



# Real space topology for moiré materials

Christophe Mora



Laboratoire Matériaux et Phénomènes Quantiques

Christophe Mora

Topology and Geometry Beyond Perfect Crystals, Nordita 2025

#### I. Chern and fractional Chern insulators in 2D materials

#### II. Layer skyrmion in adiabatic twisted TMD and chiral TBG

III. Real-space topology and ensembles of Bloch wavefunctions

# Chern and fractional Chern insulators in 2D materials



REPORTS

#### Observation of fractional Chern insulators in a van der Waals heterostructure

#### Eric M. Spanton,<sup>1\*</sup> Alexander A. Zibrov,<sup>2\*</sup> Haoxin Zhou,<sup>2</sup> Takashi Taniguchi,<sup>3</sup> Kenji Watanabe,<sup>3</sup> Michael P. Zaletel,<sup>4</sup> Andrea F. Young<sup>2</sup>

<sup>1</sup>California Nanosystems Institute, University of California, Santa Barbara, CA 93106, USA. <sup>2</sup>Department of Physics, University of California, Santa Barbara, CA 93106, USA. <sup>3</sup>Advanced Materials Laboratory, National Institute for Materials Science, Tsukuba, Ibaraki 305-0044, Japan. <sup>4</sup>Department of Physics, Princeton University, Princeton, NJ 08544, USA.



Topology and Geometry Beyond Perfect Crystals, Nordita 2025



TBG  $\theta = 1.05^{\circ}$ 



Moiré pattern

tMoTe<sub>2</sub> 40(a) 35C = 130[meV] 25C=1Ē 201510 $\breve{K}_{M'}$  $K_M M$ Г M

Zhang, Wang, Liu, Fan, Cao, and Xiao, Nature Comm 2024



Topology and Geometry Beyond5Perfect Crystals, Nordita 2025

Christophe Mora

#### Ferromagnetic states and Chern insulators Zondin 2020;

Zondiner, Ilani, Nature 2020 ; Wong, Yazdani, Nature 2020 ; Saito, Young, Nature Physics 2021

+1



Serlin, Tschirhart, Balents, Young, et al. Science 2020 Sharpe, Golhaber-Gordon, et al. Science 2019

#### Fractional Chern insulators in TBG

TBG



Xie, Jarillo-Herrero, Yacoby, Nature 2021



Fractional Chern insulators identified in Fan diagrams

They are stabilized above 5T

#### **Fractional Chern insulators**





### FCIs in TMDs



Yiping Wang, Jeongheon Choe, Eric Anderson, Weijie Li, Julian Ingham, Eric A. Arsenault, Yiliu Li, Xiaodong Hu, Takashi Taniguchi, Kenji Watanabe, Xavier Roy, Dmitri Basov, Di Xiao, Raquel Queiroz, James C. Hone, Xiaodong Xu, X.-Y. Zhu, arXiv:2502.21153



ν

Topology and Geometry Beyond Perfect Crystals, Nordita 2025

 $\mu_{o}H(mT)$ 

9

### FCIs in rhombohedral graphene



Z. Lu, T. Han, Y. Yao, Z. Hadjri, J. Yang, J. Seo, L. Shi, S. Ye, K. Watanabe, T. Taniguchi, and L. Ju, **Nature** 637, 1090 (2025).





Xie, Huo, Lu, Feng, Zhang, Wang, Yang, Watanabe, Taniguchi, Liu, Song, Xie, Liu & Lu. Nature Materials (2025).





Choi, Y., Choi, Y., Valentini, M., Patterson, C. L., Holleis, L. F. W., Sheekey, O. I., Stoyanov, H., Cheng, X., Taniguchi, T., Watanabe, K. & Young, A. F., **Nature**, 639, 342–347 (2025)

10

Christophe Mora

# Layer skyrmion in adiabatic TMD

# and chiral TBG

#### Layer skyrmions for ideal Chern bands and twisted bilayer graphene

Daniele Guerci,<sup>1</sup> Jie Wang,<sup>2</sup> and Christophe Mora<sup>3</sup>

