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Author

Wang, Tianle

Publication Date

2025-08-01

Peer reviewed|Thesis/dissertation

Engineering Correlation, Topology, and Coherence in Graphene-based Heterostructures

By

Tianle Wang

A dissertation submitted in partial satisfaction of the

requirements for the degree of

Doctor of Philosophy

in

Physics

in the

Graduate Division

of the

University of California, Berkeley

Committee in charge:

Professor Michael P. Zaletel, Chair

Professor Feng Wang

Professor Maciej Zworski

Summer 2025

Engineering Correlation, Topology, and Coherence in Graphene-based Heterostructures

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Tianle Wang

Abstract

Engineering Correlation, Topology, and Coherence in Graphene-based Heterostructures

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University of California, Berkeley

Professor Michael P. Zaletel, Chair

Two-dimensional van der Waals heterostructures enable unprecedented control over electronic bandwidth, symmetry, and topology—ingredients that stabilize interaction-driven correlation and coherence in flat bands. This thesis develops a cohesive framework, across four graphene-based platforms, for engineering and diagnosing correlation–topology–coherence interplay by tuning twist, substrate, stacking, and magnetic field. (1) DMRG shows that tiny heterostrain in magic-angle graphene reshapes flat bands and switches between topological and trivial intervalley-coherent order and metallic states. (2) Transition-metal-dichalcogenide proximity introduces spin–orbit coupling that selects flat-band topology, yielding valley Chern and time-reversal topological insulators. (3) In rhombohedral multilayers aligned to hBN, interactions produce an isolated $|C| = 1$ Chern band and an anomalous Hall crystal that survives even without moiré potential. (4) In quantum-Hall bilayers, we propose a gate-defined exciton-condensate Josephson junction with realistic readouts for supercurrent response. Together, these results chart complementary pathways to flatten bands, select topology, and reveal phase coherence in graphene systems, offering concrete device principles for interaction-enabled quantum electronics.

To my grandmother, for her lifelong care and support.

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Acknowledgments

Reflecting on my academic journey, I am reminded of the proverb, “It takes a village to raise a child.” It is impossible to name everyone who, at different times and from different perspectives, supported my life and career. First and foremost, thank you to all who cared for me, lent a hand, and shared your wisdom. Whether or not you are named below – I will surely miss some – and regardless of order, you are an indispensable part of my memories.

I have been extraordinarily fortunate to work with my Ph.D. advisor, Mike Zaletel. His intellectual range – from the most abstract mathematics to the most subtle details of experiment – taught me that curiosity need not be bounded. He offered unwavering material and intellectual support, encouraged me to pursue the directions that excited me most, and was always ready with candid advice and sharp insight when I needed it. Moreover, his care extended through politically difficult times and beyond the completion of my degree. My gratitude to him is far greater than I can put into words.

The faculty of the Berkeley Physics Department have been a constant source of support and inspiration. I am indebted to Ehud Altman, Joel Moore, Norman Yao, Mike Crommie, Feng Wang, Dan Stamper-Kurn, Dung-Hai Lee and Hitoshi Murayama for many stimulating conversations that expanded my research horizons and continue to shape my work. Outside the department, I would like to thank Maciej Zworski and Lin Lin for insightful discussions. I am equally grateful to many faculty beyond Berkeley whose role models in research – and personal warmth – has been catalytic in my development; they are too numerous to name individually.

I cannot imagine how my research would have progressed without the daily mentoring and encouragement from my senior collaborators and colleagues. I thank Nick Bultinck, Shubhayu Chatterjee, Tomohiro Soejima, Daniel Parker, Johannes Hauschild, Zhehao Dai, Ruihua Fan, Chunxiao Liu, and Sam Garrett for their direct and enduring support. I am likewise grateful to Yanqi Wang, Yimu Bao, Mit Naik, Dan Borgnia, Aaron Szasz, Yantao Wu, Ethan Lake, Zhihuan Dong, and many others at Birge for insightful conversations and practical help at key junctures.

I owe a special debt to the peers with whom I spent countless hours – who taught me in both theory and experiment and kept me moving forward: Taige Wang, Sajant Anand, Stefan Divic, Zack Weinstein, Jaewon Kim, Zhiqiang Gao, Zijian Wang, Iryan Na, Leon Lu, Rahul Sahay, Lizzy Dresselhaus, Hongyuan Li, Ruishi Qi, Ziyu Xiang, Jiahui Nie, Betty Hu, Junkai Dong, and Dachuan Lu, among many others. From absorbing lectures and wrestling with demanding problem sets to vigorous journal-club debates and close collaboration on projects, your companionship made the journey both richer and more enjoyable.

Many friends enriched my life beyond research. I am especially grateful to Zhangguanglu Wang, whose continuous support and countless happy memories sustained me during my years at Berkeley. I also cherish our meals-and-board-games cohort that emerged during the waning days of the pandemic – from gatherings at Yimu’s home to the Birge Graduate Lounge – which gave me a strong sense of community and restored my strength and confidence amid setbacks.

My journey to a new world would not have been possible without steadfast early support. I am grateful to the mentors, colleagues, and friends at my alma mater, Peking University. That vibrant, deeply rooted community nurtured my knowledge, vision, and curiosity, and inspired me to pursue my passions. I especially thank my undergraduate advisors, Biao Wu and Hong Yao, for leading me into cutting-edge research and supporting my path to Berkeley, and then-postdoc Zixiang Li for wholeheartedly helping me get settled here early on.

In the era of AI, I would like to acknowledge the assistance of ChatGPT in helping with research exploration and the organization of this thesis. While imperfect and prone to error, it lowered the barrier to new topics and freed time for core ideas. I also thank Jamie Simons for introducing me and colleagues to the BIG-bench project in 2021; experimenting with early large-language models was both instructive and fun.

Above all, I thank my family for their unconditional love and support. Few parents would be content to let their only child cross an ocean in pursuit of a dream—especially during a period marked by separation and uncertainty—but mine did so with courage and faith. They bridged time zones with late-night calls, celebrated each small milestone, and never stopped teaching me to be a better person.

Chapter 1

Introduction

Two-dimensional (2D) materials have become a fertile ground for discovering and engineering collective quantum phenomena of electrons. Since the isolation of monolayer graphene via “scotch-tape” exfoliation [1], the ability to tear, rotate, and stack atomically thin crystals has blossomed into the broader field of van der Waals (vdW) heterostructures. These systems combine 2D materials as “Lego blocks,” enabling moiré superlattices, proximity effects, and electrostatic control that realize phases inaccessible in the individual constituents. The phase diagram is further enriched by tunable experimental knobs such as electron doping and external electric and magnetic fields, which allow us to tune the band structure and interactions with unprecedented precision.

Graphene remains central to this landscape thanks to its many special properties. Specifically, its band structure realizes two “Dirac points” at the corners of the Brillouin zone where the electron bands cross the Fermi surface with uniform linear dispersion [2]. These Dirac points lead to many favorable properties for further engineering: first, they endow electrons with nontrivial topology in terms of Berry phase in momentum space, which act as an effective magnetic field that leads to various exotic phenomena [3, 4]; second, they are effectively decoupled at low energy due to their large momentum mismatch, leading to emergent “valley” degrees of freedom that enrich the resulting physics. However, the band dispersion of monolayer graphene is so large that it only realizes semi-metallic physics. To discover more diverse correlated phases where the interplay between electrons through Coulomb interaction is non-negligible, it is crucial to introduce “band flattening”: suppressing the kinetic energy of electrons so that interactions become dominant. The following chapters of this thesis will demonstrate various methods for achieving band flattening that heralds strongly correlated physics.

Among the realized phases to be discussed here, a unifying feature is “coherence”: interactions organize electron wavefunctions to share a common dynamical phase, which can then be observed through anomalous response or interference. Classic examples include ferromagnets that carry a gapless Goldstone mode, and superconductors that realize zero-resistance transport response. Generally, strongly correlated phases manifest coherence through spontaneously breaking a $U(1)$ symmetry, which acts trivially on the Hamiltonian but applies a

nontrivial phase rotation on the ground-state wavefunction. The examples above break $U(1)$ spin rotation and charge number conservation respectively, and other coherent phenomena can be introduced by breaking other $U(1)$ symmetries.

Graphene manifests a wide range of coherence phenomena thanks to its rich internal degrees of freedom. For example, ferromagnetism can be realized in flat-band graphene structures through the Stoner mechanism, where Coulomb interaction favors spin polarization that reduces the exchange energy of electrons. Moreover, one can also realize “pseudospin” ferromagnetism regarding the valley degree of freedom, where electrons live in the superposition of two valleys and break the emergent $U(1)$ valley charge symmetry. The resulting state has a distinct observable feature: a “Kekulé” charge-density wave pattern that breaks the translation symmetry of the graphene lattice. This results from the wavefunction interference between the two valleys that carry different momenta. Finally, superconductivity has also been surprisingly reported in twisted graphene systems [5], which maximize the correlation effect by fine-tuning the twist at “magic” angles. These coherent phases can compete or collaborate, sometimes further coupling to nontrivial topology, and the outcome is exquisitely sensitive to how we engineer band structure. Understanding how to control these orders and identify them in experiments is a key goal of this thesis.

Below, we summarize the four complementary scenarios that structure the thesis: (1) moiré twisting, (2) substrate proximity, (3) rhombohedral stacking, and (4) strong magnetic field. Together, they illustrate distinct routes to band-flattening and topology, and trace how coherent orders emerge, compete, and can be harnessed.

In **Chapter 2**, we use large-scale DMRG to determine the ground state of magic-angle twisted bilayer graphene near filling $\nu = -3$ when realistic heterostrain is included. We find that tiny strain reorganizes the competition among intervalley-coherent order with nontrivial topology, Kekulé-type trivial intervalley coherence, and a normal symmetric metal. The result reconciles disparate experimental reports within a single, strain-tuned picture. The message for the chapter is conceptual: minute changes in band shape can flip which coherent order wins, so careful control of the experimental parameter is crucial to realize the desired phase. The content of this chapter is based on [6].

In **Chapter 3**, we study magic-angle graphene placed on a TMD and show how proximity-induced spin-orbit coupling determines how the flat bands are gapped out and whether they host nontrivial topology. We map where valley Chern insulators and topological insulators are realized at different integer fillings—establishing proximity as a practical, symmetry-aware lever to choose the topological backdrop for correlation. The content of this chapter is based on [7].

In **Chapter 4**, we tackle rhombohedral multilayer graphene aligned to hBN at zero magnetic field and show that interactions can promote an isolated $|C| = 1$ Chern band with quantized Hall response at low electron fillings. The Chern band hosts favorable quantum geometry such that it can host fractional quantum Hall orders at fractional dopings. Strikingly, the Chern band and the associated quantized Hall response survives even as the moiré potential is dialed away, predicting a ground state that spontaneously breaks lattice translation on top of the time-reversal symmetry: an anomalous Hall crystal. This reveals a

general, moiré-independent mechanism for Chern-band formation driven by correlation and symmetry breaking. The content of this chapter is based on [8], where Junkai, Taige, and I shared equal contribution.

In **Chapter 5**, we switch gears to consider a flat-band graphene system realized by Landau level quantizations from an external magnetic field. We consider a bilayer system that realizes “exciton condensates”, which breaks $U(1)$ layer charge symmetry and carries a supercurrent counter-propagating between layers. We propose a novel design of a gate-defined, in-plane Josephson junction between two quantum-Hall exciton condensates, where the coupling is mediated not by single-electron tunneling but by a tunable pseudospin texture across a nearly layer-polarized junction. We outline electrical readouts—counterflow current and microwave-frequency reflectometry—that directly access the current–phase relation. This provides a clean, phase-sensitive probe of excitonic coherence in a regime where superconductivity cannot survive. The content of this chapter is based on [9].

In summary, these chapters argue that by choosing the right knob – twist, proximity, stacking, or field – we can steer the balance between correlation, topology, and coherence, and design clean experimental probes that diagnose the resulting order. The results presented in this thesis provide both theoretical frameworks and practical device ideas for realizing these quantum phases, paving the way toward new electronics and quantum technologies.

Chapter 2

Ground-state order in magic-angle twisted bilayer graphene

2.1 Introduction

In recent years, the nature of strongly correlated states in magic-angle twisted bilayer graphene (TBG), in particular at integer fillings $\nu \in (-4, +4)$, has been the center of experimental investigations. However, consensus on the ground state order has still not been achieved. Comparing numerous experimental reports [10–23] (see also Appendix A.1) reveals a persistent puzzle: Although these reports reach consensus at all even fillings $\nu = 0, \pm 2$ and one odd filling $\nu = +3$, all identified as correlated insulators, results at other fillings remain inconsistent. This is particularly acute at filling $\nu = -3$, where metals, insulators, and even superconductors have all been observed. Such a rich phenomenology hints at a subtle competition between orders — a mystery that must be unravelled to understand the proximate superconductor phase between $-3 \leq \nu \leq -2$.

Theoretically, ground-state studies of TBG have primarily taken a strong-coupling approach [24–27], wherein the small dispersion of the flat band is treated perturbatively on top of the Coulomb interaction. The resulting possible phases at $\nu = -3$ include quantum anomalous Hall (QAH) ferromagnets [26] and charge-density-wave insulators [28, 29], which are supported numerically from self-consistent Hartree-Fock (SCHF) [29–34], density renormalization group (DMRG) [28] and exact diagonalization (ED) [35, 36]. However, these approaches neglect a crucial facet of realistic TBG devices: heterostrain. Heterostrain [37–42] is a mismatch in the strains of the two graphene layers, with typical experimental values in the range 0.03 – 0.7% [43–47]. This seemingly insignificant amount of heterostrain amplifies the kinetic energy of the flat bands enormously, boosting their bandwidth to the same order as the interaction scale [Fig. 2.1(b)]. In this realistic intermediate coupling regime, a chief phase candidate is the “incommensurate Kekulé spiral” (IKS) phase, identified at mean-field level in [32, 48].

Connecting these proposals to experiment requires an unbiased solution of the many-

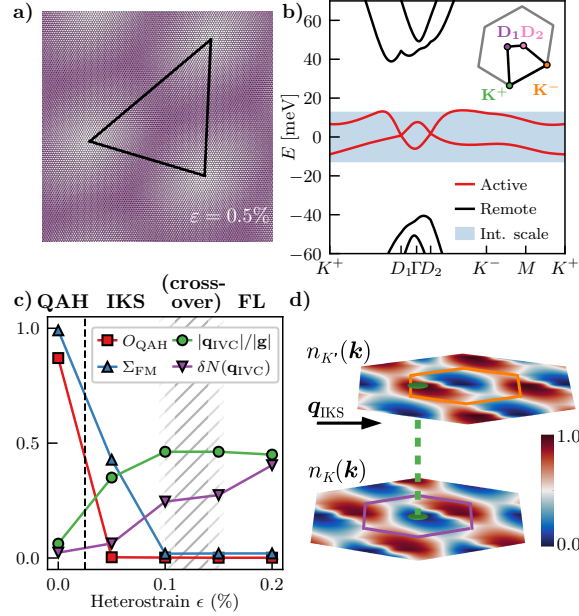


Figure 2.1: (a) Moiré pattern from two graphene lattices with 1° relative twist and $\varepsilon_{\text{Gr}} = 0.5\%$ uniaxial heterostrain. Strain is amplified at the superlattice scale, significantly distorting the moire unit cell. (b) Non-interacting bandstructure of TBG with $\varepsilon_{\text{Gr}} = 0.3\%$ heterostrain. Heterostrain shifts the Dirac nodes $D_{1,2}$ close to the Γ point (inset). (c) Phase diagram of TBG at $|\nu| = 3$ obtained from DMRG up to bond dimension $\chi = 24576$. The phase transitions are identified with their characteristic order parameters: Chern band polarization O_{QAH} , ferromagnetic order magnitude Σ_{FM} , intervalley coherence wavevector $\mathbf{q}_{\text{IVC}}$, and deviation of valley-summed electron density from uniform filling $\delta N(\mathbf{q}_{\text{IVC}})$ (see main text for the definition). (d) Valley-nested DMRG electron occupations of the first Brillouin zone in the IKS phase (parameters match Fig. 2.2, $L_y = 6$). The relative shift $\mathbf{q}_{\text{IKS}}$ makes the total occupations uniform while Γ is depleted in both valleys.

body problem at $\nu = -3$. SCHF, for instance, can be biased towards insulating states [49] (which could explain its failure to find metallic states at $|\nu| = 3$.) On the other hand, the large number of degrees of freedom makes ED or DMRG computationally demanding. The largest ED on *unstrained* TBG has at most 3×3 unit cells at $|\nu| = 3$ when keeping valley and spin degrees of freedom. But such small systems may be biased when trying to capture an incommensurate state such as the IKS. Similarly, DMRG calculations performed on MATBG to date assume valley/spin polarization to reduce computational cost [28, 39, 50], excluding several promising ground state candidates. Quantum monte carlo suffers from a sign problem away from $\nu = 0$, making it impractical [51, 52]. It is therefore imperative to perform full-scale DMRG studies with all flavors of electrons to resolve the competition among *all* ground state candidates.

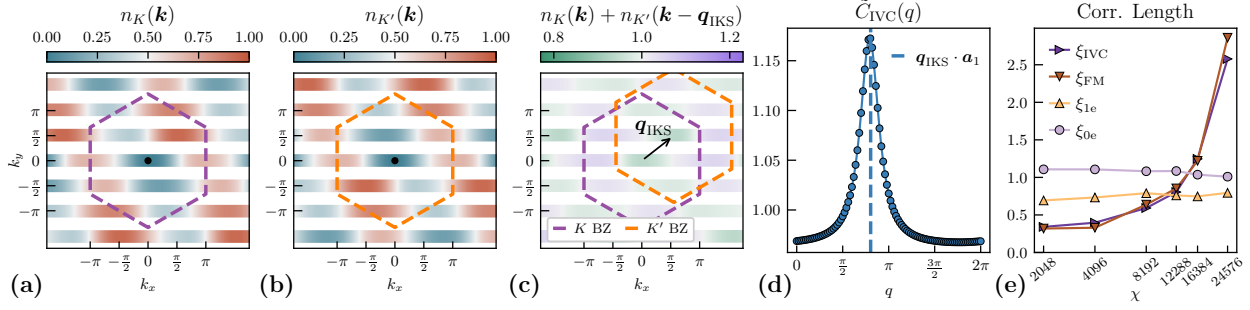


Figure 2.2: IKS at $\varepsilon_{\text{Gr}} = 0.05\%$. (a,b) Valley-resolved electron density of TBG at $\nu = -3$. Dashed hexagons denote the first Brillouin zone, and the dot in the middle is the Γ point. (c) Total electron density $N_{\mathbf{q}_{\text{IKS}}}(\mathbf{k})$ in Eq.(2.12), after a relative boost by $\mathbf{q}_{\text{IKS}}$, whereupon the density becomes uniform. (d) Fourier transform of the IKS correlation function. The peak at $q \approx 0.80\pi$ matches $\mathbf{q}_{\text{IKS}} \cdot \mathbf{a}_1$ from (c). (e) Scaling analysis of correlation lengths of several order parameters, showing that IVC and FM dominate at large bond dimensions $\chi > 16384$.

