singlet Halperin 332 state at $\nu = 2/5$
- Possibly Halperin 332 particle-hole conjugate at $\nu = 3/5$

- Spin-polarized FCI at $\nu = 1/3$ in $C = 2$ band!
- It could be thought of as a weakly interacting state of composite fermions with negative flux attachment!

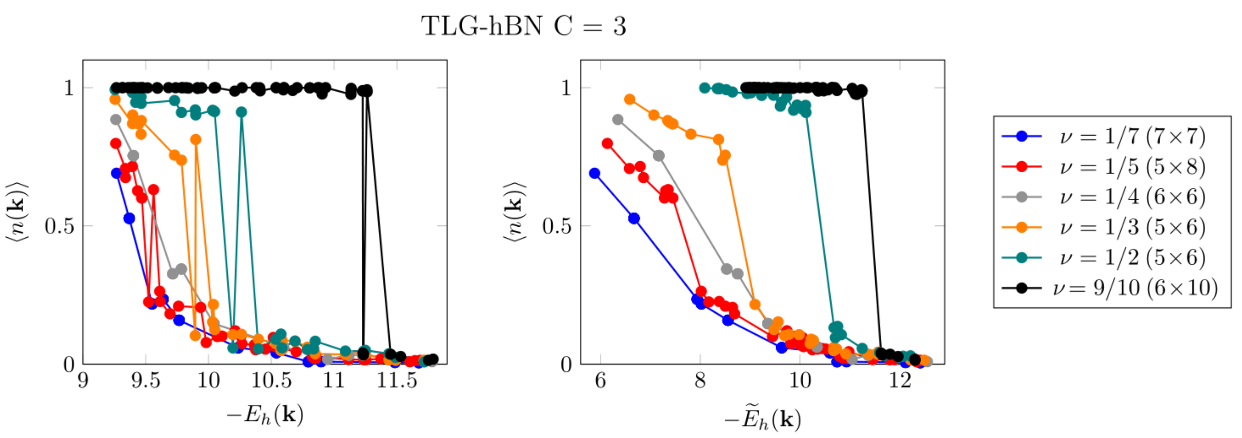
Full details in Phys. Rev. Lett. **126**, 026801

A series of FCIs in TDBG!

- We predict TDBG as candidate ***real*** material for a variety of spin-singlet and spin-polarized FCI states at different fillings and Chern numbers without the need of any magnetic field.

- Access to different topological phases by tuning the twist angle and the electric field!

A closer look at the particle-hole asymmetry



$$H_{\text{proj}} = \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} V_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} c^\dagger_{\mathbf{k}_1} c^\dagger_{\mathbf{k}_2} c_{\mathbf{k}_3} c_{\mathbf{k}_4}$$

Particle-Hole Transformation, $c_{\mathbf{k}} \to d^\dagger_{\mathbf{k}}$

$$H_{\text{proj}} \to \sum_{\mathbf{k}} E_h(\mathbf{k}) d^\dagger_{\mathbf{k}} d_{\mathbf{k}} + \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} V^*_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} d^\dagger_{\mathbf{k}_1} d^\dagger_{\mathbf{k}_2} d_{\mathbf{k}_3} d_{\mathbf{k}_4}$$

$$E_h(\mathbf{k}) = \sum_{\mathbf{k}'} \left(V_{\mathbf{k}'\mathbf{k}\mathbf{k}'\mathbf{k}} + V_{\mathbf{k}\mathbf{k}'\mathbf{k}\mathbf{k}'} - V_{\mathbf{k}\mathbf{k}'\mathbf{k}'\mathbf{k}} - V_{\mathbf{k}'\mathbf{k}\mathbf{k}\mathbf{k}'}\right)$$

Why is $E_h(\mathbf{k})$ a good approximation??