<sup>1</sup>Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA
 <sup>2</sup>Department of Physics, Temple University, Philadelphia, Pennsylvania, 19122, USA
 <sup>3</sup>Université Paris Cité, CNRS, Laboratoire Matériaux et Phénomènes Quantiques, 75013 Paris, France

#### arXiv:2408.12652v1

Topology and Geometry Beyond Perfect Crystals, Nordita 2025 11

#### Continuum model for twisted TMD - WSe<sub>2</sub> MoTe<sub>2</sub>



$$I_{\rm sp}^{K} = \begin{pmatrix} -\frac{\hbar^{2}(\mathbf{k} - \mathbf{K}^{b})^{2}}{2m^{*}} + V_{b}(\mathbf{r}) & T(\mathbf{r}) \\ T^{\dagger}(\mathbf{r}) & -\frac{\hbar^{2}(\mathbf{k} - \mathbf{K}^{t})^{2}}{2m^{*}} + V_{t}(\mathbf{r}) \end{pmatrix}$$

$$T(\mathbf{r}) = w(1 + e^{-i\mathbf{g}_2 \cdot \mathbf{r}} + e^{-i\mathbf{g}_3 \cdot \mathbf{r}})$$

Parameters chosen to fit ab initio DFT calculations



7.1

6.7

Wu, Lovorn, Tutuc, Martin, MacDonald PRL 2019

$$H_{sp}^{K} = -\frac{(\hbar \mathbf{k})^{2}}{2m^{*}}\sigma_{0} + \boldsymbol{\Delta}(\mathbf{r}) \cdot \boldsymbol{\sigma} + \Delta_{0}(\mathbf{r})\sigma_{0},$$



Topology and Geometry Beyond Perfect Crystals, Nordita 2025 12



Christophe Mora

Topology and Geometry Beyond Perfect Crystals, Nordita 2025 13



Topology and Geometry Beyond Perfect Crystals, Nordita 2025 14

#### Wavefunction zeros in the adiabatic approximation

$$\left\{-\frac{(-i\hbar\nabla - e\tilde{\mathbf{A}}(\mathbf{r}))^2}{2m^*} + \tilde{V}(\mathbf{r})\right\}\Phi_k(\mathbf{r}) = \varepsilon_k\Phi_k(\mathbf{r})$$

$$\boldsymbol{\psi}_{\boldsymbol{k}}(\boldsymbol{r}) = \boldsymbol{\chi}(\boldsymbol{r}) \, \Phi_{\boldsymbol{k}}(\boldsymbol{r})$$

The Aharonov-Bohm phase imposes one zero and an associated vortex for each unit cell (Riemann-Roch theorem)

These zeros are perturbatively not stable. They are lifted by deviations from the adiabatic limit

A real-space Berry connection can be defined

$$A(\mathbf{r}) = -i\chi^{\dagger}(\mathbf{r})\nabla_{\mathbf{r}}\chi(\mathbf{r})$$



The real-space Berry curvature integrates to -1.

### Twisted bilayer graphene – chiral limit

Chiral limit: vanishing AA (BB) hoppings

$$H = \begin{pmatrix} 0 & \mathcal{D}^{\dagger} \\ \mathcal{D} & 0 \end{pmatrix} \qquad \qquad \mathcal{D} = -i\partial_{\bar{z}} + \begin{pmatrix} 0 & f_2(\boldsymbol{r}) \\ f_1^*(\boldsymbol{r}) & 0 \end{pmatrix}$$



Zero-energy solution is also a zero mode of  $\,\mathcal{D}\,$ 

$$\begin{cases} \mathcal{D} \psi_K(\boldsymbol{r}) = 0 \\ \psi_k(\boldsymbol{r}) = g(z)\psi_K(\boldsymbol{r}) \end{cases} \longrightarrow \mathcal{D} \psi_k(\boldsymbol{r}) = 0 \\ g(z) \text{ is an arbitrary holomorphic function of } z \end{cases}$$

Same structure as the lowest Landau level (vortexability)

### Landau level correspondence for chiral TBG

At the magic angle (and chiral limit), decomposition of the WF into scalar LLL and a spinor