In this chapter, we perform 8-flavor DMRG to establish the ground state phase diagram of TBG at $|\nu| = 3$ with heterostrain ε_{Gr} . To the best of our knowledge, this is the first DMRG study to accomplish this feat. We find a phase diagram, summarized in Fig. 2.1(c), that unifies all previous phase candidates. The key results are four-fold.

1. The ground state at vanishing strain carries spin-polarized QAH order with intervalley coherence (QAH-IVC), which is nearly degenerate with the valley-polarized variant (QAH-VP) identified in past studies. We expect electron-phonon coupling (EPC) observed in recent experiments [53] to favor QAH-IVC.
2. Low strain stabilizes the spin-polarized IKS state, reinforcing the recent prediction from the mean-field study [32] to a much more robust level.
3. Intermediate strain drives a transition from flavor-polarized IKS to fully-symmetric Fermi liquid (FL), with close energy competition in their crossover region.
4. There is a large low-energy manifold of “ Γ -depleted” orders — states where the electron occupation is low in the vicinity of the Γ point. The IKS phase is one such order, but others such as commensurate spin spirals (CSS) appear as close competitors.

Our study highlights the complex competition between a large manifold of distinct orders and selects the global ground state of TBG at $\nu = 3$ among various proposals. Equipped with this unbiased prediction from DMRG, we conclude with concrete near-term experiments that would confirm these predictions.

2.2 Model and Heterostrain

We use a standard Bistritzer-MacDonald (BM) model [54] of TBG at twist angle $\theta = 1.08^\circ$, and add realistic heterostrain [38] and strong Coulomb interactions. We take chiral ratio $\kappa = w_{AA}/w_{AB} = 0.65$, where $w_{AA/AB}$ are interlayer tunneling strengths for different sublattices, in the realistic range $0.5 - 0.8$ to account for some lattice relaxation [55–57]. Heterostrain modifies the Hamiltonian as an effective layer-dependent vector potential $-i\nabla \rightarrow -i\nabla + \mathbf{A}_\ell$ [38, 55, 58–67]:

$$\mathbf{A}_\ell = -\frac{\ell}{2} \frac{\beta\sqrt{3}}{2a} (\epsilon_{xx} - \epsilon_{yy}, -2\epsilon_{xy}), \quad (2.1)$$

and also distort lattice vectors $\mathbf{a}_i$ (and reciprocal vectors $\mathbf{g}_i$) such that C_{3z} and C_{2x} are strongly broken, while C_{2z} and time-reversal are preserved [38].

Fig. 2.1(b) shows the band structure for a single valley and spin in the presence of strain. Crucially, even sub-percent level of heterostrain can dramatically increase the flat band dispersion of TBG as much as tenfold. The reason graphene-scale heterostrain ε_{Gr} has such a large effect is that the strain $\varepsilon_{\text{moiré}}$ it produces on the moiré superlattice is amplified by a factor of inverse twist angle $1/\theta \sim 100$ (see Appendix A.2):

$$\varepsilon_{\text{moiré}} \propto \frac{\varepsilon_{\text{Gr}}}{\theta}. \quad (2.2)$$

Quantitatively, the narrow bands of TBG have bandwidth of 2.5 meV without heterostrain, which increases to 16 meV at $\varepsilon_{\text{Gr}} = 0.2\%$ and 40 meV by $\varepsilon_{\text{Gr}} = 0.5\%$ — comparable to the Coulomb scale of 30 – 50 meV. Heterostrain is therefore an experimental parameter of paramount importance to accurately determine the ground state phase diagram of TBG.

We consider interacting physics within the eight narrow (‘flat’) bands of TBG. A complete description of the model is given in Appendix A.3. We use a Chern or ‘maximally sublattice polarized’ [26] basis $\hat{c}_{\mathbf{k}\sigma\tau s}^\dagger$ where $(\sigma, \tau, s) = (A/B, K/K', \uparrow/\downarrow)$ label sublattice, valley, and spin. These bands have Chern number $C = \sigma\tau$. Below we will use corresponding Pauli matrices $\sigma^\mu, \tau^\mu, s^\mu$. The Hamiltonian is

$$\hat{H} = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^\dagger h_{\mathbf{k}} \hat{c}_{\mathbf{k}} + \frac{1}{2} \sum_{\mathbf{q}} V_{\mathbf{q}} : \hat{\rho}_{\mathbf{q}} \hat{\rho}_{-\mathbf{q}} :, \quad (2.3)$$

where $\hat{\rho}_{\mathbf{q}}$ is the (8×8) component flat band density operator at momentum $\mathbf{q}$ and $V_{\mathbf{q}}$ is the double gate-screened Coulomb interaction, normal ordered relative to the background. As usual, the dispersion $h_{\mathbf{k}}$ is the BM part minus a correction to avoid double-counting Coulomb interactions [26, 50]. The model studied here has approximate particle-hole symmetry [32], so ground states at $\nu = -3$ and 3 are nearly identical; we take $\nu = -3$.

Our DMRG calculations are performed on an infinite cylinder geometry with a circumference of L_y moiré unit cells. We choose a computational ‘cylinder’ basis $\hat{c}_{n,k_y,\sigma\tau s}$ of hybrid Wannier orbitals that are maximally (exponentially) localized at the n^{th} unit cell along the

cylinder axis, but have definite momentum k_y around the cylinder [28, 50, 68]. Fourier transformed, our model captures L_y line cuts through the moiré Brillouin zone at $k_y = \frac{2\pi m}{L_y}$, $-L_y \leq 2m < L_y$. The long-range interactions in the Hamiltonian, encoded as matrix product operators (MPO) in DMRG, are faithfully compressed [50, 69] to accuracy $< 10^{-2}$ meV at all distances. Our simulations required significant numerical resources. The $L_y = 4$ Hamiltonian has MPO bond dimension $\chi_{\text{MPO}} \approx 2000$, and we consider states up to bond dimension $\chi = 24576$. Our algorithm conserves electron occupation in each spin and valley ($U(1)_{\uparrow K} \times U(1)_{\downarrow K} \times U(1)_{\uparrow K'} \times U(1)_{\downarrow K'}$) as well as crystalline momentum along the circumference of the cylinder. We focus on the spin/valley unpolarized $(\tau^z, s^z) = (0, 0)$ sector with zero crystalline momentum. See Appendix A.4 for details. Each unit cell on our cylinder consists of $L_y \times 8$ orbitals (already beyond normal exact diagonalization), and each datapoint requires ~ 40000 core-hours.

2.3 Vanishing strain: QAH-IVC order

We start near zero strain, where strong coupling theories [26, 27] predict a ground state with quantized anomalous Hall order. Previous numerical studies [29–36] have singled out QAH states with spin and valley polarization (QAH-VP), even when allowing $U_V(1)$ symmetry breaking. If we assume valley-polarization, DMRG recapitulates this finding. However, our treatment of all eight flavors allows us to drop this assumption. With total spin and valley charge zero, we find a new ground state candidate: a QAH insulator with intervalley coherent order (QAH-IVC). We briefly detail these states to introduce our method and notation, then consider larger strains.

QAH states have a time-reversal breaking order parameter

$$O_{\text{QAH}} = \frac{1}{N_k} \sum_{\mathbf{k}} \langle \hat{c}_{\mathbf{k}}^\dagger \sigma^z \tau^z \hat{c}_{\mathbf{k}} \rangle \quad (2.4)$$

that measures the polarization of the Chern bands. Despite their similar names, QAH-VP and QAH-IVC have unequal flavor polarizations, and hence strikingly different charge density patterns at the graphene scale. These orders are adiabatically connected to ‘model’ Slater determinant states specified by correlation matrices $P_{\alpha\beta}(\mathbf{k}) = \langle \hat{c}_{\mathbf{k},\beta}^\dagger \hat{c}_{\mathbf{k},\alpha} \rangle$. Explicitly, the ‘model’ QAH-VP state at $\nu = -3$ has $O_{\text{QAH}} = 1$:

$$P_{\text{QAH-VP}}(\mathbf{k}) = \left(\frac{1 + \sigma^z \tau^z}{2} \right) \left(\frac{1 + \tau^z}{2} \right) \left(\frac{1 + s^z}{2} \right), \quad (2.5)$$

with flavor polarization $(\tau^z, s^z) = (1, 1)$. By contrast, the ‘model’ QAH-IVC state with spin along x is

$$P_{\text{QAH-IVC}} = \left(\frac{1 + \sigma^z \tau^z}{2} \right) \left(\frac{1 + \sigma^x \tau^x}{2} \right) \left(\frac{1 + s^x}{2} \right), \quad (2.6)$$

with zero flavor polarization $(\tau^z, s^z) = (0, 0)$. This state also has $O_{\text{QAH}} = 1$.

Fig. 2.1c shows O_{QAH} versus ε_{Gr} in the $(0, 0)$ sector. At $\varepsilon_{\text{Gr}} \approx 0$, we find $O_{\text{QAH}} \approx 0.87$ (slightly depolarized due to band hybridization), signaling QAH order before an abrupt transition at $\varepsilon_{\text{Gr}} \approx 0.05\%$. To confirm this as QAH-IVC order, we define intervalley coherent (IVC) and ferromagnetic (FM) order parameters (used repeatedly below):

$$\hat{\Delta}_{\text{IVC}} = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^{\dagger} \sigma^x \tau^+ \hat{c}_{\mathbf{k}}, \quad \hat{\Delta}_{\text{FM}} = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}}^{\dagger} s^+ \hat{c}_{\mathbf{k}}. \quad (2.7)$$

As these 2-electron operators are off-diagonal in the conserved quantities τ^z/s^z , they identically vanish; we must instead measure a 4-electron correlator of their Fourier transform (see Appendix A.4 for details and the relation to Hohenberg-Mermin-Wagner theorem). Explicitly, for

$$\hat{\Delta}_{\text{FM}}(n) = \sum_{k_y} \hat{c}_{n, k_y}^{\dagger} s^+ \hat{c}_{n, k_y}, \quad (2.8)$$

we consider

$$C_{\text{FM}}(n) = \langle \hat{\Delta}_{\text{FM}}(0) \hat{\Delta}_{\text{FM}}^{\dagger}(n) \rangle, \quad \Sigma_{\text{FM}} \equiv \sum_n |C_{\text{FM}}(n)|, \quad (2.9)$$

and define $C_{\text{IVC}}, \Sigma_{\text{IVC}}$ analogously. Since $\Sigma_{\text{FM/IVC}}$ captures how fast $C_{\text{FM/IVC}}$ decays, a large $\Sigma_{\text{FM/IVC}}$ quantitatively distinguishes long-range FM/IVC ordering from other short-range phases with smaller $\Sigma_{\text{FM/IVC}}$. (We provide more precise distinctions in Appendix A.5 and A.7)

Fig. 2.1c shows $\Sigma_{\text{FM}} \approx 1$ at $\varepsilon_{\text{Gr}} = 0\%$ and we find Σ_{IVC} is also large, confirming QAH-IVC order in the $(\tau^z, s^z) = (0, 0)$ sector at vanishing strain. Appendix A.6.1 examines the valley-polarized sector $(1, 1)$, finding QAH-VP order. These two QAH states are nearly degenerate, with QAH-VP lower by 0.1 meV per electron at $\varepsilon_{\text{Gr}} = 0\%$ — two orders of magnitude below the Coulomb scale. This near degeneracy is due to the proximity of our system to the ‘chiral limit’ [70], where these QAH states are related by an emergent $U(4)_{\pm}$ symmetry [26]. Following the analysis of Ref. [71], the electron-phonon coupling will split the degeneracy in favor of the QAH-IVC state. Our results so far match strong coupling theory, but strains of only 0.05% change the picture entirely.

2.4 Low strain: IKS order

At low strains $\varepsilon_{\text{Gr}} = 0.05 - 0.1\%$ we now show the ground state has an *incommensurate* valley spiral order and identify the phase as the incommensurate Kekulé spiral (IKS) [32]. Previous work on this phase was limited to mean-field level, leaving open the reasonable scenario this incommensurate order is destroyed by strong fluctuations. Our key result here is that IKS is indeed stable to fluctuations — partially due to its ‘T-depletion’ property, as we explain below — making it the many-body ground state at intermediate strain.

We briefly overview the IKS phase and then provide numerical results. IKS order breaks both moiré translation symmetry $\hat{T}_{\mathbf{a}_{1,2}}$ as well as $U(1)_{\text{valley}} = e^{i\theta_v \tau^z}$ symmetry down to a

combined symmetry

$$\hat{T}_{\mathbf{a}_i}^{\text{IKS}} = \hat{T}_{\mathbf{a}_i} e^{i\mathbf{q}_{\text{IKS}} \cdot \mathbf{a}_i \tau^z / 2}. \quad (2.10)$$

This produces an *incommensurate* real space spiral of the order parameter: $\theta_v(\mathbf{r} + \mathbf{a}_i) = \theta_v(\mathbf{r}) + \mathbf{a}_i \cdot \mathbf{q}_{\text{IKS}}$, observable in STM as a slowly-changing Kekulé order between unit cells [47, 72]. At $\nu = -3$, the IKS phase is an insulator with ferromagnetic and intervalley coherent order, similar to QAH-IVC. Unlike QAH-IVC, IKS order preserves time-reversal symmetry (so $O_{\text{QAH}} = 0$) and has intervalley coherence only at wavevector $\mathbf{q}_{\text{IKS}}$, condensing

$$\hat{\Delta}_{\text{IKS}} = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{q}_{\text{IKS}}}^\dagger \sigma^x \tau^x \hat{c}_{\mathbf{k}}. \quad (2.11)$$

A ‘model’ correlation matrix for IKS order must reflect $\hat{\Delta}_{\text{IKS}}$ via coherence between the two valleys at $\mathbf{k}$ and $\mathbf{k} + \mathbf{q}_{\text{IKS}}$.

We now show these distinctive features of IKS order in DMRG. Fig. 2.2(a,b) shows the electron density $n_{\text{K/K}'}(\mathbf{k})$ for each valley. The valleys are related by time-reversal symmetry $n_{\text{K}}(\mathbf{k}) = n_{\text{K}'}(-\mathbf{k})$. The region near Γ is depleted in both valleys; we comment below why this crucial feature minimizes the energy of IKS. Remarkably, a shift by $\mathbf{q}_{\text{IKS}} = 0.40\mathbf{g}_1 + 0.25\mathbf{g}_2$ reveals a nearly uniform electron density as shown in Fig. 2.2(c):

$$N_{\mathbf{q}_{\text{IKS}}}(\mathbf{k}) = n_{\text{K}}(\mathbf{k}) + n_{\text{K}'}(\mathbf{k} - \mathbf{q}_{\text{IKS}}) \approx 1, \quad (2.12)$$

consistent with a ‘model’ correlation matrix for the IKS insulator $P_{\text{IKS}} \sim \langle \hat{c}_{\mathbf{k}+\mathbf{q}_{\text{IKS}}}^\dagger \sigma^\mu \tau^x \hat{c}_{\mathbf{k}} \rangle$ with uniform filling. To examine this quantitatively, we compute q_{IVC} that minimizes

$$\delta N(\Delta \mathbf{q}) = \max_{\mathbf{k}} |n_{\text{K}}(\mathbf{k}) + n_{\text{K}'}(\mathbf{k} - \Delta \mathbf{q}) - 1|, \quad (2.13)$$

and plot it in Fig. 2.1(c). We find δN is small while $|\mathbf{q}_{\text{IVC}}|$ is large, consistent with IKS order.

Next, we directly analyze the IVC and FM orders within the IKS phase, providing another determination of $\mathbf{q}_{\text{IKS}}$. Fig. 2.1(c) shows FM order Σ_{FM} is has the same order of magnitude as in the QAH-IVC phase. The IVC order, on the other hand, needs to be generalized with translation breaking to capture IKS:

$$\Delta_{\text{IKS}}(n; q_y) = \sum_{k_y} \hat{c}_{n, k_y + q_y}^\dagger \sigma^x \tau^+ \hat{c}_{n, k_y}. \quad (2.14)$$

In this way, the corresponding correlator $C_{\text{IKS}}(n; q_y)$ will show the phase spiral at wavevector $\mathbf{q}_{\text{IKS}}$:

$$\text{Arg}[C_{\text{IKS}}(n; q_y = q_{\text{IKS}}^y)] \sim (\mathbf{q}_{\text{IKS}} \cdot \mathbf{a}_1)n. \quad (2.15)$$

In Fig. 2.2(d) we show the Fourier transform of $C_{\text{IKS}}(n; q_y)$ with the expected $q_{\text{IKS}}^y = 0.25|\mathbf{g}_2|$: $\tilde{C}_{\text{IKS}}(q) = \mathcal{F}[C_{\text{IKS}}(n; q_{\text{IKS}}^y)]$, which indeed exhibits a sharp peak at $q = \mathbf{q}_{\text{IKS}} \cdot \mathbf{a}_1 / 2\pi \approx 0.40$. This suggests that $\mathbf{q}_{\text{IKS}} = 0.40\mathbf{g}_1 + 0.25\mathbf{g}_2$, which is consistent with that determined from the electron occupation.