A closer look at the particle-hole asymmetry

$$H_{\text{proj}} = \sum_{\mathbf{k}} E_h(\mathbf{k}) d^\dagger_{\mathbf{k}} d_{\mathbf{k}} + \sum_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} V^*_{\mathbf{k}_1\mathbf{k}_2\mathbf{k}_3\mathbf{k}_4} d^\dagger_{\mathbf{k}_1} d^\dagger_{\mathbf{k}_2} d_{\mathbf{k}_3} d_{\mathbf{k}_4}$$

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$$\mathrm{V}_{\mathbf{k}_1,\mathbf{k}_2,\mathbf{k}_3,\mathbf{k}_4} \sim \sum_{\mathbf{q}} V(\mathbf{q}) \lambda(\mathbf{k}_4, \mathbf{q}) \lambda(\mathbf{k}_3, -\mathbf{q}) \delta_{\mathbf{q},\mathbf{k}_1-\mathbf{k}_4}$$

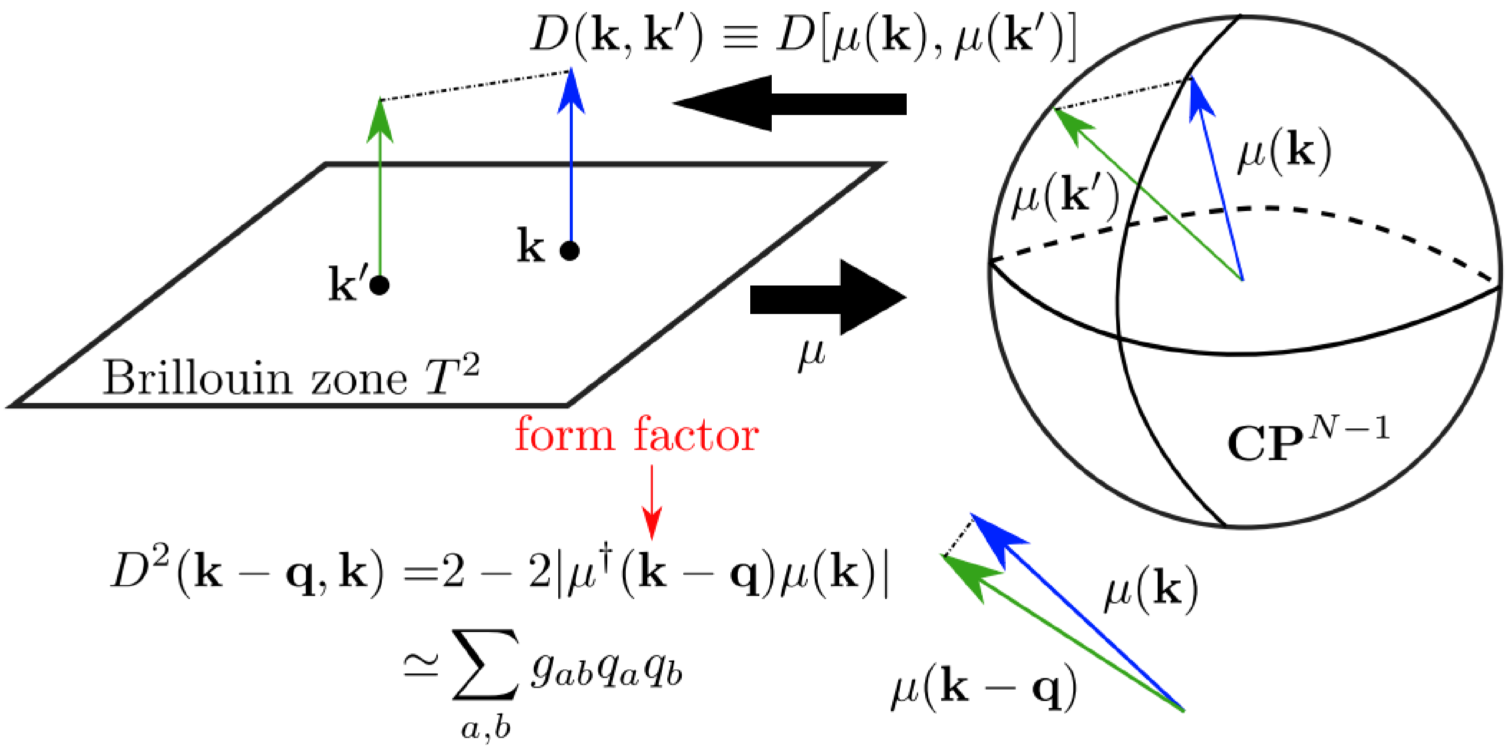
$$\lambda(\mathbf{k}, \mathbf{q}) = \mu^\dagger(\mathbf{k} - \mathbf{q}) \mu(\mathbf{k})$$