Again, one zero in the LLL WF per unit cell

Skyrmion texture in real space for chiral TBG

Guerci, Wang, Mora Arxiv 2024

$$\boldsymbol{\psi}_{\boldsymbol{k}}(\boldsymbol{r}) = \boldsymbol{\chi}(\boldsymbol{r}) \Phi_{\boldsymbol{k}}^{LLL}(\boldsymbol{r}) \qquad \qquad \boldsymbol{\chi}(\boldsymbol{r}) = \begin{pmatrix} \chi_1(\boldsymbol{r}) \\ \chi_2(\boldsymbol{r}) \end{pmatrix} \qquad \qquad A(\mathbf{r}) = -i\chi^{\dagger}(\mathbf{r})\nabla_{\mathbf{r}}\chi(\mathbf{r})$$



Layer skyrmion texture for a Chern C=1 band



Real-space Chern number = Pontryagin index = -1

Summary: adiabatic twisted TMD and chiral TBG

LL – spinor decomposition  $\psi_k(r) = \chi(r) \Phi_k(r)$ 

Scalar part experiences an effective magnetic field with a flux quantum through the unit cell

One zero per unit cell, unstable against perturbation

Skyrmion texture for the spinor. Real-space Chern number or Pontryagin index of -1



19

# **Real-space topology and ensemble**

## of Bloch wavefunctions



Topology and Geometry Beyond Perfect Crystals, Nordita 2025 20

### Beyond the ideal cases (TMDs or TBG)

Mathematical theorem. If  $\psi_k(r)$  is never vanishing and periodic over the lattice : the real-space Chern number is always zero.

$$u_{\mathbf{k}}(\mathbf{r}) = \chi(\mathbf{r})\Phi_{\mathbf{k}}(\mathbf{r}) + \epsilon\Delta u_{\mathbf{k}}(\mathbf{r})$$



Example in TBG at angle with realistic corrugation

Lifting of the zero (perturbation) : small region with strong positive contribution to the real-space Chern number.

Compensate the negative part.

#### **Real-space skyrmion for TMD**

$$u_{\mathbf{k}}(\mathbf{r}) = \chi(\mathbf{r})\Phi_{\mathbf{k}}(\mathbf{r}) + \epsilon\Delta u_{\mathbf{k}}(\mathbf{r})$$

Non-adiabatic limit

$$\hat{\boldsymbol{n}}_{\mathbf{k}}(\mathbf{r}) = \frac{u_{\mathbf{k}}^{\dagger}(\mathbf{r})\boldsymbol{\sigma}u_{\mathbf{k}}(\mathbf{r})}{u_{\mathbf{k}}^{\dagger}(\mathbf{r})u_{\mathbf{k}}(\mathbf{r})}$$

Reduces to (in the adiabatic limit)

$$\boldsymbol{\hat{n}}(\mathbf{r}) = \chi^{\dagger}(\mathbf{r})\boldsymbol{\sigma}\chi~(\mathbf{r})$$





### Real-space topology – individual vs ensemble of WFs

So far, we explored individual (at fixed momentum) WF

$$u_{\mathbf{k}}(\mathbf{r}) = \chi(\mathbf{r})\Phi_{\mathbf{k}}(\mathbf{r}) + \epsilon\Delta u_{\mathbf{k}}(\mathbf{r})$$

Generally, they have zero real-space Chern number, despite exhibing (close to) skyrmion textures



We introduce an ensemble average – similar to tunneling density of states

$$\boldsymbol{A}(E,\mathbf{r}) = \sum_{\mathbf{k}} u_{\mathbf{k}}^{\dagger}(\mathbf{r})\boldsymbol{\sigma} u_{\mathbf{k}}(\mathbf{r})\delta(\boldsymbol{\epsilon}_{\mathbf{k}} - E) \qquad \qquad \boldsymbol{\hat{n}}_{E}(\mathbf{r}) =$$

 $\frac{\boldsymbol{A}(E,\mathbf{r})}{|\boldsymbol{A}(E,\mathbf{r})|}$ 

#### **Ensemble of WFs - TMDs**



Adiabatic vs individual WF vs ensemble

24

#### **Real-space Chern number from ensemble**



The real-space Chern number extracted from the ensemble average is consistently -1 - for the topmost two bands with (momentum) Chern number +1