Finally, we establish (quasi-)long-range order corresponding to IVC and FM order parameters. To do so, we extract the correlation length $\xi_{\text{FM/IVC}}$ from the long distance behavior of the correlator $|C_{\text{FM,IKS}}(n)| \approx e^{-n/\xi_{\text{FM,IKS}}}$. If the state has (quasi-)long-range order, ξ should diverge with the DMRG bond-dimension χ . In Fig. 2.2(e), we plot the correlation length ξ corresponding to various operators, and observe that $\xi_{\text{FM/IKS}}$ indeed sharply increases with χ . On the other hand, correlation lengths for operators with no long-range order, such as $\hat{\Delta}_{1e} \sim \hat{c}_{\mathbf{k}}$, $\hat{\Delta}_{0e} \sim \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}'}$, do not increase with χ . We conclude that, even in the presence of fluctuations, the many-body ground state at low strains is the IKS phase.

2.5 Intermediate strain: Fermi liquid

At yet-higher strains, the increasingly large dispersion renders IKS less favorable than a conventional Fermi liquid (FL). The Fermi liquid is the ‘normal’ state with a fully symmetric occupation in each valley and spin that partially fills the (interaction-renormalized) band structure. This is the state found in DMRG at $\varepsilon_{\text{Gr}} = 0.2\%$. On the other hand, the ground states at lower strains show a “mixed” order with both metallic and flavor-polarized features, highlighting the close competition of different orders at the IKS-FL crossover region.

Fig. 2.1(c) and Fig. 2.3 show the key features of the FL phase at $\varepsilon_{\text{Gr}} = 0.2\%$. Unlike IKS, the electron density $n_{\text{K/K'}}(\mathbf{k})$ shown in Fig. 2.3(a,b) is concentrated into a few small pockets that cannot be nested into close-to-uniform filling, with $\delta N(\mathbf{q}_0) \approx 0.4$ even at the minimizing wavevector $\mathbf{q}_0$. Moreover, these pockets are reminiscent of Fermi surfaces of metallic states, which closely match those obtained from symmetry-enforced SCHF as shown in Fig. 2.3(c). A closer look at momentum wire $k_y = \pi/2$ is displayed in Fig. 2.3(d): although no sharp Fermi surfaces are observed due to the quasi-1D geometry, the DMRG state does manifest drops/increases of $n(\mathbf{k})$ where the Fermi surfaces are expected from SCHF. $n(k) \neq 0, 1$ in DMRG are expected from a combination of finite bond dimension and non-unity quasiparticle weight. Finally, both IVC and FM orders are small in the ground state compared to the IKS phase, suggesting the absence of flavor order. Therefore, we conclude that $\nu = -3$ ground state at $\varepsilon_{\text{Gr}} = 0.2\%$ is consistent with a symmetric Fermi liquid in 2D.

For $\varepsilon_{\text{Gr}} = 0.1\text{--}0.15\%$ (Fig. 2.1(c), shaded region), DMRG is inconclusive about the nature of the state. These states exhibit features of both the FL state, such as large variations in $n(\mathbf{k})$, and small FM and IVC order. However, the state also shows a spin density wave not present in either the FL or IKS phases (Appendix A.7.3). We attribute this to the extremely close competition between FL and IKS here, not resolved at our largest bond dimensions.

2.6 Strain favors Γ -depleted states

A key conclusion from the previous section is the importance of the Γ point: away from zero strain, all DMRG ground states in $(0,0)$ sector feature electron depletion at Γ point. The reason can be understood at the mean-field level even without symmetry breaking. The

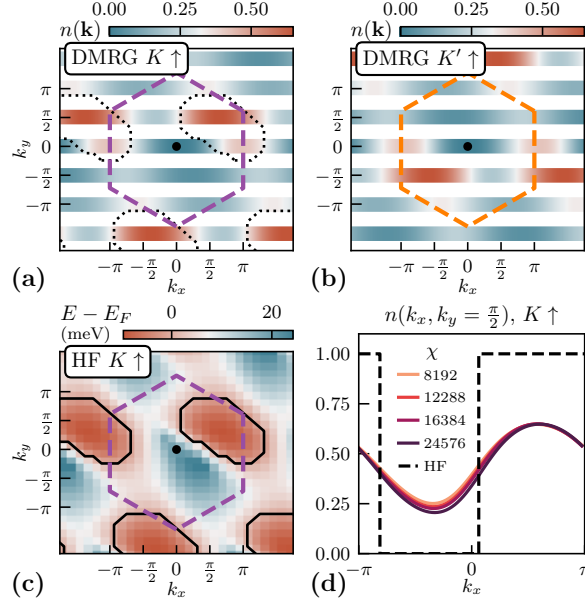


Figure 2.3: FL at $\varepsilon_{\text{Gr}} = 0.2\%$. (a,b) Spin-up electron density in $K^{(l)}$ valley, plotted similarly to Fig. 2.2. The spin-down sector is related by the spin-flip symmetry s^x and shows identical occupations. Dotted lines in (a) circled the Fermi surfaces predicted from fully-symmetric SCHF. (c) Energy $E(k)$ of the partially occupied band from SCHF. The electron only occupies the regions circled in solid lines, forming sharp Fermi surfaces. (d) The DMRG electron occupations in $(K, \uparrow)$ sector along the $k_y = \frac{\pi}{2}$ wire at various bond dimensions, where the filled/emptied regions closely matches that of SCHF (dashed lines).

combination of the Hartree potential and strain-induced dispersion creates a sharp peak in the mean-field bandstructure, Fig. 2.3(c) (see also Appendix A.4). Therefore, any state that occupies this region incurs a substantial kinetic energy penalty, favoring Γ -depleted states. Below we show that this is in fact a general feature of ground-state competition of TBG: Γ -depleted states form a low-energy manifold, wherein an intricate competition picks out the true ground state.

In Fig. 2.4(a), we compare the ground state energy of DMRG ground state in $(0, 0)$ sector to those in other (τ^z, s^z) sectors, which feature different ground-state orders under enforced flavor polarization (see Appendix A.6 for their phase identification). At vanishing strain ε_{Gr} , energy competition is tight between different sectors, as they all manifest QAH-VP or QAH-IVC. However, at larger strains there is a clear energy separation between $(1, 1)$ sector and other sectors, which increases linearly with strain. This is explained by Fig. 2.4(c), where all low-energy states share the Γ -depleted feature. Meanwhile, the energy difference within the low-energy manifold is only around 0.3 meV, which is hardly resolved at the largest bond dimension (Fig. 2.4(b)). We speculate that the difficulty of resolving the IKS to FL transition

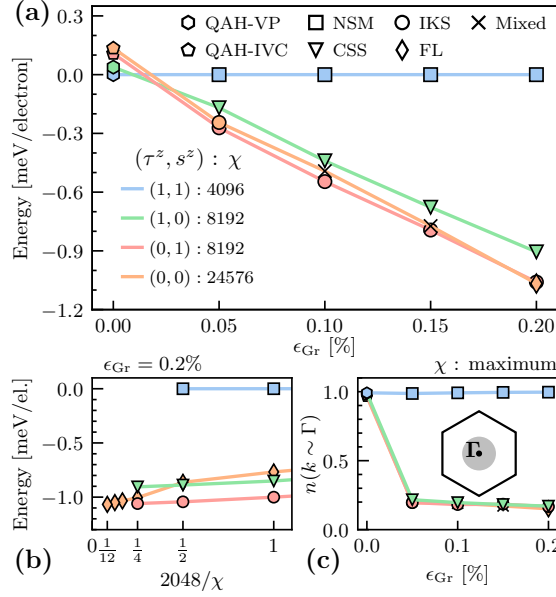


Figure 2.4: (a) DMRG energies in all four sectors as a function of heterostrain $\epsilon_{Gr} \leq 0.2\%$. The (1,0) sector was not computed beyond $\epsilon_{Gr} = 0.2\%$, but is expected to be above (0,0) and (0,1) in energy. (b) The energy of different flavor sectors as a function of χ at $\epsilon_{Gr} = 0.2\%$. (c) Electron density per momentum near Γ : $n(k \sim \Gamma) = \sum_{|k| < 1/5|g_1|} n(k)$. Parameters match Fig. 2.2.

within DMRG is likely due to this proliferation of low-energy states.

2.7 Discussion and Implications

Our realistic microscopic model, Eq. (2.3), has reasonably neglected a number of effects at the 0.1 meV level, such as intervalley scattering terms in the Coulomb interaction and anisotropy [26]. However, there are also a number of possible phenomena on the 1 meV scale that we have not yet included, such as lattice relaxation, particle-hole symmetry breaking [73] and, notably, the electron-phonon coupling (EPC) uncovered in recent studies [71]. Quantitatively determining the contribution of each perturbation is crucial to identify the accurate phase diagram. For example, it is argued in Ref. [71] that EPC lowers the energy of intervalley orders by order of 0.5 meV, which clearly favors QAH-IVC and IKS over their competitive counterparts. This, in particular, suggests the Chern insulators found at finite magnetic field [74] may be connected to QAH-IVC. We leave the implementation of these perturbations to future work.

Experimentally, our results suggest that the amount of heterostrain present in virtually all experimental samples is more than sufficient to push TBG into the intermediate coupling

regime. In this regime, our numerics suggest IKS as the primary insulating ground state candidate at $|\nu| = 3$, which is consistent with the great majority of experiments (Table in Appendix A.1) at $\nu = 3$. (We do note this is specific to samples *not* aligned to an hBN substrate; alignment strongly favors the QAH phase [75, 76].) We also suggest FL as a competitive ground-state candidate at the intermediate-strain region, which might explain why most experiments find a metallic state near $\nu = -3$ (e.g. selected by particle-hole breaking effects). We also note that QAH-IVC might be identified in the rare ultra-low strain samples [47].

The predicted phases at $|\nu| = 3$ could be directly confirmed by atomically-resolved STM experiments [72, 77]: the IVC order in QAH-IVC and IKS will result in charge density wave on the graphene lattice at “Kekulé” wavevector $\mathbf{Q} = \mathbf{K} - \mathbf{K}'$, and the phase spiral of IKS is reflected in the changing pattern of such charge density wave on the moiré lattice at wavevector $\mathbf{q}_{\text{IKS}}$. We note that both of these phenomena have been successfully identified in recent STM experiments focusing on $|\nu| = 2$ [47], confirming the physical relevance of IKS order.

Chapter 3

Flat-band topology of magic angle graphene on a transition metal dichalcogenide

3.1 Introduction

Recent experimental progress [5, 10, 14, 15, 17–20, 43–45, 74, 76, 78–86] has maintained continued interest in the study of twisted bilayer graphene (TBG) in the magic angle regime, where the twist angle between the two graphene layers is approximately one degree. Near this magic angle, the TBG band spectrum structure contains eight bands near the charge neutrality point with a very small bandwidth. When the Fermi level lies within these flat bands, interactions play an important role and lead to the appearance of correlated insulating states at certain integer fillings. Interestingly, the flat bands were also found to have a subtle but non-trivial form of band topology [87–93].

In this work, we consider the band spectrum of magic angle graphene in the presence of a transition metal dichalcogenide (TMD) substrate. For some first experimental results on such TBG-TMD devices, at angles $\theta = 0.79^\circ\text{--}0.97^\circ$ somewhat below the first magic angle, see Ref. [82]. The heavy atoms in a TMD substrate are known to introduce significant spin-orbit coupling (SOC) in graphene via the proximity effect. Because of their small bandwidth, the flat bands are expected to be significantly reconstructed by the SOC terms, and the band topology of the SOC bands can potentially be very different from the band topology of the original BM bands. Studying how the flat band topology changes in the presence of SOC is not purely a theoretical exercise, but is also an important step towards understanding the interacting phase diagram. One of the main reasons is that magic angle graphene has a large approximate $U(4)\times U(4)$ symmetry [26, 28], as a result of which there are many different candidate symmetry-breaking states which are very close in energy, as is seen for example in numerical Hartree-Fock [26, 31, 44, 94], density matrix renormalization group [28] and quantum Monte Carlo [95] studies. Because of this close intrinsic competition, small extrinsic

effects coming from the substrate can tip the balance between different symmetry-breaking states. For example, the two-fold in-plane rotation symmetry breaking staggered sublattice potential which is induced by an aligned hexagonal Boron-Nitride substrate has already been observed to drastically change the interacting phase diagram of magic angle graphene [76, 80, 84]. This is in agreement with the numerical Hartree-Fock study of Ref. [26], where it was found that a staggered sublattice potential as small as 10 meV can change the nature of the ground state at charge neutrality.

There are multiple different ways to combine TBG with TMD substrates, depending on whether a TMD substrate is placed on only one or on both sides of the TBG device, and depending on the in-plane orientation of the TMD relative to the graphene layers. In this work, we consider all these possibilities and find that the different devices have very different band structures. We also find that $\mathcal{C}'_{2x}$, the spinful two-fold rotation symmetry around the in-plane x -axis, plays an important role in explaining the differences in band structure. In particular, our results show that TBG-TMD heterostructures which are $\mathcal{C}'_{2x}$ symmetric have Dirac points near the Γ point, even though the spinful $\mathcal{C}_{2z}\mathcal{T}$ symmetry is broken, while $\mathcal{C}'_{2x}$ breaking heterostructures have a gapped band spectrum. Interestingly, we find that the gapped band structures have a pair of bands which are extremely flat around the $K^\pm$ point. For a representative band structure displaying this pair of flat bands, see Figs. 3.1(b) and 3.1(c), where the band structure is shown along a path between high-symmetry points in the mini-Brillouin zone. We develop an intuitive understanding of the spin-orbit coupled band structures, and in particular how they are affected by the different proximity-induced terms, by doing a $k \cdot p$ analysis at the different Dirac points.

For the devices with a gapped band spectrum, we calculate the Chern numbers of the different isolated bands. We find a very rich phase diagram depending on the relative strength of the different proximity-induced terms. We identify the parameter regions and integer filling factors where valley Chern insulators and topological insulators protected by time-reversal symmetry are realized. Interestingly, we find that for realistic values of the proximity-induced terms, it is possible to obtain topological insulators both at filling $\nu = -2$ and $\nu = 2$, i.e. at the filling factors obtained by doping either two holes or two electrons per moiré unit cell into the system.

The remainder of this paper is organized as follows. In Section 3.2, we start by reviewing the continuum model of twisted bilayer graphene. In Section 3.3 we consider the different TBG-TMD heterostructures, and discuss the proximity-induced terms that appear in the TBG Hamiltonian, together with their symmetries. We then first study the effect of only the leading Rashba spin-orbit coupling terms in Section 3.4. We use a $k \cdot p$ analysis to develop an understanding of the effects of Rashba spin-orbit coupling on the TBG flat bands, and we investigate the symmetry protection of the different Dirac cones in the bands with spin-orbit coupling. In Section 3.5, we add the remaining subleading proximity induced terms, and analyze the resulting flat bands. Again, we resort to a $k \cdot p$ analysis to develop an intuitive understanding of the effects of the subleading terms. Next, we focus on the heterostructures which can have gapped flat bands, and we calculate the corresponding Chern numbers in Section 3.6. We also discuss the different topological phases that can be realized in these

devices. We end with a discussion of our results in Section 3.7.

3.2 Twisted bilayer graphene continuum model

In this section, we first review the continuum model describing twisted bilayer graphene (TBG) [54, 96, 97]. We start by defining the single-valley, spinless moiré Hamiltonian, which can be written as

$$H_K = \sum_{\mathbf{k}} H_0(\mathbf{k}) + H_T(\mathbf{k}). \quad (3.1)$$

The first term $H_0(\mathbf{k})$ is the intra-layer term, given by

$$H_0(\mathbf{k}) = \sum_l f_l^\dagger(\mathbf{k}) h_{l\theta/2}(\mathbf{k}) f_l(\mathbf{k}). \quad (3.2)$$

Here, $f_l^\dagger(\mathbf{k})$ denotes the electrons from layer l , each having two components from the two sublattices. $l = +/ -$ is the index of top/bottom layer, and $h_\theta(\mathbf{k})$ is the monolayer graphene Hamiltonian with twist angle θ and Fermi velocity v_F :

$$h_\theta(\mathbf{k}) = \hbar v_F (k_x \sigma^x + k_y \sigma^y) e^{-i\theta \sigma^z}, \quad (3.3)$$

where σ acts on the electron sublattices. The top and bottom layer in $H_0(\mathbf{k})$ are rotated by $\pm\theta/2$ respectively, so the two layers have a relative twist angle θ .

The second term in Eq. (3.1), $H_T(\mathbf{k})$, is the inter-layer tunneling term given by

$$H_T(\mathbf{k}) = \sum_{j=1}^3 f_+^\dagger(\mathbf{k} + \mathbf{q}_j) T_j f_-(\mathbf{k}) + h.c.. \quad (3.4)$$

The momentum transfer $\mathbf{q}_1$ is defined as $\mathbf{q}_1 = \mathbf{K}_- - \mathbf{K}_+$, i.e. it corresponds to the momentum difference between the Dirac points of the bottom and top layer. The other two momentum transfers $\mathbf{q}_2$ and $\mathbf{q}_3$ are related to $\mathbf{q}_1$ by the three-fold rotation symmetry: $\mathbf{q}_2 = \mathcal{C}_{3z}\mathbf{q}_1$, $\mathbf{q}_3 = \mathcal{C}_{3z}\mathbf{q}_2$. The inter-layer hopping matrices T_j are defined as

$$T_j = w_0 \sigma^0 + w_1 \sigma^x e^{\frac{2\pi i}{3}(j-1)\sigma^z}. \quad (3.5)$$

The two parameters w_0, w_1 respectively correspond to the sublattice diagonal (AA/BB) and sublattice off-diagonal (AB/BA) hopping strengths respectively. In this work, we use $w_1 = 110$ meV and $w_0 = 0.75w_1$, which takes into account corrugation effects [55, 98, 99]. For these values of the inter-layer hopping, the single-valley TBG Hamiltonian has two very flat bands around charge neutrality for twist angles close to the first magic angle value $\theta^* \sim 1.08^\circ$.