Bloch wavefunction of the flat band

Form factor

- The key is in the form factor!
- If it decays fast enough then perhaps higher order corrections are suppressed?
- How does it decay?

Form factors and the Fubini-Study metric



$$2g_{ab}(\mathbf{k}) = \partial_a\mu^\dagger(\mathbf{k})\partial_b\mu(\mathbf{k}) - [\partial_a\mu^\dagger(\mathbf{k})\mu(\mathbf{k})][\mu^\dagger(\mathbf{k})\partial_b\mu(\mathbf{k})] + (a \leftrightarrow b)$$

J. Provost and G. Vallee, "Riemannian structure on manifolds of quantum states," Communications in Mathematical Physics 76, 289–301 (1980)

Form factors and the Fubini-Study metric

in the limit of small q

- The form factor $|\lambda(\mathbf{k},\mathbf{q})| \approx 1 - \frac{1}{2}\sum_{ab} q_a q_b g_{ab}(\mathbf{k}) \overset{?}{\approx} e^{-\sum_{ab}\frac{1}{2}q_a q_b g_{ab}(\mathbf{k})}$

- Moiré systems have lots of bands (N ~ 10^3) so the eigenvectors could spread out in distance in $\mathbf{CP}^{N-1}$ so that the form factor decays quickly!

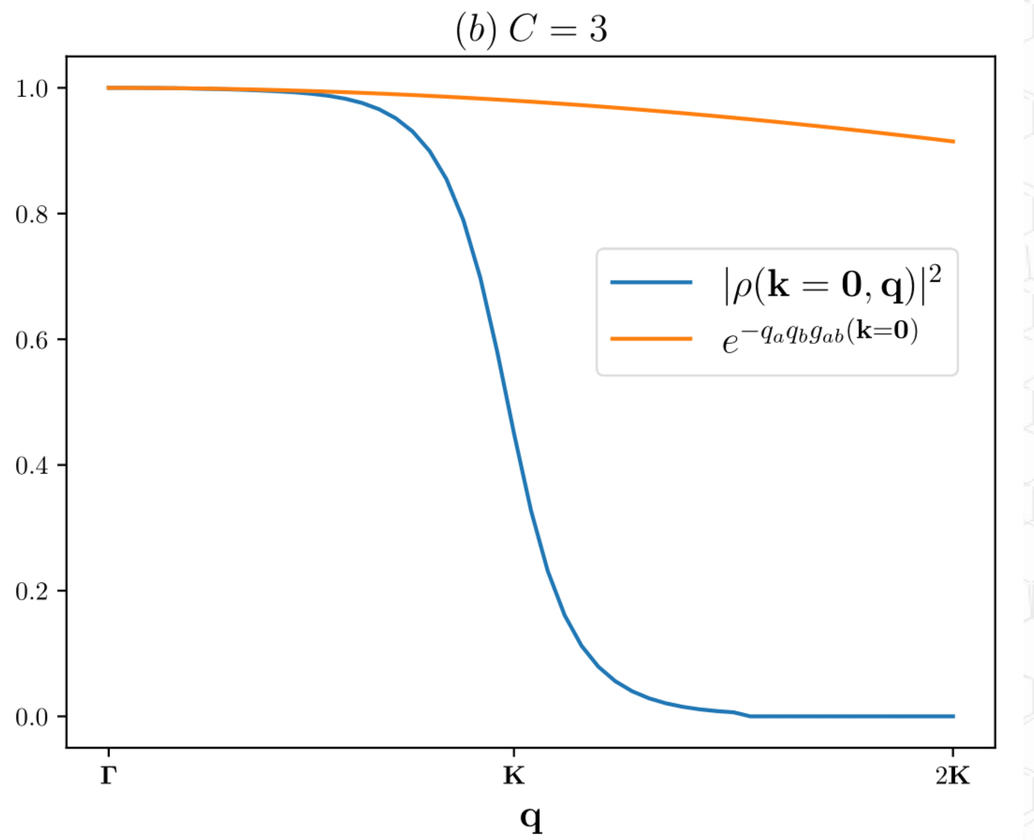
- Fast enough decaying form factors are controlled mainly by the metric $g_{ab}(\mathbf{k})$