Christophe Mora

#### **Ensemble of WFs - TBG**

Real-space Berry curvatures



### **Topological Heavy fermion model**



Six-band model reproduces the spectrum of TBG:2 local Wannier orbitals (non-dispersive)4 topological conduction bands

Successful in describing the coexistence of local moments and itinerants electrons

Song & Bernevig Phys Rev Lett 2022 Clugru Borovkov Lau Coleman Song & Bernevig, Low Temp Phys 2023 Shi & Dai Phys Rev B 2022

### Real-space topology in the topological Heavy fermion model

Electronic distributions for the six different orbitals

Real-space Berry curvature for the six orbital WFs



28

#### Real-space topology in the topological Heavy fermion model

Electronic distributions for the six different orbitals

Real-space Berry curvature for the six orbital WFs



29

#### Symmetries for TMDs

In contrast with individual Bloch WFs (at fixed k), the ensemble-average inherits the (spatial) symmetries of the model

$$\begin{aligned} \mathbf{A}(E,\mathbf{r}) &= \sum_{\mathbf{k}} u_{\mathbf{k}}^{\dagger}(\mathbf{r}) \boldsymbol{\sigma} u_{\mathbf{k}}(\mathbf{r}) \delta(\epsilon_{\mathbf{k}} - E) \\ \hat{\boldsymbol{n}}_{E}(\mathbf{r}) &= \frac{\mathbf{A}(E,\mathbf{r})}{|\mathbf{A}(E,\mathbf{r})|} \end{aligned}$$

ôn

Example of TMDs : two symmetries  $C_{3z}$  and  $C_{2y}T$  – assuming valley polarization

$$\hat{\boldsymbol{n}}_E(C_{3z}\mathbf{r}) = R_z(\mathbf{b}_1 \cdot \mathbf{r})\hat{\boldsymbol{n}}_E(\mathbf{r})$$
$$\hat{\boldsymbol{n}}_E(C_{2y}\mathbf{r}) = M_z\hat{\boldsymbol{n}}_E(\mathbf{r})$$

$$AAB = 1.0$$

$$0.5$$

$$0.0$$

$$-0.5$$

$$-1.0$$

$$egin{aligned} egin{aligned} egin{aligned} egin{aligned} eta_E(AA)ert_z &= 0 \ eta_E(AB) &= (0,0,\pm 1) \ eta_E(BA) &= (0,0,\mp 1) \end{aligned}$$

### Symmetry indicators for real-space topology



$$\begin{aligned} \hat{\boldsymbol{n}}_E(AA)|_z &= 0\\ \hat{\boldsymbol{n}}_E(AB) &= (0, 0, \pm 1)\\ \hat{\boldsymbol{n}}_E(BA) &= (0, 0, \mp 1) \end{aligned}$$

Symmetry indicators relate the Chern number to the  $C_{3z}$  eigenvalues at high-symmetry positions

$$e^{i2\pi C[\hat{\boldsymbol{n}}_E]/3} = \theta(AA)\theta(AB)\theta(BA) = \pm 1 \mod 3$$

For twisted TMDs, the real-space Chern number is always non-trivial !

#### Same non-trivial real-space Chern number in TBG

Same symmetries,  $C_{3z}$  and  $C_{2y}T$  apply in TBG – assuming valley and sublattice polarization

The resulting real-space Chern number is therefore also always non-trivial



#### Experiments on layer-skyrmions textures

#### $WSe_2$







Zhang, Morales-Durán, Li, Yao, Su, Lin, Dong, Liu, Chen, Kim, Watanabe, Taniguchi, Li, Robinson, MacDonald & Shih. Nature Physics, 2024

Thompson, Chu, Mesple, Zhang, Hu, Zhao, Park, Cai, Anderson, Watanabe, Taniguchi, Yang, Chu, Xu, Cao, Xiao & Yankowitz. Nature Physics, 2024.