Adding the spin and valley degrees of freedom, the complete moiré Hamiltonian for TBG takes the form

$$H_{TBG} = \begin{pmatrix} H_K(\mathbf{k}) & \\ & H_{\bar{K}}(\mathbf{k}) \end{pmatrix}_\tau \otimes s^0, \quad (3.6)$$

where $\tau \in \{+, -\}$ labels the two valleys, and s^μ correspond to the identity matrix and the three Pauli matrices in spin space. The moiré Hamiltonians coming from different valleys are related by time reversal: $H_{\bar{K}}(\mathbf{k}) = H_K^*(-\mathbf{k})$.

The Hamiltonian H_{TBG} preserves the following symmetries: (1) Time-reversal symmetry $\mathcal{T}$; (2) $\mathcal{C}_{3z}$ rotation around the out-of-plane z -axis; (3) $\mathcal{C}_{2z}$ rotation around the z -axis and (4) $\mathcal{C}_{2x,2y}$ rotation around the in-plane x - and y -axes. For the purposes of this work, the most relevant symmetries are $\mathcal{T}$, $\mathcal{C}_{2z}$ and $\mathcal{C}_{2x}$, which respectively act as $\mathcal{T} = \tau^x \mathcal{K}$ ($\mathcal{K}$ is complex conjugation), $\mathcal{C}_{2z} = \tau^x \sigma^x$ and $\mathcal{C}_{2x} = l^x \sigma^x$. Note in particular that both $\mathcal{T}$ and $\mathcal{C}_{2z}$ interchange valleys, and are therefore absent in the single-valley moiré Hamiltonian $H_K(\mathbf{k})$. As expected from their geometrical definition, all two-fold rotations interchange the sublattices, and only rotations about in-plane axis interchange the two layers.

$H_0(\mathbf{k})$ contains two Dirac cones which are coupled in the presence of $H_T(\mathbf{k})$. As a result, $H_{TBG}(\mathbf{k})$ has two Dirac cones in each valley with renormalized Fermi velocity [54]. Importantly, the Dirac cones are protected by the $\mathcal{C}_{2z}\mathcal{T}$ symmetry, which acts within a single valley.

3.3 Combining TBG with a TMD substrate

As is known from previous work [100], placing graphene on a transition metal dichalcogenide (TMD) substrate (such as MoS₂) can induce significant spin-orbit coupling (SOC) for the graphene electrons. From ab initio calculations, it was found for example in Ref. [101] that the effect of a TMD substrate on the low-energy spectrum of graphene can be well approximated by a spatially-independent perturbation H_{SOC} on the graphene layer closest to the substrate. Physically, the moiré potential coming from the TMD substrate can be ignored for two reasons: (i) the large bandgap of the TMD, and (ii) the large mismatch between the lattice constants of graphene and the TMD. The large TMD bandgap will lead to an overall weaker moiré potential, and the large mismatch in lattice constants results in a moiré pattern with large reciprocal lattice vectors such that only graphene Bloch states with large energy differences are coupled.

The most important SOC terms which are induced by the TMD substrate are the Ising SOC, which takes the form

$$H_{SOC_I} = \lambda_I \tau^z s^z, \quad (3.7)$$

and the Rashba SOC, which is given by

$$H_{SOC_R} = \lambda_R (\tau^z \sigma^x s^y - \sigma^y s^x), \quad (3.8)$$

where τ, σ, s act on the graphene layer proximate to the TMD. Note that magnitudes of the SOC terms in principle depend on the angle of the TMD-graphene alignment. In particular, the TMD is not invariant under a $\mathcal{C}'_{2z}$ rotation, leading to the $\mathcal{C}'_{2z}$ -odd term H_{SOC_I} : if the alignment is rotated by 180°, $\lambda_I \rightarrow -\lambda_I$. In recent experiments, the typical strengths of the different proximity-induced terms in each layer were found to be $\lambda_R \approx 16$ meV, $\lambda_I \approx 1$ meV and $u \approx 1$ meV [101–105].

In magic angle graphene the kinetic energy of the electrons is quenched and the SOC strength becomes comparable to the bandwidth of the nearly flat bands. For this reason, the SOC can potentially have a drastic effect on the moiré bands. We note that the effect of SOC on TBG was also studied previously in Ref.[82] using the same model studied here, but in the regime below the magic angle ($\theta \sim 0.8^\circ$).

In addition to the SOC terms, the TMD also induces a finite sublattice splitting, given by

$$H_{SL} = u\sigma^z. \quad (3.9)$$

The sublattice splitting is also induced by an aligned hexagonal Boron-Nitride substrate [106–111], and has been observed experimentally to have a non-trivial effect on the correlated phase diagram of TBG [76, 80, 84].

Because of the SOC, the TBG-TMD heterostructures is no longer invariant under the spinless symmetries mentioned in the previous section. We therefore need to consider the spinful generalizations of the three relevant symmetries discussed above, which are given by $\mathcal{T}' = i\tau^x s^y \mathcal{K}$, $\mathcal{C}'_{2z} = i\tau^x \sigma^x s^z$ and $\mathcal{C}'_{2x} = il^x \sigma^x s^x$. This will help us determine how the signs of λ_I , λ_R and u depend on the relative orientation of the TMD layer to the TBG. Namely, the $\mathcal{C}'_{2z}$ operation, which is equivalent to a 180° rotation of the TMD layer, anti-commutes with H_{SOC_I} and H_{SL} but commutes with H_{SOC_R} . This means that the λ_I and u terms will change sign upon changing the TMD orientation, but λ_R term will not. We will denote the proximity-induced terms with a $\pm$ superscript, which corresponds to their relative sign on both layers (i.e., λ_I^+ denotes Ising coupling with the same sign on both layers).

In this work, we focus on three different kinds of TBG-TMD heterostructures: (1) a TMD-TBG-TMD heterostructure with the same TMD orientation on both sides (“even”), (2) a TMD-TBG-TMD heterostructure with opposite TMD orientation on both sides (“odd”), and (3) a one-sided TBG-TMD heterostructure. The even/odd heterostructures add even/odd proximity-induced terms to the TBG Hamiltonian, respectively given by

$$H_e^{PI} = \frac{u^+}{2}\sigma^z + \frac{\lambda_I^+}{2}\tau^z s^z + \frac{\lambda_R^-}{2}l^z(\tau^z \sigma^x s^y - \sigma^y s^x), \quad (3.10)$$

$$H_o^{PI} = l^z \left(\frac{u^-}{2}\sigma^z + \frac{\lambda_I^-}{2}\tau^z s^z + \frac{\lambda_R^-}{2}(\tau^z \sigma^x s^y - \sigma^y s^x) \right). \quad (3.11)$$

Note that the Rashba term is required to have opposite sign on the two graphene layers by the layer-exchanging $\mathcal{C}'_{2x}$ symmetry. The one-sided TBG-TMD stacking only has proximity-induced terms on one layer, and can be written as a combination of the even and odd proximity-induced terms:

$$H_{1s}^{PI} = \frac{1+l^z}{2} \left(\frac{u}{2}\sigma^z + \frac{\lambda_I}{2}\tau^z s^z + \frac{\lambda_R}{2}(\tau^z \sigma^x s^y - \sigma^y s^x) \right). \quad (3.12)$$

In Table 3.1, we list all the proximity-induced terms (Ising SOC, Rashba SOC and sublattice splitting) in both the even and odd form, and their transformation properties under

m	$(\mathcal{T}, \mathcal{T}')$	$(\mathcal{C}_{2z}, \mathcal{C}'_{2z})$	$(\mathcal{C}_{2x}, \mathcal{C}'_{2x})$	$\mathcal{C}'_{2z}\mathcal{T}'$	$\mathcal{C}'_{2y}\mathcal{T}'$
u^+	$(\checkmark, \checkmark)$	$(\times, \times)$	$(\times, \times)$	$\times$	$\checkmark$
λ_I^+	$(\times, \checkmark)$	$(\times, \times)$	$(\checkmark, \times)$	$\times$	$\checkmark$
λ_R^+	$(\times, \checkmark)$	$(\times, \checkmark)$	$(\checkmark, \times)$	$\checkmark$	$\times$
u^-	$(\checkmark, \checkmark)$	$(\times, \times)$	$(\checkmark, \checkmark)$	$\times$	$\times$
λ_I^-	$(\times, \checkmark)$	$(\times, \times)$	$(\times, \checkmark)$	$\times$	$\times$
λ_R^-	$(\times, \checkmark)$	$(\times, \checkmark)$	$(\times, \checkmark)$	$\checkmark$	$\checkmark$

Table 3.1: Symmetry transformation properties of the proximity-induced terms in Eqs. (3.10), (3.11) and (3.12). A “ $\times$ ” entry in the table means that the term on that row is odd under the symmetry labeling the column, i.e. the symmetry is broken. A “ $\checkmark$ ” entry means that the proximity-induced term is even and therefore symmetry-preserving.

time-reversal and different two-fold rotations. From the table, we see that the different TBG-TMD heterostructures are distinguished by their transformation properties under $\mathcal{C}'_{2x}$. In particular, H_e breaks $\mathcal{C}'_{2x}$, while H_o is invariant under it. Importantly, because of the Ising SOC and sublattice splitting, all heterostructures necessarily break not only the spinless $\mathcal{C}_{2z}$ symmetry, but also the spinful $\mathcal{C}'_{2z}$ symmetry. All proximity-induced terms, however, do respect the spinful time-reversal symmetry $\mathcal{T}'$. As in the original TBG continuum model, the single-valley moiré Hamiltonians of the TBG-TMD heterostructures are interchanged by time-reversal symmetry.

3.4 Flat bands from Rashba spin-orbit coupling

As mentioned in the last section, Rashba SOC is the dominant term introduced by the proximity effect of TMD. Therefore, we will first isolate its effect on the flat band spectrum of TBG, and later add the Ising SOC and sublattice splitting as small perturbations. We note that a recent work has also discussed TBG in the presence of Rashba SOC [112].

We first consider a TBG-TMD heterostructure with both even and odd Rashba SOC terms:

$$H_R = H_{TBG} + \frac{1}{2} (\lambda_R^+ + \lambda_R^- l^z) (\tau^z \sigma^x s^y - \sigma^y s^x) \quad (3.13)$$

H_R features four flat bands in each valley, with opposite valleys related by $\mathcal{T}'$ symmetry. In Fig. 3.1, we highlight the four flat bands of H_R from the K valley, with both $(\lambda_R^+, \lambda_R^-) = (16, 0)$ meV and $(\lambda_R^+, \lambda_R^-) = (0, 16)$ meV. The band spectrum with $\lambda_R^- = 0$, as shown in Fig. 3.1(a), remains almost two-fold degenerate and is not very different from the original BM band spectrum. The heterostructure with $\lambda_R^+ = 0$, on the other hand, has a very intricate band

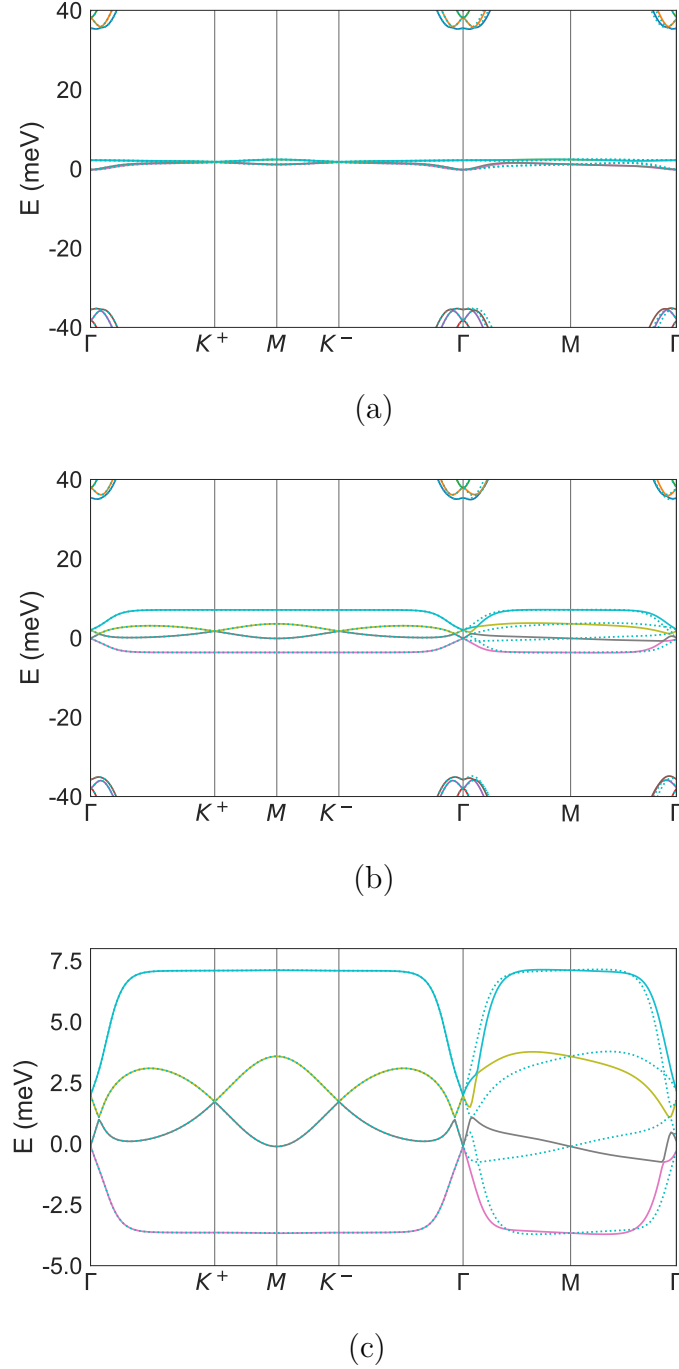


Figure 3.1: (a) Band structure along a high symmetry line of the BM Hamiltonian with a Rashba SOC term given by $\lambda_R^+(\tau^z \sigma^x s^y - \sigma^y s^x)$. The twist angle is $\theta = 1.08^\circ$, and $\lambda_R^+ = 16$ meV. (b) Same as above, but now with the Rashba SOC as $\lambda_R^-(\tau^z \sigma^x s^y - \sigma^y s^x)$ which has opposite sign on both layers, and $\lambda_R^- = 16$ meV. (c) Same as (b) but zoomed in to highlight the flat bands. The solid and dotted lines represent the flat bands from different valleys.

structure with several remarkable features as shown in Figs. 3.1(b) and (c). First, near the $K^\pm$ points there is one pair of well-separated bands which are extremely flat, while the other two bands have Dirac cones at $K^\pm$. Second, we find that in total there are sixteen different linear band crossings or Dirac points, all of which are protected by the spinful $\mathcal{C}_{2z}'\mathcal{T}'$ symmetry. Note that because of the spin-orbit coupling, the two-band single-valley BM model becomes a four-band model. As a result, the chirality of these sixteen Dirac points is no longer well defined, and it is more appropriate to think about the Dirac points as carrying a non-Abelian charge [93, 113].

The sixteen Dirac cones are scattered over the mini-BZ as follows. Two of the Dirac points are located at the Γ point, and they are displaced in energy, i.e. one Dirac point is between the top two bands and one Dirac point is between the bottom two bands. The three different $\Gamma - M$ lines each contain two linear band crossings, one between the top two bands, and one between the bottom two bands. The six final Dirac points are very close to, but not exactly on, the $\Gamma - K^+$ and $\Gamma - K^-$ lines. For the parameter values we used, we find that the Dirac points along the $\Gamma - M$ and $\Gamma - K^\pm$ are all located very closely to the Γ point. In Appendix B.1, we plot the energy difference between the top two bands, and the energy difference between the middle two bands, for both $\lambda_R = 2$ meV and $\lambda_R = 16$ meV. On these figures, one can clearly identify the location of all sixteen Dirac points (the location of the Dirac cones in the lower two bands is the same as the location of the Dirac cones in the upper two bands), and see how they move around as a function of λ_R .

Below, we use a $k \cdot p$ analysis around both the $K^\pm$ and Γ points to develop an understanding of the drastically different effects of the even and odd Rashba SOC on the BM bands, and analyze the symmetry properties of the Dirac points along the $\Gamma - M$ lines.

Before diving into the details, the fundamental difference between λ_R^- [Fig. 3.1(b)] and λ_R^+ [Fig. 3.1(c)] can be summarized as follows. While far from the magic angle the two mini-Dirac points at $K^\pm$ are localized onto one-or the other layer, near the magic angle the interlayer-tunneling causes the flat bands to be delocalized 50-50 between the two layers. And as explained in more detail below, we also find the flat band states to have a relative phase difference of i between the two layers. As a result, when projecting H_R into the flat band, one finds that the effect of λ_R^+ on the two layers cancels, leaving the band structure almost unaffected, while for λ_R^- they add. The flatness of the band throughout most of the mBZ is simply a result of the momentum-independence of the Rashba coupling.

3.4.1 Analysis of the Dirac points at $K^\pm$

For our $k \cdot p$ analysis near the $K^\pm$ points, we start by considering the approximation of the "chiral limit" of tBLG, which corresponds to artificially putting $w_0 = 0$ in the BM Hamiltonian [70, 114]. In the chiral limit, the Bloch states of the flat bands around both the $K^\pm$ points can be taken to be completely localized on one of the two sublattices (i.e A vs B). Therefore, we can write the four-component Bloch states of the spinless, single-valley BM Hamiltonian in this sublattice-polarized basis as $\psi(\mathbf{r})$ and $\chi(\mathbf{r})$, where both ψ and χ have two components corresponding to the two different layers, but live on different sublattices.

The chiral Bloch states for the complete moiré Hamiltonian are then given by $\psi_{\mathbf{k}}(\mathbf{r})$, $\chi_{\mathbf{k}}(\mathbf{r})$, $\psi_{\bar{\mathbf{k}}}(\mathbf{r})$ and $\chi_{\bar{\mathbf{k}}}(\mathbf{r})$, where $\{\mathbf{k}, \bar{\mathbf{k}}\}$ denote the $K/\bar{K}$ valleys, and two spins are represented by the same Bloch states.