How do they decay?

- Very fast!

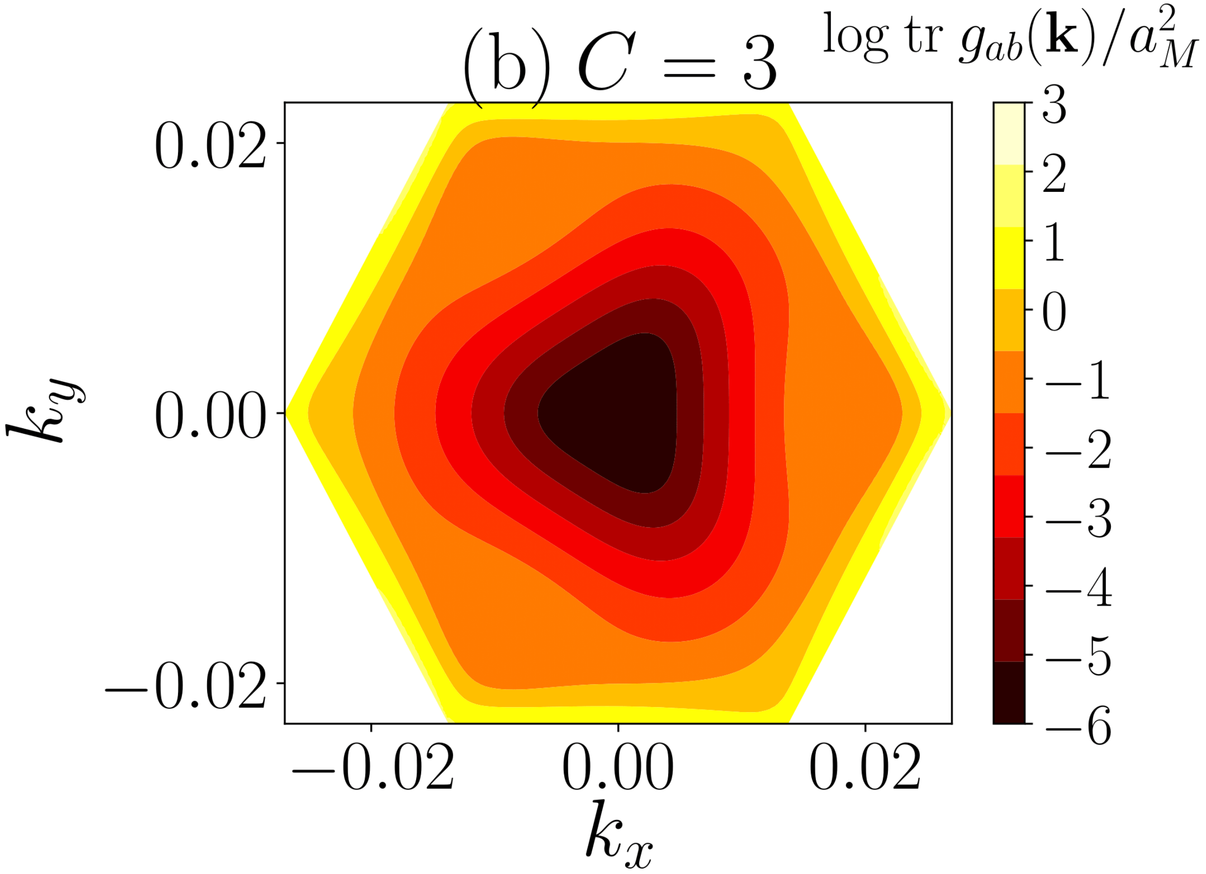
- The form factor appears clearly in the hole energy!