### Acknowledgments



Kryštof Kolář



Felix von Oppen



Kang Yang



Daniele Guerci



Jie Wang

### Conclusion

Kolar, K. Wang, von Oppen, Mora PRB 2024 Guerci J. Wang, Mora Arxiv 2408.12652 Kolar, K. Wang, von Oppen, Mora, in preparation

Decomposition of the WF into a LL and a spinor with a layer-skyrmion texture in twisted TMDs in the adiabatic limit and chiral TBG

Non-trivial real-space Chern number associated with the skyrmion

Fragile outside the adiabatic and chiral limits : Chern is zero

Ensemble of wavefunctions: defines a robust real-space Chern number. Always non-zero in TMDs and TBG because of spatial symmetries



Topology and Geometry Beyond Perfect Crystals, Nordita 2025 35

### Adiabatic approximation

Morales-Durán, Wei, Shi, and MacDonald, 2024. Phys. Rev. Lett. 132, 096602.

Zhai and Yao,Bruno, Dug2020. Phys. Rev.TaillefumierMater. 4, 094002.Rev. Lett. 9

Bruno, Dugaev, and Taillefumier, 2004. Phys. Rev. Lett. 93, 096806.

#### $tMoTe_2$

E. Thompson, K. T. Chu, F. Mesple, X.-W. Zhang, ...., X. Xu, T. Cao, D. Xiao, and M. Yankowitz, Arxiv 2024

tWSe<sub>2</sub>

F. Zhang, N. Morales-Duran,..., J. A. Robinson, A. H. Macdonald, and C.-K. Shih, Arxiv 2024





Pontryagin density (or Berry phase) of a skyrmion texture  

$$\hat{\boldsymbol{n}}(\mathbf{r}) = \frac{\boldsymbol{\Delta}(\mathbf{r})}{|\boldsymbol{\Delta}(\mathbf{r})|} \qquad \qquad \tilde{B}(\mathbf{r}) = -\frac{\hbar}{2e} \hat{\mathbf{n}}(\mathbf{r}) \cdot \partial_x \hat{\mathbf{n}}(\mathbf{r}) \times \partial_y \hat{\mathbf{n}}(\mathbf{r})$$

# Layer skyrmions in twisted bilayer graphene

#### Layer skyrmions for ideal Chern bands and twisted bilayer graphene

Daniele Guerci,<sup>1</sup> Jie Wang,<sup>2</sup> and Christophe Mora<sup>3</sup>

<sup>1</sup>Center for Computational Quantum Physics, Flatiron Institute, New York, New York 10010, USA <sup>2</sup>Department of Physics, Temple University, Philadelphia, Pennsylvania, 19122, USA <sup>3</sup>Université Paris Cité, CNRS, Laboratoire Matériaux et Phénomènes Quantiques, 75013 Paris, France

#### arXiv:2408.12652v1

#### Ledwith, Tarnopolsky, Khalaf, Vishwanath, PRR 2020 Magnetic boundary condition Wang, Cano, Millis, Liu, Yang, PRL 2021 Twisted bilayer graphene (chiral) Twisted TMDs $\psi_{\boldsymbol{k}}(\boldsymbol{r}) = \boldsymbol{\chi}(\boldsymbol{r}) \Phi_{\boldsymbol{k}}^{LLL}(\boldsymbol{r})$ Bloch BC Magnetic translation BC Berry phase of the spinor (under winding) screens the magnetic phase $x/a_M$ $\sqrt{3}$ 0 $\boldsymbol{\chi}(\boldsymbol{r}+\boldsymbol{a}_{j})=e^{-i(\boldsymbol{a}_{j}\times\boldsymbol{r})/2l_{B}^{2}}\boldsymbol{\chi}(\boldsymbol{r})$ $\Delta_z(\mathbf{r}) \,(\text{meV})_{40}$ 20

#### Skyrmions texture for the layer index

Twisted bilayer graphene (chiral)



Triangular Skyrme texture in the layer index

Realistic twisted bilayer graphene (non-chiral)



### Fractional Chern insulators in MoTe<sub>2</sub>

Graphite hBN V<sub>tg</sub> V<sub>bg</sub>\_ θ



Twist angle around  $\theta = 3.7^{\circ}$ 

#### Capacitance (compressibility)



Cai, Anderson, Wang, Zhang, Liu, Holtzmann, Zhang, Fan, Taniguchi, Watanabe, Ran, Cao, Fu, Xiao, Yao, and Xu, Nature 2023

Zeng, Xia, Kang, Zhu, Knüppel, Vaswani, Watanabe, Taniguchi, Mak, and Shan, 2023. Nature 622, 69–73.