We can use the symmetries of the BM model to relate the different chiral Bloch states. First, H_{TBG} is invariant under $\mathcal{C}_{2z}\mathcal{T} = \sigma^x\mathcal{K}$ symmetry, which exchanges the sublattices. Therefore the Bloch states of H_{TBG} which live on different sublattices transform into each other by $\mathcal{C}_{2z}\mathcal{T}$, which implies that $\chi_{\mathbf{k}}(\mathbf{r}) = \psi_{\mathbf{k}}^*(-\mathbf{r})$. Similarly, H_{TBG} is also invariant under $\mathcal{T} = \tau^x\mathcal{K}$ symmetry, giving the following relation between other basis functions: $\{\psi_{\bar{\mathbf{k}}}(\mathbf{r}), \chi_{\bar{\mathbf{k}}}(\mathbf{r})\} = \{\psi_{-\mathbf{k}}^*(\mathbf{r}), \chi_{-\mathbf{k}}^*(\mathbf{r})\}$. These relations allow us to fix all chiral Bloch states given a single Bloch state $\psi_{\mathbf{k}}(\mathbf{r})$.

For the purpose of our $k \cdot p$ analysis, we are only interested in the chiral Bloch state $\psi_{\mathbf{k}}(\mathbf{r})$ near the $K^\pm$ points. We have observed numerically that in this region the chiral Bloch states are to a very good approximation given by the following simple form:

$$\psi_{K^\pm}(\mathbf{r}) \sim \begin{pmatrix} 1 \\ -i \end{pmatrix} f(\mathbf{r}), \quad (3.14)$$

where $f(\mathbf{r})$ is some envelope function which ensures that the wavefunction amplitude is concentrated on the AA regions. Eq. (3.14) thus implies that the wavefunction components on different layers have the same magnitude and a relative phase difference of $\pi/2$. Importantly, we find that away from the chiral limit, and even for realistic values of w_0 , one can still find a basis for the flat bands where the expression in Eq. (3.14) remains a very good approximation for the basis states. This basis precisely corresponds to the sublattice polarized basis introduced in Ref. [26]. The observation that we can work in a basis of the form in Eq. (3.14) at realistic values of w_0 will help us understand many of the results obtained below.

Now we explain how we construct the $k \cdot p$ Hamiltonian near the $K^\pm$ points. We start with numerically diagonalizing H_{TBG} at the $K^\pm$ points. Because the bands at the $K^\pm$ are degenerate, the corresponding eigenbasis is not uniquely defined. To remedy this, we fix the eigenbasis by imposing that the $\mathcal{C}_{2z}'\mathcal{T}$ symmetry acts as $i\sigma^x s^x \mathcal{K}$. Next, we project $H_R(\mathbf{k})$ in the neighborhood of the $K^\pm$ points into the symmetry-fixed eigenbasis, and obtain the following matrix:

$$\left(\tilde{H}_{R,K^\pm}(\mathbf{k}) \right)_{ij} \equiv \langle i | H_R(\mathbf{k}) | j \rangle, \quad (3.15)$$

where $|i\rangle \in \{|\psi_{K^\pm}\rangle, |\chi_{K^\pm}\rangle, |\psi_{\bar{K}^\pm}\rangle, |\chi_{\bar{K}^\pm}\rangle\}$. This procedure gives us the following effective $k \cdot p$ Hamiltonian to first order in $\mathbf{k}$:

$$\tilde{H}_{R,K^\pm}(\mathbf{k}) = E_{0,K} + \tilde{v}_K(k_x\sigma^x + k_y\tau^z\sigma^y) + \frac{\tilde{\lambda}_R^-}{2}(\tau^z\sigma^x s^y - \sigma^y s^x), \quad (3.16)$$

where $\tilde{v}_K$ is the renormalized Dirac velocity of the tBLG. Note that under the flat band projection, the even Rashba SOC term (λ_R^+) vanishes, and therefore it has no effect on the band spectrum in first order perturbation theory. The odd Rashba terms λ_R^- , on the

other hand, is unaffected by the projection. One can explicitly check these properties of the even and odd Rashba terms under projection into the flat bands by using the approximate expression for the flat band basis states given in Eq. (3.14).

In each valley, the projected odd Rashba SOC in Eq. (3.16) has eigenvalues $\{-\tilde{\lambda}_R^-, 0, 0, \tilde{\lambda}_R^-\}$. This separates two of the four zero-energy bands with quantum number $\sigma^z s^z \tau^z = -1$ with a band gap $\Delta = 2\tilde{\lambda}_R^-$, producing the flat bands in Figs. 3.1(b) and (c), while the other two bands remain unchanged and retain their Dirac crossing. These Dirac points are protected by the $\mathcal{C}'_{2z}\mathcal{T}'$ symmetry of H_R .

3.4.2 Analysis of the Dirac points on the $\Gamma - M$ lines

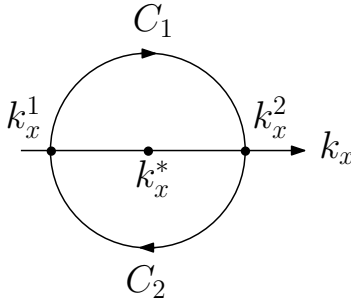


Figure 3.2: $\mathcal{C}'_{2x}$ symmetric contour around a Dirac point at $\mathbf{k}^* = (k_x^*, 0)$. The contour consists of two parts C_1 and C_2 , which are related by $\mathcal{C}'_{2x}$. k_x^1 and k_x^2 are the begin (end) and end (begin) points of C_1 (C_2).

Having analyzed the Dirac cones at the K -points, we now turn our attention to those Dirac cones in the band structure of Fig. 3.1(c) which lie on the three different $\Gamma - M$ lines. Our goal is to identify the symmetries which protect these Dirac points. Let us first consider the Dirac cones at the Γ point, and focus on the case with $\lambda_R^+ = 0$. As a first step, we again perform a $k \cdot p$ analysis. We do this by numerically diagonalizing H_R at the Γ point, and then using the eigenstates to construct the $k \cdot p$ Hamiltonian. To fix the eigenbasis, we impose different symmetry representations with a new basis $\{\tau, \tilde{\sigma}, \tilde{s}\}$: $\tilde{\mathcal{T}}' = i\tau^y \mathcal{K}$, $\tilde{\mathcal{C}}'_{2z} \tilde{\mathcal{T}}' = \mathcal{K}$, and $\tilde{\mathcal{C}}'_{2x} = i\tau^z \tilde{\sigma}^z \tilde{s}^z$. Here, τ still refers to the valley degree of freedom, but $\tilde{\sigma}$ and $\tilde{s}$ no longer represent the original sublattices or spins, as they are now hybridized by the Rashba SOC. Instead, $\tilde{\sigma}^z$ distinguishes the pair of high energy ($\tilde{\sigma}^z = +$) and the pair of low energy bands ($\tilde{\sigma}^z = -$) at Γ , and $\tilde{s}^\mu$ acts within each pair of high or low energy bands. Note that in this basis, the $\tilde{\mathcal{C}}'_{2x}$ operator is diagonal matrix, which will be helpful for our later discussions.

After projecting $H_R(\mathbf{k})$ in the neighborhood of the Γ point into this eigenbasis, we obtain the following effective $k \cdot p$ Hamiltonian to first order in $\mathbf{k}$:

$$\tilde{H}_{R,\Gamma} = (E_{0,\Gamma} + \tilde{m}\tilde{\sigma}^z) + \tilde{v}_\Gamma \tau^z (k_x \tilde{s}^z + k_y \tilde{\sigma}^z \tilde{s}^x) \quad (3.17)$$

In each valley, H_R has two separated Dirac cones at the Γ point. Similar to the Dirac cones in the BM band spectrum, they are protected by the valley-charge conservation symmetry and $\mathcal{C}'_{2z}\mathcal{T}'$.

From the $k \cdot p$ analysis we also observe that all valley-diagonal mass terms, i.e. the terms $\tau^{0,z}\tilde{\sigma}^{0,z}\tilde{s}^y$, not only break the $\tilde{\mathcal{C}}'_{2z}\tilde{\mathcal{T}}'$ symmetry, but also the $\tilde{\mathcal{C}}'_{2x}$ symmetry. As a next step, we will show that this is no accident, and that the Dirac cone at Γ is protected by the $\mathcal{C}'_{2x}$ symmetry. At the same time, we will also show that the additional Dirac points along the $\mathcal{C}'_{2x}$ -invariant $\Gamma - M$ line are also protected by $\mathcal{C}'_{2x}$, and that the Dirac points along the two $\Gamma - M$ lines which are interchanged by $\mathcal{C}'_{2x}$ are protected by a combination of the $\mathcal{C}'_{2x}$ and $\mathcal{C}'_{3z}$ symmetries, where the latter is the spinful three-fold in-plane rotation symmetry.

To show that Dirac cones along the $\mathcal{C}'_{2x}$ invariant line are protected by $\mathcal{C}'_{2x}$, let us consider the general situation where there is a Dirac point at momentum $\mathbf{k}^* = (k_x^*, 0)$. For generality, we will also allow the $\mathcal{C}'_{2z}\mathcal{T}'$ symmetry to be broken. Denoting the cell-periodic part of the Bloch states as $|u_{\mathbf{k},n}\rangle$, the $\mathcal{C}'_{2x}$ symmetry implies that

$$D(\mathcal{C}'_{2x})|u_{\mathbf{k},n}\rangle = e^{i\alpha_n(\mathbf{k})}|u_{\mathcal{C}_{2x}\mathbf{k},n}\rangle, \quad (3.18)$$

where $\mathcal{C}_{2x}\mathbf{k} = (k_x, -k_y)$, $D(\mathcal{C}'_{2x})$ is the $\mathcal{C}'_{2x}$ representation acting on the periodic part of the Bloch states, and $e^{i\alpha_n(\mathbf{k})}$ is a gauge-dependent phase factor. Note that we always work in a continuous gauge, such that $\alpha_n(\mathbf{k})$ is a continuous function of momentum. Since $\mathcal{C}_{2x}^2 = -1$, the phase factors $e^{i\alpha_n(\mathbf{k})}$ satisfy $\exp(i[\alpha_n(\mathbf{k}) + \alpha_n(\mathcal{C}_{2x}\mathbf{k})]) = -1$. Along the $\mathcal{C}_{2x}$ -invariant momentum line, the phase factors $\exp(i\alpha_n(\mathbf{k})) = \pm i$ are the $\mathcal{C}'_{2x}$ eigenvalues of the Bloch states. From the $\mathcal{C}'_{2x}$ transformation property in Eq. (3.18), it follows that the Berry connection $\mathbf{A}_n(\mathbf{k}) = i\langle u_{\mathbf{k},n}|\nabla|u_{n,\mathbf{k}}\rangle$ satisfies

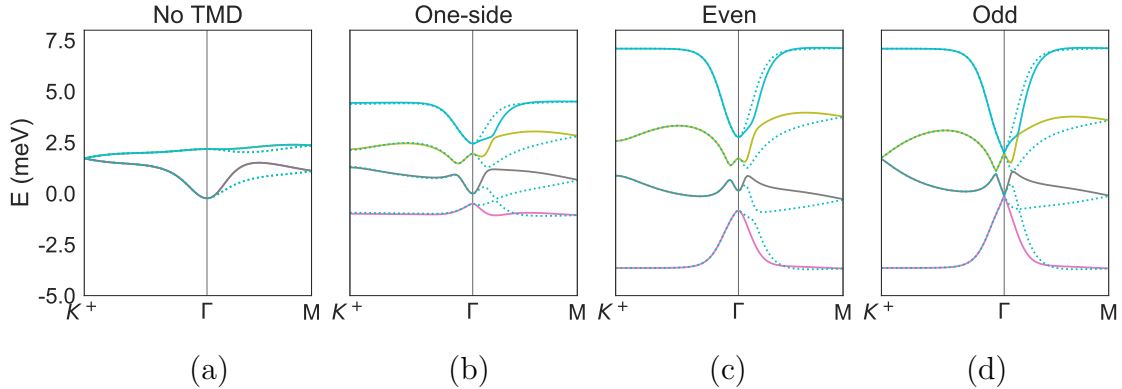


Figure 3.3: Example of band spectra along $\Gamma - K^+$ line and $\Gamma - M$ line in four different kinds of devices: (a) TBG without TMD substrate; (b) one-sided TBG-TMD heterostructures; (c) even TMD-TBG-TMD heterostructures; (d) odd TMD-TBG-TMD heterostructures. The strengths of proximity-induced terms are $(\lambda_R, \lambda_I, u) = (16, 1, 2)$ for all figures.

$$\mathbf{A}_n(\mathbf{k}) = \mathcal{C}_{2x} \mathbf{A}_n(\mathcal{C}_{2x} \mathbf{k}) - \nabla \alpha_n(\mathbf{k}). \quad (3.19)$$

Note that Eq. (3.19) implies that the Berry curvature $F(\mathbf{k}) = \partial_x A_{n,y}(\mathbf{k}) - \partial_y A_{n,x}(\mathbf{k})$ is odd under $\mathcal{C}'_{2x}$.

Next, we consider a $\mathcal{C}_{2x}$ symmetric contour C encircling the Dirac point at $\mathbf{k}^*$. This contour consists of two parts C_1 and C_2 , which are related by $\mathcal{C}_{2x}$. The two parts C_1 and C_2 meet at the points k_x^1 and k_x^2 on the $\mathcal{C}_{2x}$ -invariant line $k_y = 0$. See Fig. 3.2 for an example of the contour C . The Berry phase along the closed contour C is given by

$$\oint_C \mathbf{A}_n(\mathbf{k}) \cdot d\mathbf{k} = \int_{C_1} \mathbf{A}_n(\mathbf{k}) \cdot d\mathbf{k} + \int_{C_2} \mathbf{A}_n(\mathbf{k}) \cdot d\mathbf{k} \quad (3.20)$$

Using Eq. (3.19), we can write the contribution to the Berry phase of the C_2 section of the contour as

$$\int_{C_2} \mathbf{A}_n(\mathbf{k}) \cdot d\mathbf{k} = - \int_{\mathcal{C}_{2x} C_1} \mathbf{A}_n(\mathbf{k}) \cdot d\mathbf{k} \quad (3.21)$$

$$= - \int_{C_1} \mathcal{C}_{2x} \mathbf{A}_n(\mathcal{C}_{2x} \mathbf{k}) \cdot d\mathbf{k} \quad (3.22)$$

$$= - \int_{C_1} (\mathbf{A}_n(\mathbf{k}) + \nabla \alpha_n(\mathbf{k})) \cdot d\mathbf{k}, \quad (3.23)$$

where the minus sign in the first line comes from the fact that C_2 and $\mathcal{C}_{2x} C_1$ have different orientations, and in the third line we have used Eq. (3.19).

Combining Eqs. (3.20) and (3.23), we find that the Berry phase is given by

$$\oint_C \mathbf{A}_n(\mathbf{k}) \cdot d\mathbf{k} = \alpha_n(k_x^1, 0) - \alpha_n(k_x^2, 0). \quad (3.24)$$

Because the Berry curvature is odd under $\mathcal{C}'_{2x}$, and because the contour C is $\mathcal{C}_{2x}$ symmetric, we know that the only contribution to the Berry phase can come from the Dirac cone at $\mathbf{k}^*$. This means that the Berry phase is equal to π . From Eq. (3.24), it then follows that the $\mathcal{C}'_{2x}$ eigenvalues of the Bloch states along the $\mathcal{C}_{2x}$ -invariant line have to change sign on crossing the Dirac point. This implies that every band has to cross an even number of Dirac points along the $\mathcal{C}_{2x}$ -invariant momentum line. In a gapped $\mathcal{C}'_{2x}$ -symmetric band spectrum, the $\mathcal{C}'_{2x}$ eigenvalues of the Bloch states have to be constant along the $\mathcal{C}_{2x}$ -invariant line $k_y = 0$, so Eq. (3.24) implies that the Dirac cones are protected by the $\mathcal{C}'_{2x}$ symmetry.

The above result thus shows that the Dirac points on the $\mathcal{C}'_{2x}$ -invariant $\Gamma - M$ line are protected by $\mathcal{C}'_{2x}$. The spinful three-fold rotation symmetry $\mathcal{C}'_{3z}$ then implies that also the Dirac points on the two $\Gamma - M$ lines which are interchanged by $\mathcal{C}'_{2x}$ cannot be gapped, which means that these Dirac crossing are protected by the combination of the $\mathcal{C}'_{2x}$ and $\mathcal{C}'_{3z}$ symmetries.

We can explicitly check the above conclusions by revisiting the $k \cdot p$ Hamiltonian in Eq. (3.17). The $k \cdot p$ Hamiltonian along the $k_y = 0$ line takes the form $\tilde{H}_{R,\Gamma}(k_y = 0) = E_{0,\Gamma} + \tilde{m}\tilde{\sigma}^z + \tilde{v}_\Gamma k_x \tau^z \tilde{s}^z$, and the $\mathcal{C}'_{2x}$ symmetry acts as $i\tau^z \tilde{\sigma}^z \tilde{s}^z$. From these expressions, it immediately follows that each band will indeed have opposite $\mathcal{C}'_{2x}$ eigenvalues at different sides of the Dirac points at Γ . We have also numerically computed the $\mathcal{C}'_{2x}$ eigenvalues of the four flat bands along the entire $\Gamma - M$ line, and we observed that the four bands change their $\mathcal{C}'_{2x}$ eigenvalue not only at Γ , but also on crossing the other Dirac points on the $\Gamma - M$ line. This confirms that these Dirac points are indeed protected by the $\mathcal{C}'_{2x}$ symmetry.

3.5 Effects of sublattice splitting and Ising SOC

After our analysis of the effect of Rashba SOC on the BM bands, we will now include the Ising SOC and sublattice splitting terms in our analysis. Specifically, we consider the even and odd TBG-TMD heterostructure, where the Ising SOC ($\lambda_I^\pm$) and sublattice splitting ($u^\pm$) are introduced according to Eqs. (3.10) and (3.11) respectively:

$$H_{e,o} = H_{TBG} + H_{e,o}^{PI}, \quad (3.25)$$

and they can be treated as perturbations to H_R in Eq. (3.13), with $\lambda_R^+ = 0$ and $\lambda_R^- \neq 0$. A similar treatment can be applied to one-sided TBG-TMD heterostructure

$$H_{1s} = H_{TBG} + H_{1s}^{PI}, \quad (3.26)$$

but the conclusion would be similar, as we found in the previous section that the λ_R^+ term in H_{1s} has only a small effect.