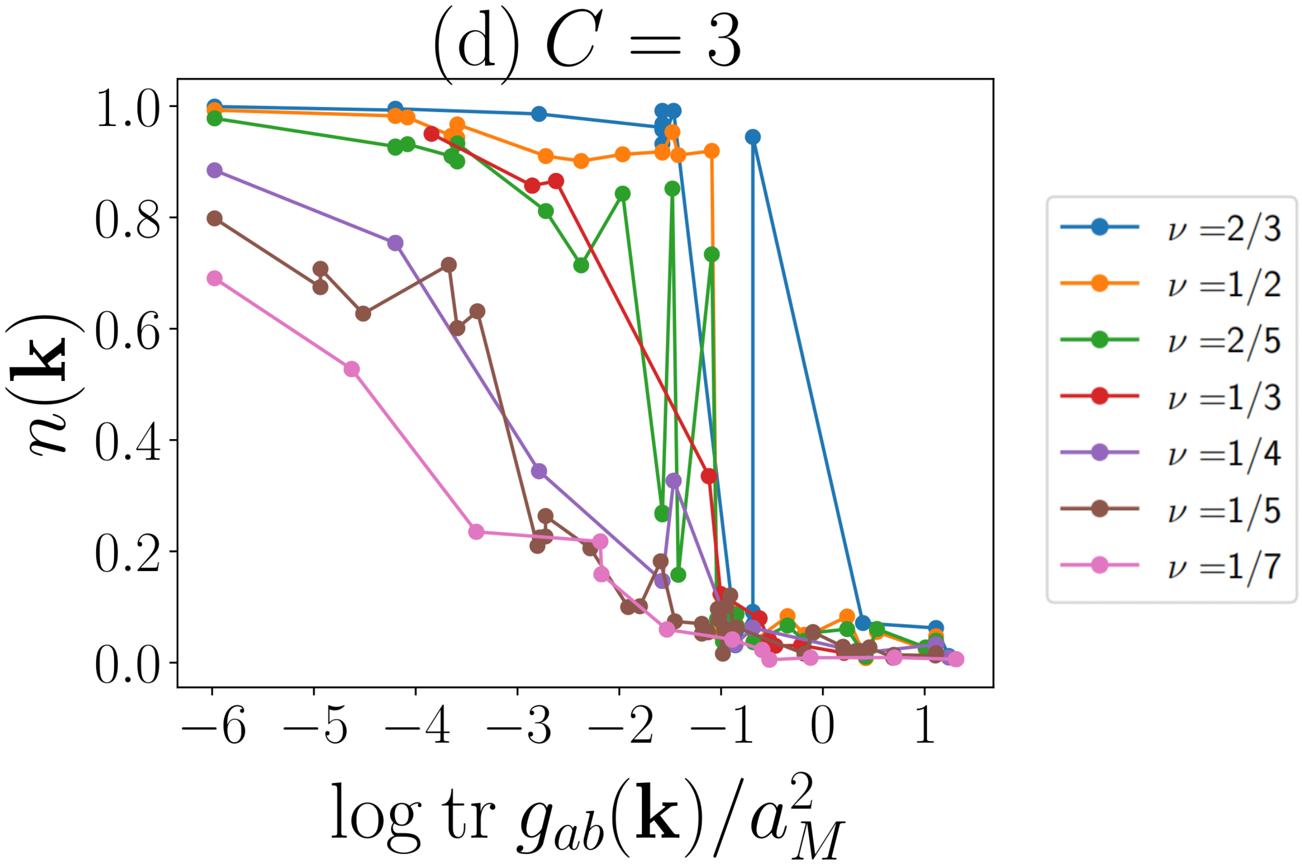
$$E_h(\mathbf{k}) = \sum_{\mathbf{q}} V(\mathbf{q})|\lambda(\mathbf{k},\mathbf{q})|^2 \approx \sum_{\mathbf{q}} V(\mathbf{q})(1 - q_a q_b g_{ab}(\mathbf{k}))$$