Christophe Mora

#### Continuum model in a magnetic field

Herzog-Arbeitman, Chew, Bernevig PRB 2022

$$H_{\rm sp}^{K} = \begin{pmatrix} -\frac{\hbar^2 (\mathbf{k} - \mathbf{K}^b)^2}{2m^*} + V_b(\mathbf{r}) & T(\mathbf{r}) \\ T^{\dagger}(\mathbf{r}) & -\frac{\hbar^2 (\mathbf{k} - \mathbf{K}^t)^2}{2m^*} + V_t(\mathbf{r}) \end{pmatrix}$$

Minimal coupling  $\mathbf{k} \rightarrow \mathbf{\Pi} = \mathbf{k} - e\mathbf{A}/\hbar$ 

Gauge invariant method

Commensurate flux 
$$\frac{\Phi}{\Phi_0} = \frac{p}{q}$$

Set of commutating operators: kinetic energy and magnetic translations

 $\Pi \qquad T_{q\mathbf{a}_1} \qquad T_{\mathbf{a}_2/p}$ 

$$\begin{aligned} \left(\Pi_x^2 + \Pi_y^2\right) |n, \mathbf{k}\rangle &= (n + \frac{1}{2}) \frac{1}{l_B^2} |n, \mathbf{k}\rangle \\ T_{q\mathbf{a}_1} |n, \mathbf{k}\rangle &= e^{iq\mathbf{a}_1 \cdot \mathbf{k}} |n, \mathbf{k}\rangle \\ T_{\mathbf{a}_2/p} |n, \mathbf{k}\rangle &= e^{i\frac{1}{p}\mathbf{a}_2 \cdot \mathbf{k}} |n, \mathbf{k}\rangle \end{aligned}$$



#### **Bloch Landau levels**

$$\begin{aligned} \text{Implicit solution, eigenstate of} \quad \mathbf{II}, T_{q\mathbf{a}_{1}}, T_{\mathbf{a}_{2}/p} \\ \hline |n, \mathbf{k}\rangle &= e^{i\mathbf{k}\cdot\mathbf{R}} |n, 0\rangle \\ \text{guiding center} \end{aligned} \qquad \mathbf{Lattice} \qquad \text{Reciprocal space} \\ \mathbf{k}', n'|e^{i(m_{1}\mathbf{b}_{1}+m_{2}\mathbf{b}_{2})\cdot\mathbf{r}}|n, \mathbf{k}\rangle &= \delta_{\mathbf{k}', \mathbf{k}+m_{2}\mathbf{b}_{2}} \exp\left(-i\pi m_{1}m_{2}\frac{q}{p}\right) \\ \exp\left(-i2\pi k_{1}[k_{2}+m_{2}/p]\right) \exp\left\{i2\pi(k_{2}p+m_{2})\frac{q}{p}m_{1}\right\} \\ &\times (z^{*})^{n'-n}\sqrt{\frac{n'!}{n!}}L_{n'}^{n-n'}(|z|^{2})\exp(-|z|^{2}/2)} \end{aligned} \qquad \mathbf{z} = (m_{1}b_{1}+m_{2}b_{2})\frac{\ell_{B}}{\sqrt{2}} \\ \text{Explicit form of the Bloch LL is not needed. Gauge invariant construction.} \end{aligned}$$

#### (Fractional) Chern insulator in MoTe<sub>2</sub>





 $C \neq$ 

C = 1

Г

M

Watanabe, Taniguchi, Shan, and Mak, 2024. Nature 628, 522-526.

Kang, Shen, Qiu, Zeng, Xia,

#### Streda formula

 $\theta = 1^{\circ}$ 



Topology and Geometry Beyond Perfect Crystals, Nordita 2025 44