Similar to Rashba SOC, the additional proximity-induced terms in H_e and H_o will change the band structure of H_{TBG} . In Fig. 3.3, we show the band spectra of H_e , H_o and H_{1s} along high-symmetry lines. We see that all the band spectra are gapped at the $K^\pm$ points where the gapless Dirac cones are broken by the proximity-induced terms, but the band gap in $H_{e,1s}$ are much larger than that of H_o . As for the Γ point, $H_{e,1s}$ and H_o also show different characters: H_o still retains the two gapless Dirac cones along the $\Gamma - M$ line, while $H_{e,1s}$ have all of these Dirac cones gapped out. The three Hamiltonians also gap out the Dirac cones away from high-symmetry lines, but the difference between the resulting spectra is less significant. Overall, it is expected that H_{1s} has a band spectrum similar to H_e since they share the same perturbation terms, and we will now explain the different band features of H_e and H_o in the perspective of both symmetry protection and $k \cdot p$ analysis.

We can understand the different band gaps in H_e and H_o from symmetry considerations. According to Table 3.1, both the $u^\pm$ and $\lambda_I^\pm$ terms in $H_{e,o}$ break the $\mathcal{C}'_{2z}\mathcal{T}'$ symmetry, removing the protection on the Dirac cones at the $K^\pm$ points. However, the u^- and λ_I^- terms in H_o preserve the $\mathcal{C}'_{2x}$ symmetry protecting the Dirac cones along the $\Gamma - M$ line, therefore they will not induce a band gap. The u^+ and λ_I^+ terms, on the other hand, do not preserve $\mathcal{C}'_{2x}$, so we do expect those Dirac cones to be gapped in H_e , but not in H_o .

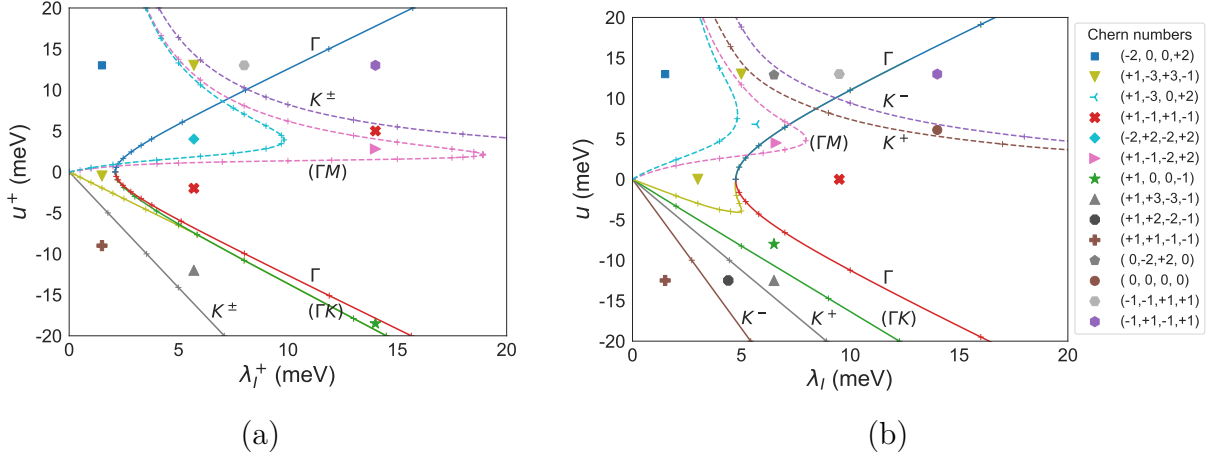


Figure 3.4: Topological phases diagram of (a) even and (b) one-sided TBG-TMD heterostructures regarding (u, λ_I) parameters. Each phase is characterized by the Chern numbers of the four flat bands in K valley shown on the right. The sketched phase boundaries are where the band gap vanishes, either between the middle two bands (solid) or the top/bottom two bands (dashed), and the labels represent the position of gap closing in the momentum space.

The arguments above can be made explicit by using our $k \cdot p$ analysis at the $K^\pm$ and Γ points. At the $K^\pm$ points, we use the same approximate Bloch states as in the previous section to obtain a $k \cdot p$ Hamiltonian. In this way, we obtain the following effective Hamiltonians for $H_{e,o}$ near the $K^\pm$ points:

$$\tilde{H}_{e,K^\pm} = \tilde{H}_{R,K^\pm} + \tilde{u}^+ \sigma^z + \tilde{\lambda}_I^+ \tau^z s^z; \quad (3.27)$$

$$\tilde{H}_{o,K^\pm} = \tilde{H}_{R,K^\pm}. \quad (3.28)$$

In H_e , the additional terms in Eq. (3.27) gap out the Dirac cone, as they indeed break the $\mathcal{C}'_{2z} \mathcal{T}' = i\sigma^x s^x \mathcal{K}$ symmetry. Note that the $\tilde{u}^+$ and $\tilde{\lambda}_I^+$ terms commute, which implies that they are competing mass terms. As for H_o , we find that u^- and λ_I^- simply vanish under the projection involved in the $k \cdot p$ construction. This can easily be checked explicitly by using the simple approximate form for the BM Bloch states around the $K^\pm$, as discussed in detail in the previous section. Even so, u^- and λ_I^- terms still gap out the Dirac cones as these terms break the $\mathcal{C}'_{2z} \mathcal{T}'$ symmetry. The Dirac mass generated by these two terms, however, will only appear in second order perturbation theory, and will therefore be much smaller than the Dirac masses in H_e . From Fig. 3.3, we indeed see that the gaps at the $K^\pm$ points in H_o are significantly smaller than the corresponding gaps in H_e , which are barely visible on this scale.

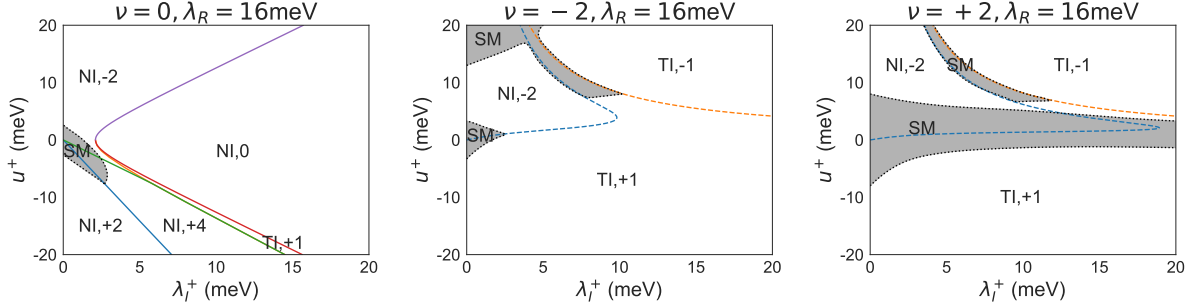


Figure 3.5: The topological phase diagram of an even-aligned TBG-TMD heterostructure at $\nu = 0$, $\nu = -2$ and $\nu = +2$ filling. Each phase is labeled by the Chern number from the occupied bands in K valley, and categorized into semimetal (SM), normal insulator (NI), and topological insulator (TI) by the $\mathbb{Z}_2$ classification of TI and whether the phase is gapped or not.

At the Γ point, the $k \cdot p$ Hamiltonians corresponding to $H_{e,o}$ are

$$\tilde{H}_{e,\Gamma} = \tilde{H}_{R,\Gamma} + \tilde{u}^+ \tau^z \tilde{\sigma}^y \tilde{s}^z + \tilde{m}_I^+ \tau^z \tilde{\sigma}^z \tilde{s}^y, \quad (3.29)$$

$$\tilde{H}_{o,\Gamma} = \tilde{H}_{R,\Gamma} + (\tilde{u}^- + \tilde{m}_I^-) \tau^z \tilde{\sigma}^y \tilde{s}^x, \quad (3.30)$$

With the symmetry representations $\tilde{\mathcal{C}}'_{2z} \tilde{\mathcal{T}}' = \mathcal{K}$ and $\tilde{\mathcal{C}}'_{2x} = i\tau^z \tilde{\sigma}^z \tilde{s}^z$, we see that $\tilde{H}_{e,\Gamma}$ breaks both of these symmetries, while $\tilde{H}_{o,\Gamma}$ breaks $\tilde{\mathcal{C}}'_{2z} \tilde{\mathcal{T}}'$ but not $\tilde{\mathcal{C}}'_{2x}$. This means that only H_e lifts all the symmetry protection on the Dirac cones and obtains a fully gapped bands in first order perturbation. On the other hand, H_o will only renormalize but not gap out these Dirac cones, as they are still under the protection of $\mathcal{C}'_{2x}$.

3.6 Valley Chern numbers and topological insulators

In the previous section we found that both for the even and one-sided TBG-TMD heterostructures the flat bands can be fully gapped in the presence of all proximity-induced terms. This allows us to define Chern numbers for these isolated bands and determine their topological properties. In this section, we examine how these Chern numbers depend on the proximity-induced terms, and what topological phases can be realized in different parameter regimes and for different fillings.

We obtain the Chern numbers for the different isolated bands, as well as for different heterostructures, as follows. First, we note that since all heterostructures preserve time-reversal symmetry $\mathcal{T}'$, we only need to calculate the Chern numbers for the four flat bands in a single valley, as the bands in different valleys related by $\mathcal{T}'$ will have opposite Chern number. The Chern numbers of the isolated bands in one of the valleys are computed using the method of Ref.[115].

Since the band gaps are mainly determined by the strengths of Ising SOC λ_I and sublattice splitting u , we fix the Rashba SOC strength $\lambda_R = 16$ meV, and focus on how the Chern numbers depend on both u and λ_I . The resulting phase diagrams of the single-valley moiré Hamiltonians (in valley $\tau = +$) corresponding to both the even and one-sided heterostructures are shown in Fig. 3.4. Note that it is sufficient to consider the parameter regime where $\lambda_I > 0$ because the $u^\pm$ and $\lambda_I^\pm$ change sign under $\mathcal{C}'_{2z}\mathcal{T}'$, which implies that the bands with parameters $(-u, -\lambda_I)$ have opposite Chern numbers from those with $(+u, +\lambda_I)$.

From the phase diagrams in Fig. 3.4, we can identify the different parameter regimes where, based on a single-particle picture, non-trivial gapped topological phases are realized in the heterostructures. In Fig. 3.5, we show the possible phases in the even heterostructure at fillings $\nu = -2, 0, 2$, where bands can fill in $\mathcal{T}'$ -related pairs. The different topological phases are characterized by the Chern numbers of the occupied bands, and are distinguished physically in several ways. The most robust phases are those which have an odd total Chern number in each valley. These states are topological insulators which are protected by the $\mathcal{T}'$ Kramers symmetry, and are characterized by gapless helical edge modes. The phases which have an even but non-zero total Chern number in each valley are “valley-Hall” states protected only by the valley-charge conservation symmetry. In the bulk, the valley-charge conservation symmetry is preserved to a very good approximation, but it can be significantly broken along the edge of the device. Therefore, the insulators with an even but non-zero valley Chern number are separated from both the trivial and topological insulators by a bulk gap closing, even though their edge modes will acquire a small mass because of the valley- $U(1)$ breaking terms on the edge (while we do not attempt this analysis, these phases are presumably classified by different symmetry-protected distinctions between atomic insulators). It is reasonable to expect the gap of the edge modes is smaller than the bulk gap, such that transport experiments on a device with non-zero even valley Chern number will measure a significantly smaller gap compared to devices with zero valley Chern number.

We can summarize the most relevant experimental implications of our results as follows. First, for the even and one-sided TBG-TMD heterostructure, it is possible to realize a variety of topological phases by tuning the strength of proximity-induced coupling and the filling fraction of the electron flat bands. At filling $\nu = 0$, gapped phases can be realized with valley Chern numbers $C_V = \pm 2, \pm 4$ in two-sided even heterostructures, and also $C_V = \pm 1, \pm 3$ in one-sided heterostructures. As for filling $\nu = \pm 2$, there is a large and physically realistic parameter regime where phases with $C_V = \pm 1$ can be realized, which correspond to non-trivial topological insulators protected by time-reversal symmetry.

3.7 Discussion and outlook

To summarize, we have analyzed the band structures of different TBG-TMD heterostructures near the magic angle. First, the effect of the dominant Rashba SOC on the TBG flat bands was examined, and the resulting spin-orbit coupled band spectrum was found to

exhibit some remarkable features such as a pair of very flat bands near the $K^\pm$ points, and a very high number of Dirac cones. Based on an approximation of the BM Bloch states near the $K^\pm$ point, we provided a simple explanation for how the Rashba SOC gives rise to the very flat bands. We also analyzed the stability of the different Dirac cones, and found that to gap out all Dirac cones one does not only need to break the spinful $\mathcal{C}'_{2z}\mathcal{T}'$ symmetry, but also the $\mathcal{C}'_{2x}$ symmetry, as the latter protects the Dirac cones on the three $\Gamma - M$ lines (as explained above, some of these Dirac cones additionally require $\mathcal{C}'_{3z}$ to be protected). Having understood the effect of the Rashba SOC, we then included the subleading Ising SOC and sublattice splitting terms. We found that $\mathcal{C}'_{2x}$ breaking heterostructures generically have a fully gapped band spectrum containing eight isolated bands, with the Ising SOC and sublattice splitting terms behaving as competing mass terms driving various phase transitions between different gapped phases. Away from the phase transitions we calculated the Chern numbers of the isolated bands, and we obtained a rich phase diagram with many topologically non-trivial phases. We explicitly identified the parameter regimes where topological insulators and valley-Hall insulators are realized at filling factors $\nu = -2, 0, 2$.

The results of this paper are expected to hold when the TBG twist angle is small enough, and sufficiently close to the first magic angle. The twist angle should be small enough such that the continuum model with two decoupled $\tau = \pm$ valleys used in this work is applicable. A small twist angle is, however, not sufficient. We should also be close enough to the first magic angle in order to have (i) a large enough gap between the eight active bands and the remote bands, and (ii) a bandwidth for the eight active bands that is smaller than or comparable to the SOC terms induced by the TMD substrate. If the bandwidth is too large, then the Rashba SOC will not be strong enough to reconstruct the active bands and generate the pair of extremely flat bands around the K -points in the mini-BZ.

We hope that the analysis presented here can be the starting point for future experimental and theoretical work on TBG-TMD heterostructures close to the magic angle. One possible improvement on the results presented here is to take the effects of lattice relaxation and particle-hole symmetry breaking into account, which can be done straightforwardly using the results of Refs. [55, 56, 116]. Because most of our arguments rely on spatial symmetries which are not broken by lattice relaxation and the particle-hole symmetry breaking terms of Refs. [56, 116], we expect that our results will be largely unaffected. However, the phase diagrams and corresponding phase boundaries discussed in Sec. 3.6 are expected to change slightly.

Another important open question is how the band structures found in this work will be affected by the Coulomb interaction. It would especially be interesting to see how the phase diagram at the magic angle as a function of doping changes in the presence of SOC, as this could potentially provide insight into the nature of the different correlated insulators and superconducting domes. On the theoretical side, it would be interesting to apply a mean-field analysis and see if the same dominant ordering tendencies are found as in the case without SOC, and whether at the integer fillings there is perhaps a clear candidate symmetry-breaking order which has significantly lower energy. At filling factors $\nu = \pm 2$, it would be especially interesting if no sign of additional symmetry breaking is found in

Hartree-Fock, and the topological insulators survive in the presence of interactions, at least on the mean-field level. We leave the study of these questions for future work.

Chapter 4

Anomalous Hall crystals in rhombohedral multilayer graphene

4.1 Introduction

Tunable experimental platforms that host correlated topological states are fertile grounds for exotic phenomena. In recent years, a menagerie of candidates have arisen, including twisted graphene multilayers [5, 11–23, 118–133], twisted transition metal dichalcogenide (TMD) bilayers [134–166], and rhombohedral multilayer graphene (RMG) [117, 167–186]. Topological phenomena have been reported in RMG systems with $N_L = 2 - 5$ layers, both with [168, 169, 172] and without [167, 170, 171, 182] moiré potentials due to an hBN substrate. A number of theoretical studies have examined this hBN moiré potential [187–191] and the resulting topological bands [183–186, 192]. A recent experiment [117] reported that rhombohedral pentalayer graphene aligned to an hBN substrate hosts a $|C| = 1$ quantized anomalous Hall (QAH) insulator, and a whole series of fractional quantum anomalous Hall (FQAH) states that spontaneously break time-reversal symmetry.

Finding Chern bands that are favorable to realize such fractional states is an ongoing challenge [193–198]. In initial realizations of fractional Chern insulators (FCI), magnetic field was necessary to induce [173], or improve the Chern band [118, 199] in order to favor fractional states. A zero-field fractional quantum Hall effect was only recently realized in MoTe_2 [138–141]. For all of the aforementioned systems, the Chern band has been understood at a single-particle level, with interactions providing isospin polarization and thence the fractional states [31, 89, 143, 162, 200, 201]. In contrast, the origin and the character of the Chern band in rhombohedral pentalayer graphene [117] has so far been a mystery.