- How does the metric $g_{ab}(\mathbf{k})$ affect the electron occupation $\langle n(\mathbf{k})\rangle = \langle c^\dagger_{\mathbf{k}} c_{\mathbf{k}}\rangle$?

Let's look again



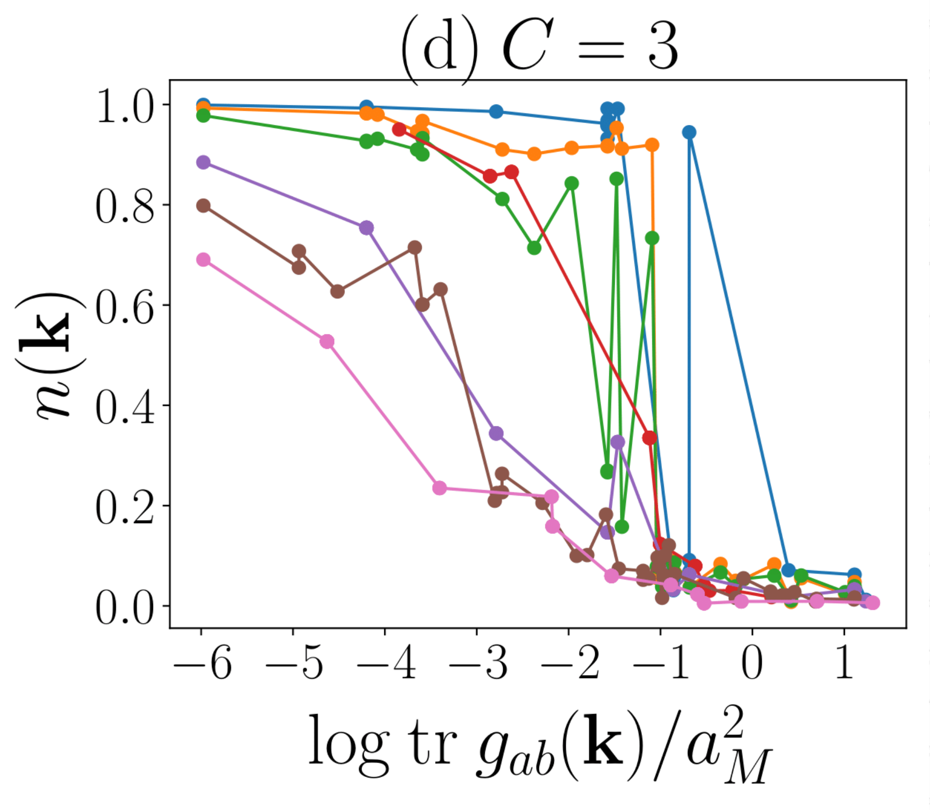


- Guiding principle :

Electrons tend to occupy states with the lowest hole-energy. ⟺ Electrons tend to occupy states with the lowest Fubini-Study metric trace!

The Fermi Liquids in TLG-hBN are metric-induced!

- Electrons prefer to occupy states with lower Fubini-Study metric.
- If the Fubini-Study metric fluctuations are large enough, it could become energetically favorable to form a Fermi Liquid.



- More general framework for Moiré systems in arXiv:2202.10467

Take home message

- Moiré systems are promising platforms for fractional quantum Hall physics (and even more)
- The particle-hole asymmetry of interactions in a single band has dramatic consequences.
- The Fubini-Study metric is a very relevant quantity to the low energy physics of Moiré materials.

Thank You!