In this work, we shed light on this mystery by numerically solving the interacting many-body problem in $N_L = 4 - 6$ layer RMG with an hBN potential. Using self-consistent Hartree-Fock (SCHF) calculations, we find that interactions open a gap at filling $\nu = 1$, stabilizing an isolated $|C| = 1$ Chern band. Using exact diagonalization (ED) and density-matrix renormalization group (DMRG) calculations, we confirm that this Chern band hosts

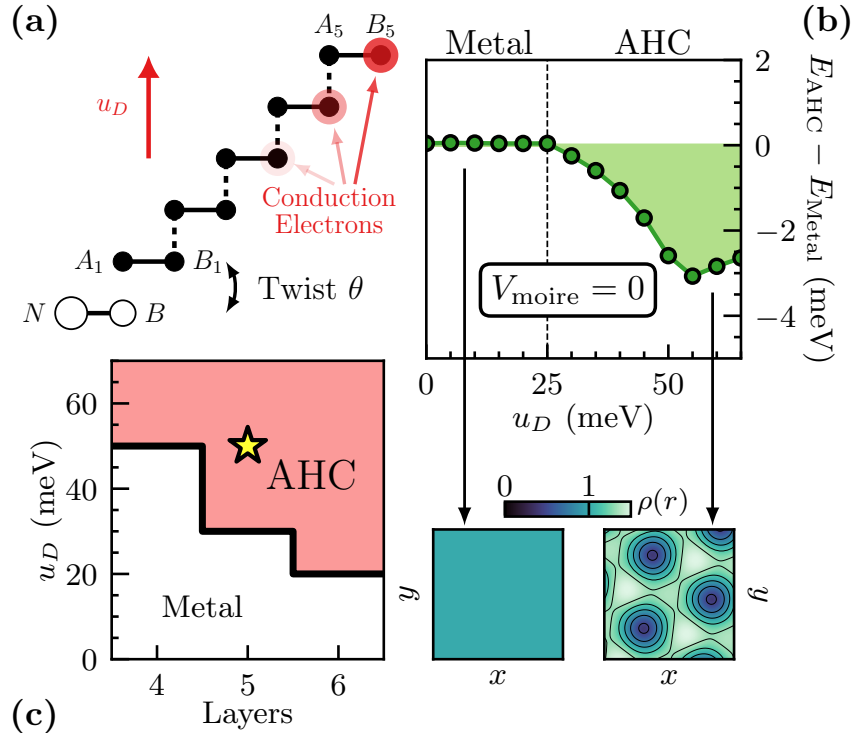


Figure 4.1: (a) Side view of rhombohedral pentalayer graphene aligned to an hBN substrate on the bottom with a twist angle θ . The potential $u_D > 0$ polarizes electrons away from the hBN, making them “moiré-distant”. (b) The energy difference per electron between a graphene translation symmetric metal and an anomalous Hall crystal (AHC) within SCHF as a function of u_D in rhombohedral pentalayer graphene at *zero* moiré potential $V_1 = 0$. The AHC is the ground state beyond $u_D = 25$ meV. Typical charge densities $\rho(r)$ (lower right) show spontaneous translation symmetry breaking in the AHC. (c) Phase diagram of rhombohedral multilayer graphene for $N_L = 4 - 6$ layers with phase boundary from SCHF. The critical displacement field u_D^* decreases with increasing N_L . Yellow star: estimated experimental parameters [117].

an FQAH state.

The Chern band is remarkably robust to perturbations. Crucially, it arises when the electrons are polarized *away* from the aligned hBN substrate, which we refer to as the “moiré-distant” case (Fig. 4.1(a)). It follows that the Chern band is insensitive to many details; similar Chern bands arise for different moiré potentials, different hopping parameters, and for $N_L = 4 - 6$ rhombohedral layers (Fig. 4.1(c)). In fact, the Chern band persists even as the moiré potential is turned off within our SCHF calculations (Fig. 4.1(b), 4.3(a)(d)). This is reminiscent of the “Hall crystal” phase proposed in [202, 203], where electrons in a

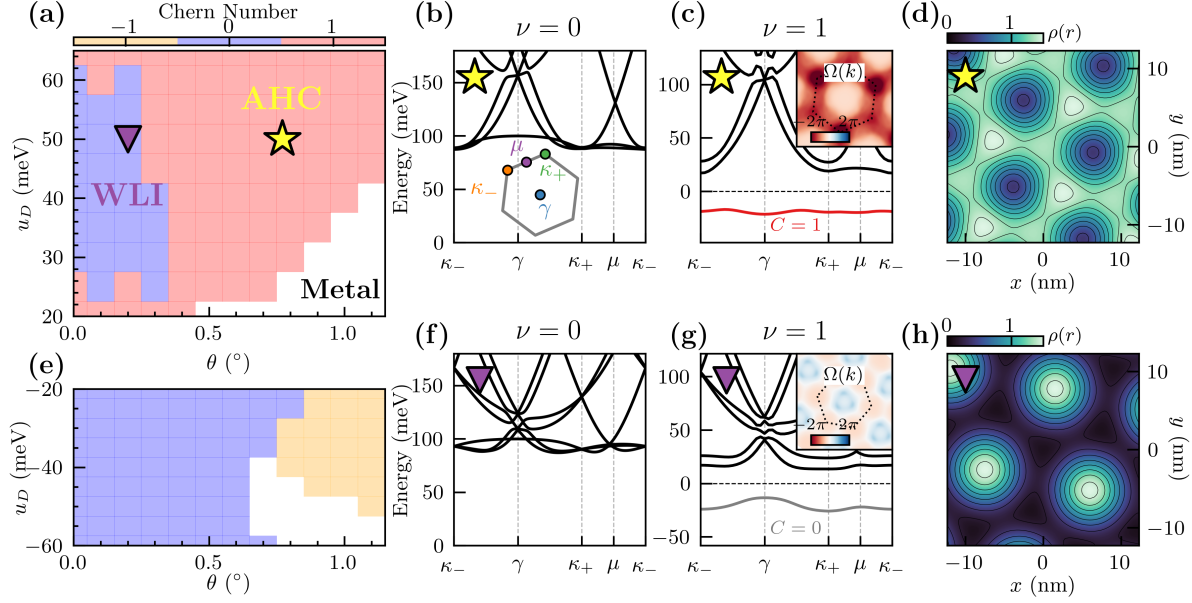


Figure 4.2: (a,e) The phase diagram of moiré rhombohedral pentalayer graphene as a function of the interlayer potential difference u_D , and the twist angle θ . The colors label the Chern number of the SCHF ground states, with gapless regions shown in white. On the moiré-distant side ($u_D > 0$), the anomalous Hall crystal (AHC) phase has $C = 1$, whereas the Wigner-like insulator (WLI) has $C = 0$. (b,f) Non-interacting band structures at the yellow star (u_D, θ) = (50 meV, 0.77°) and purple triangle (u_D, θ) = (50 meV, 0.2°). Inset in (b): plot of the moiré Brillouin zone. (c,g) SCHF bandstructure at $\nu = 1$, finding an AHC and WLI at the yellow star and purple triangle respectively. Insets: Berry curvature $\Omega(\mathbf{k})$ of the occupied band. (d,h) Charge densities $\rho(\mathbf{r})$ of the AHC (d) and WLI (h). The AHC charge density resembles a honeycomb lattice, whereas the WLI charge density resembles a triangular lattice.

magnetic field crystallize into a state with nonzero Hall conductance. Thus, we propose that the Chern insulator at $\nu = 1$ is an anomalous Hall crystal (AHC) state that spontaneously breaks both continuous translation symmetry and time reversal symmetry (with the moiré potential providing a pinning field). This establishes an entirely new mechanism for Chern band formation that arises from the interplay of translation breaking and topology.

4.2 Microscopic Model

We consider a model [204, 205] of RMG with a moiré potential [187] due to an hBN substrate at twist angle θ (Fig. 4.1(a)):

$$\hat{H} = \hat{h}_{\text{kin}} + \sum_{\mathbf{q}} \frac{U_{|\mathbf{q}|}}{2A} : \hat{\rho}_{\mathbf{q}} \hat{\rho}_{-\mathbf{q}} :, \quad U_q = \frac{2\pi \tanh(qd)}{\epsilon_r \epsilon_0 q}, \quad (4.1)$$

where $\hat{\rho}_{\mathbf{q}}$ is the density operator at momentum $\mathbf{q}$, A is the sample area, normal ordering is relative to the charge neutrality gap of RMG in the presence of displacement field, and the screened Coulomb potential $U_{|\mathbf{q}|}$ has gate distance $d = 250 \text{ \AA}$ and dielectric constant $\epsilon_r = 5$.

The kinetic term in the K -valley takes the form

$$h_{\text{kin}} = h_{RG}^{(N_L)} + h_D + V_{\text{hBN}}, \quad (4.2)$$

where $h_{RG}^{(N_L)}$ is a standard model [169] for N_L -layer rhombohedral graphene with in-layer and interlayer hoppings t_{0-4} . The displacement term $[h_D]_{\ell\ell'} = u_D(\ell - 1 - (N_L - 1)/2)\delta_{\ell\ell'}$ creates a potential difference of u_D per layer with the zero point in the middle. Physically, $u_D > 0$ polarizes electrons in the conduction band *away* from the hBN moiré potential. The potential acts on the bottom layer as $V_{\text{hBN}}(\mathbf{r}) = V_0\sigma^0 + V_1\mathbf{f}(\mathbf{r}, \psi) \cdot \boldsymbol{\sigma}$, which is a sum of first harmonics with strength V_1 and phase ψ , plus a layer potential shift V_0 (σ^μ are sublattice Pauli matrices). While a variety of models have been proposed for V_{hBN} [187–190], our focus is on the moiré-distant side $u_D > 0$, which we find is largely V_{hBN} -independent. As the displacement field and moiré potential break C_{2x} and M_x symmetries of standalone RMG, the moiré Hamiltonian $\hat{H}$ retains only C_{3z} rotation, time-reversal, and moiré translation symmetries. See Appendix C.1 for complete model details.

4.3 Interaction-Induced Chern Band

To understand the origin of the Chern insulator, we performed self-consistent Hartree-Fock (SCHF) calculations on up to 48×48 moiré unit cells. We project the $N_L = 5$ graphene layers to the lowest 7 conduction bands, which is well-controlled whenever $|u_D|$ is sizable. The relevant Chern insulator recently observed in rhombohedral pentalayer graphene was at electron filling $\nu = 1$, which suggests a flavor polarization into a single species. Therefore we assume polarization to a single valley and spin flavor.

We first consider $\theta = 0.77^\circ$ and $u_D = 50 \text{ meV}$, estimated to match the displacement field $D/\epsilon_0 = 0.81 \text{ V/nm}$ that stabilizes the QAH insulator experimentally¹. The single-particle band structure of moiré-distant electrons (Fig. 4.2(b)) *does not* have a direct gap above the first band. Within SCHF at $\nu = 1$ (Fig. 4.2(c)), we find interactions open a gap, where the

¹We estimate the conversion between D and u_D by comparing the reported HF phase diagram with the experiment in rhombohedral trilayer graphene [169, 206].

occupied band (red) has strictly positive Berry curvature (inset) and Chern number $|C| = 1$. We refer to this as the AHC phase, for reasons justified below. Its narrow 6 meV bandwidth and favorable quantum geometry, discussed below, make it eminently suitable for fractional topological states.

4.4 Phase Diagram at $\nu = 1$

Fig. 4.2(a,e) shows the phase diagram of moiré rhombohedral pentalayer graphene at filling $\nu = 1$. On the moiré-distant side $u_D > 0$, the AHC phase is stabilized over a broad range of twist angles and displacement fields near the experimentally relevant point (yellow star). Decreasing the displacement field drives a transition into a metallic phase, consistent with experiment [117]. Reducing the twist angle θ instead drives a transition to a $C = 0$ insulator that we call a “Wigner-like insulator” (WLI), based on its charge distribution $\rho(r)$. The band structures of a representative WLI state is shown in Fig. 4.2(g). The charge density of the state (Fig. 4.2(h)) shows that $\rho(r)$ varies strongly in the WLI, with peaks on a triangular lattice, reminiscent of a Wigner crystal. Its single-particle band structure in Fig. 4.2(f) reveals the origin of this charge density variation: at the γ point, the backfolded bands decrease in energy as θ decreases, bringing many within 30 meV of the minimum. These bands may then be strongly mixed by interactions, selecting the configuration that minimizes Hartree energy, i.e. a triangular lattice. Conversely, the AHC has a more uniform charge distribution without distinct peaks (Fig. 4.2(d)).

We comment briefly on the moiré-proximate side $u_D < 0$, where the dominant phase is a $C = 0$ insulator. Though consistent with experiment [117], we caution that this phase governed by details of V_{hBN} , and Fig. 4.3(b) shows that varying the moiré potential strength and phase can drive a transition to a metal or even a Chern insulator. Models incorporating lattice relaxation [190], other *ab initio* modelling [189, 207], and comparison with experiment [191] may be required here.²

4.5 Robustness of the Anomalous Hall Crystal

The AHC state is robust to a wide range of perturbations. In Fig. 4.3(c), we show the Chern number as a function of u_D and dielectric constant ϵ_r . The AHC state survives up to $\epsilon_r \sim 15$ for a range of u_D , showing that relatively weak interactions are sufficient to stabilize it. Fig. 4.3(a, d) shows the moiré-distant charge gap as a function of ϵ_r and moiré potential strength V_1 and phase ψ . The charge gap increases with interaction strength, but is essentially independent of the moiré potential. The charge gap is peaked near $u_D \approx 55$ meV at $\theta \approx 0.77^\circ$, despite the effective moiré potential decreasing monotonically with u_D .

²Near $u_D \approx 0$ valence bands, which we ignore, also become relevant; our model is most reliable for the moiré-distant regime $u_D > 0$.

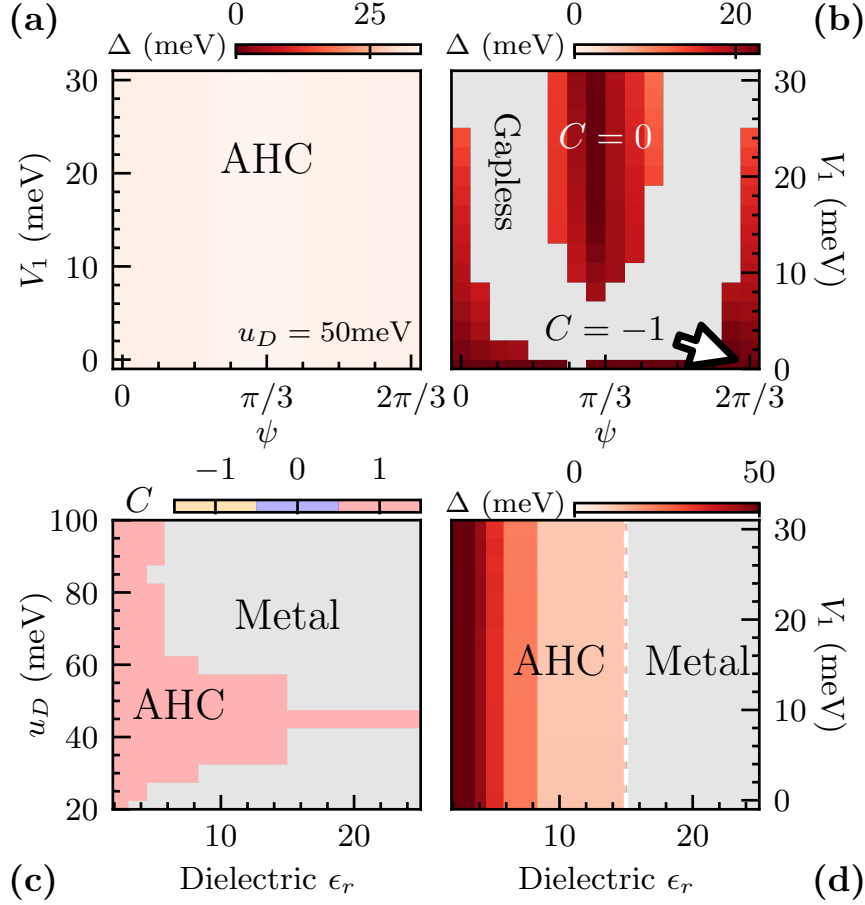


Figure 4.3: (a) The featureless charge gap of rhombohedral pentalayer graphene at $\nu = 1$ on the moiré-distant side ($u_D = 50$ meV) as the moiré strength V_1 and phase ψ vary. (b) Same on the moiré-proximate side ($u_D = -50$ meV), with a trivial insulator separated from a small Chern insulating phase by a metallic region. (c) The Chern number with respect to u_D and dielectric constant ϵ_r on the moiré-distant side, showing the AHC survives to relatively weak interaction strengths near $u_D \sim 50$ meV. (d) The charge gap at $u_D = 50$ meV versus moiré strength V_1 and dielectric ϵ_r . The AHC phase reaches $V_1 = 0$, demonstrating interaction-driven spontaneous translation symmetry breaking. All data from SCHF at $\theta = 0.77^\circ$.

(see Appendix C.2). Conversely, tuning V_1 and ψ changes the ground state on the moiré-proximate side (Fig 4.3(b)).

Remarkably, the AHC phase does not require a particular number of rhombohedral layers. Fig. 4.1(c) shows SCHF ground state at $\nu = 1$ for $N_L = 4 - 6$ layers, with an $|C| = 1$ AHC phase appearing in all cases at large u_D . Moreover, the critical u_D^* decreases significantly as the number of layers increases, easing the experimental requirement of a large displacement

field $D \propto u_D$. Finally, the phase diagram is robust to modelling differences in the hopping parameters of rhombohedral graphene. For instance, we show in the Supplemental Material that the AHC remains when all further neighbor hoppings $t_{i \geq 2}$ are set to zero.

4.6 Spontaneous translation symmetry breaking

The resilience of the $|C| = 1$ phase to the change in moiré potential raises a natural question: Is the moiré potential necessary at all for stabilizing the state? We now argue that within SCHF the ground state is an anomalous Hall crystal [202, 203] that spontaneously breaks translation symmetry.

We consider the Hamiltonian with *zero* moiré potential. Under this condition, SCHF calculations at $n \approx 0.93 \times 10^{12} \text{cm}^{-2}$ find a ground state with *spontaneously* broken graphene translation symmetry, which has much lower energy than (metallic) graphene-translation symmetric states when $u_D > 25 \text{meV}$ (Fig. 4.1(b)). We note that the AHC state is most stable compared to the metallic phase around $u_D = 55 \text{meV}$, which is consistent with our estimate for the experimental displacement field and where the charge gap reaches maximum.

The AHC state is a compressible state in the clean limit, since the lattice constant can change continuously. However, a small spatially-varying potential or disorder can pin its periodicity [203], whereupon its nontrivial Chern number can be revealed through the Streda formula and Hall conductance. This is likely the role played by moiré potential in experiment [117]: both the topology and the charge gap of the ground state are determined by the interaction effects that are already present in the moiré-less limit, but the moiré pinning field stabilizes the crystal at $\nu = 1$.

4.7 Fractional quantum anomalous Hall (FQAH) effect

One of the main features of the experimental discovery [117] was a full series of FQAH states found at fractional fillings in the absence of magnetic field. Employing exact diagonalization (ED) and density matrix renormalization group (DMRG) calculations, here we numerically confirm that partially filling the Chern band generated by the AHC gives us FQAH states.

Recent progress on the study of FCI phases has emphasized the role of quantum geometry [70, 152, 209–223], in addition to flat dispersion [193–195, 224–226]. Small trace condition violation $T = \int d^2\mathbf{k} (\text{Tr}(g_{\text{FS}}(\mathbf{k})) - \Omega(\mathbf{k}))$ gives a band suitable for finding FCIs. Here, $g_{\text{FS}}(\mathbf{k})$ is the Fubini-Study metric, and $\Omega(\mathbf{k})$ is the Berry curvature. The AHC band has both flat bandwidth and relatively small trace condition violation (Fig. 4.4(a)), making it likely to host FQAH phases. Indeed we find that a Laughlin state appears at $\nu = 2/3$ of the AHC band, with clear signatures from both ED (Fig 4.4(b)) and DMRG calculations (Fig 4.4(d)). These calculations (see Appendix C.3) are done in the many-body Hilbert space

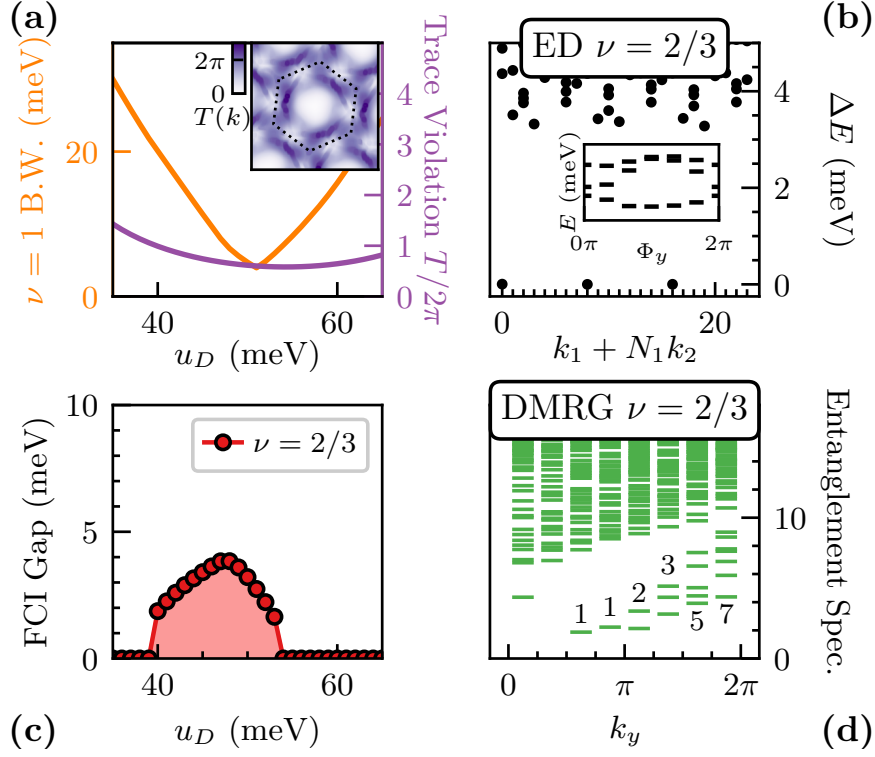


Figure 4.4: (a) Band conditions of the AHC phase as a function of u_D . Both the bandwidth and the violation of trace condition are minimized near $u_D = 50$ meV. (b) Many-body spectrum from ED on a 4×6 system at $\nu = 2/3$. Inset: spectral flow of the three degenerate ground states, a signature of the FCI ground state [193–195]. (c) The FCI gap at $\nu = 2/3$ as a function of u_D obtained in ED. The FCI gap is nonzero around 40 to 55 meV, and gives way to metals beyond this regime due to large bandwidths. (d) Entanglement spectrum obtained in DMRG at $\nu = 2/3$ with $L_y = 8$. The partition number counting of states below the entanglement gap is consistent with the chiral edge modes associated with the Laughlin states, confirming the state is an FCI [208]. Parameters: $(u_D, \theta) = (50 \text{ meV}, 0.77^\circ)$ unless specified.

of the lowest SCHF band at $\nu = 1$, assuming spin and valley polarization, which numerically biases the formation of fractional topological states. The FQAH phase yields to a competing metallic phase at small and large u_D (Fig 4.4(c)). The FQAH state is likely a ground state in the spin- and valley-polarized sector. Similar to the case in the lowest Landau level [227–229], this state is likely in competition with a spin-unpolarized state, which merits future investigation.

Examining the stability of the FQAH phases down to the zero moiré potential limit is an excellent topic for future studies, where we expect competition between an FQAH phase

with the same unit cell size, versus Wigner or anomalous Hall crystals with larger unit cells. Experimentally, the existence of the $\nu = 2/3$ plateau points to the realization of the former scenario, at least in the weak moiré potential limit, while a profusion of insulating states at smaller densities [117] might be due to the latter scenario.

4.8 Discussion

We have demonstrated the existence of the AHC phase within SCHF calculations. While such a phase can be stabilized *in principle*, SCHF is known to overestimate the tendency to crystallize, for example in Wigner crystals [230]. Pinpointing the location of the phase boundary between the AHC and the metal with more sophisticated techniques (just as variational Monte Carlo is used in the jellium model [231–233]) is left to future work. We note that the AHC phase at the optimal u_D survives even after decreasing the interaction strength by a factor of three (Fig. 4.3(c,d)), hinting at the robustness of the phase beyond mean-field theory.

The interpretation of the Chern state as an AHC clarifies an experimental mystery. Experimental phase diagrams in [117] are strongly asymmetric between positive and negative displacement fields D , suggesting that the hBN is only aligned on one side (Fig. 4.1(a)). Comparing experimental data at $\nu = 4$ [117] to SCHF calculations of the charge gap (see Appendix C.2.5), we independently infer that Chern insulator appears when the electrons are polarized away from the hBN potential (moiré-distant) instead of towards the hBN potential (moiré-proximate). We also predict that AHC in samples without moiré would have a characteristic density pattern and $\sigma^{xy} = e^2/h$ over extended density ranges.

The ubiquity of the AHC phase in our phase diagram hints at a universal physical mechanism stabilizing the formation of a Chern band, while the relatively uniform charge density of the AHC state points to a translation-breaking mechanism different from that of the Wigner crystal. A deeper analytic understanding of the origin of the AHC phase is clearly needed, which will be addressed in a forthcoming work [234].

Chapter 5

Exciton-condensate Josephson junction in graphene-based quantum Hall heterostructures

5.1 Introduction

Exciton condensate (EC) is a coherent state of electron-hole pairs predicted to exhibit many of the same phenomena as superconductivity, and its experimental demonstration remains a central pursuit in condensed matter physics [235–237]. This phase was first realized in semiconductor quantum Hall bilayer systems at unit filling [238–240], where excitons are formed by binding electrons in one layer with holes in the other. Clear evidence of dissipationless exciton transport has been observed in terms of zero resistance counterflow and perfect Coulomb drag [241, 242], in analogy to the superflow in superconductors. More recently, the EC has also been realized in van der Waals (vdW) heterostructures, such as quantum-Hall graphene bilayers [243–245] and transition metal dichalcogenides (TMD) bilayers [246–248].

Despite this progress, EC systems have yet to demonstrate signatures of macroscopic phase coherence, which in superconductors has been robustly evidenced by the Meissner effect and the Josephson effect. Although beautiful early studies of interlayer tunneling [249, 250] have identified a zero-bias conductance peak suggestive of the DC Josephson effect, discrepancies with theoretical expectations, possibly due to disorders and resistive contacts, remains to be resolved [240]. Here, we propose the in-plane Josephson junction in exciton condensates [251–254] as an ideal platform to verify the phase coherent nature of EC.

A major finding of our work is that the mechanism of excitonic Josephson coupling can differ significantly from that in superconductors, where it is mediated by electron tunneling across the junction. Due to the quenched kinetic energy of electrons in a strong magnetic field, such tunneling is greatly suppressed in quantum Hall systems — in fact, in a clean system such tunneling is forbidden by the conservation of guiding center coordinate. Previous

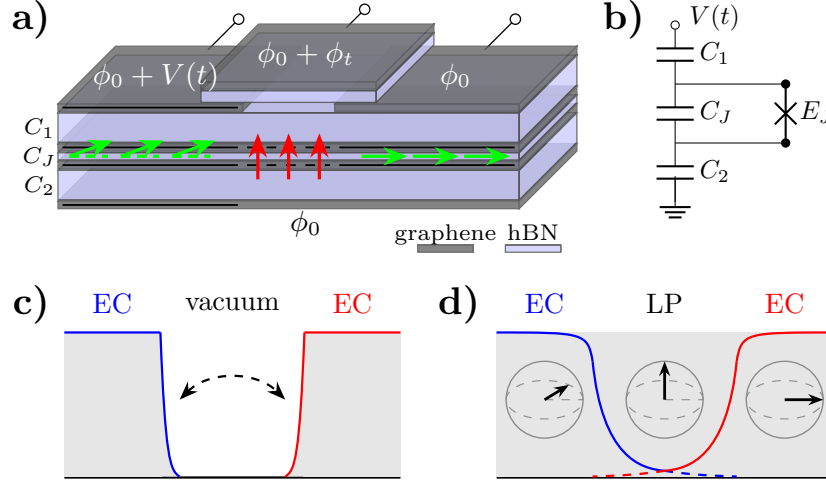


Figure 5.1: (a) Sketch of the proposed device. Dark and light slabs represent graphene (conductor) and hBN (insulator). The arrows denote the layer-pseudospin $\mathbf{m}$ orientation of the bilayer electron wavefunction at filling $\nu = 1$ of the zeroth Landau level (see Eq. (5.1)): In-plane (green) and vertical (red) arrows represent the exciton condensate (EC) and the layer-polarized state (LP) respectively. (b) Lumped-element model of the device, with each element schematic drawn in (a): C_J denotes the capacitance of electron bilayers, and E_J denotes the EC Josephson coupling energy. $V(t)$ denotes the left-gate probe voltage capacitively coupled to the bilayer via $C_{1,2}$. (c-d) Comparison of two mechanisms of EC Josephson coupling: by tunneling excitons in vacuum junctions (c), and by in-plane canted pseudospin in layer-polarized junctions (d). The height of the shade and the solid lines at each point denote the electron filling and EC order magnitude respectively.

proposals for in-plane Josephson junctions thus relied on disorder [251], which is thought to be minimal in the gate-defined structures relevant to present vdW devices [255]. Taking advantage of recent progress in fabricating gate-defined clean edges in vdW bilayers, we design a new type of exciton Josephson junction. We show that the exciton Josephson coupling can be established from the canting of electron layer polarization in the quantum Hall ferromagnet [256]. This mechanism does not rely on disorder and can be tuned via gate voltages, allowing the practical realization of a measurable EC Josephson effect in a clean quantum-Hall system.

The design of the junction is shown in Fig. 5.1(a): two spatially separated ECs sandwich a junction region above which a split top-gate is used to apply a perpendicular displacement field, where the Josephson coupling is established and controlled. Much of this work is devoted to estimating the Josephson coupling in this setup. We apply the Hartree-Fock (HF) approximation, or equivalently, a non-linear sigma model (NLsM) analysis to show that the Josephson coupling is highly tunable. Using this theory we propose a realistic design

of an exciton-condensate Josephson junction embedded in an LC resonant circuit, where the Josephson effect can be measured directly through counterflow current or indirectly by measuring the AC impedance of the gates. In particular, the oscillation frequency covers the microwave regime that is within the experimental reach.

5.2 Device and measurement protocols

We consider a bilayer quantum Hall system with negligible interlayer hopping and gate-screened Coulomb interactions [256–258]. The layer degrees of freedom can be viewed as a pseudospin, and we use $\pm$ to label the two layers. There are two separately conserved charge $U(1)$ symmetries associated with the total electron number $N_+ + N_-$ and the layer charge polarization $N_+ - N_-$. Throughout the bulk of our discussion, we focus on the unit total filling and assume that electrons stay within the zeroth Landau level (zLL). Without interactions, there would be a huge pseudospin degeneracy at total filling one. It is well known that the exchange effect from Coulomb interaction completely polarizes the pseudospin [259]. Moreover, the finite layer separation favors the in-plane polarization, namely an equal-weight superposition of the two layers, which spontaneously breaks the conservation of $N_+ - N_-$. The system thus enters the EC phase. Using $c_{+,k}$ ($c_{-,k}$) as the fermion operator for the k -th orbital of the zLL in the up (down) layer, the EC state can be well approximated by the following Slater determinant

$$|\mathbf{m}(\theta, \varphi)\rangle = \prod_k \left(\cos \frac{\theta}{2} c_{+,k}^\dagger + e^{i\varphi} \sin \frac{\theta}{2} c_{-,k}^\dagger \right) |0\rangle. \quad (5.1)$$

Here $\theta \in [0, \pi]$ measures the layer polarization and can be adjusted by applying a perpendicular displacement field, while φ characterizes the macroscopic EC phase which governs the Josephson effect. We introduce a pseudospin variable $\mathbf{m} = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta)$ to describe the charge polarization and interlayer phase coherence. The dynamics of the pseudospin is the only active degree of freedom within the variational manifold spanned by Eq. (5.1) and will play an important role in our later discussion.

We propose to realize an EC Josephson junction using the split top gate depicted in Fig. 5.1(a). Structures of this sort have been recently used, for example, to define tunable quantum point contacts [260, 261] with a junction width of 50–100 nm. The bottom gate and the split top gates to the left and right are held at equal voltages, giving rise to layer-balanced ECs [243, 244]; let this condition define the left / right top-gate voltage ϕ_0 . A small additional voltage ϕ_t is then applied to the middle top gate, increasing both the chemical potential and the displacement field along a strip in the 2DEG below. Because of the large integer quantum Hall gap ($\Delta \sim 10$ meV) at filling $\nu_T = 1$ [245], there is a range of ϕ_t where $\nu_T = 1$ remains unchanged, while the displacement field creates a layer-polarized strip between the two ECs which will define the “tunneling barrier” of our Josephson junction. We will discuss the relevant range of ϕ_t quantitatively in later sections.

Similar to the Cooper pair box, we can interpret our device as an LC circuit where the two ECs act as a single capacitor and the junction as an inductor (Fig. 5.1(b))¹. We can translate between the superconductor and the EC cases by mapping charge to layer polarization, voltage to layer voltage differences, and current to counter-flow current. This lumped-element model is applicable at low probe frequency $\nu \ll v/L_x$, with v the velocity of EC phase variation and L_x the size of EC islands; in this limit the EC phase gradient within the bulk is negligible (see Appendix D.2 for an analysis without this assumption).

The total energy of the lumped-element device depends on EC layer polarization $N_x = (N_+ - N_-)/2$ and EC phase difference φ across the junction:

$$E[N_x, \varphi] = \frac{d_\ell}{2d_g} N_x e V(t) + \frac{e^2}{2C_J} N_x^2 - E_J \cos \varphi. \quad (5.2)$$

Here d_ℓ is the distance of bilayer separation, $d_g \gg d_\ell$ is the distance between the bilayers and the top/bottom gates, $V(t)$ is the extra voltage applied on the left top gate, C_J is the effective bilayer capacitance, and E_J is the Josephson coupling energy. Curiously, C_J is larger than its geometric capacitance due to the exchange interaction in EC states, proportional to $\ell_B d_\ell^{-2}$ instead of d_ℓ^{-1} [256], which amplifies the response of the circuit. The device has a resonant frequency in response to $V(t)$

$$\nu_J = e \sqrt{E_J / C_J} / \hbar, \quad (5.3)$$

which can be probed by both conductance and capacitance measurements.

If layer-resolved contacts with the device can be established, we can connect the two layers of the right island and keep the left one floating (here C_J only includes the left EC island). We can then read out the current oscillation $I_J(t)$ across the contacts with an AC driving displacement potential $V(t) = V_1 \cos(2\pi\nu t)$:

$$\begin{aligned} \dot{Q}_J(t) &= I_J(t) = \frac{e}{\hbar} E_J \sin \varphi_J(t) \\ \dot{\varphi}_J(t) &= \frac{e}{\hbar} \left(\frac{d_\ell}{2d_g} V(t) - \frac{Q_J(t)}{C_J} \right) \end{aligned} \quad (5.4)$$

Here $Q_J = eN_x$ and $\varphi_J = \varphi$ compared to Eq. (5.2). For $I_J \ll eE_J/\hbar$ we may take $\sin \varphi_J \approx \varphi_J$ and obtain its frequency dependence, which diverges at $\nu = \nu_J$:

$$I_J(\nu) = \frac{2\pi\nu C_J}{1 - (\nu/\nu_J)^2} \frac{d_\ell}{2d_g} V_1. \quad (5.5)$$

The result is valid for $\frac{d_\ell}{d_g} e V_1 \ll \left| \frac{1 - (\nu/\nu_J)^2}{\nu/\nu_J} \right| \hbar \nu_J$.

¹We note that a single capacitor C_J can describe the layer polarization energy in both EC islands: for a fixed charge number in each layer, the layer polarization of two ECs will be equal and opposite, and C_J will be equal to the series-connected sum of their capacitances.

If good contacts are unavailable as in TMD devices, one can probe the frequency-dependent gate capacitance $\tilde{C}_g(\nu) = Q_g(\nu)/V(\nu)$ of the left gates sandwiching the EC island. Compared to the geometric capacitance C_g , we will again observe a singular response at $\nu = \nu_J$:

$$\tilde{C}_g(\nu) \sim C_g \left(1 + \frac{\ell_B}{d_g} \frac{1}{1 - (\nu/\nu_J)^2} \right) \quad (5.6)$$

Such a response can be measured, for example, by reflectometry measurements of the top gate [262].

5.3 Pseudospin-mediated Josephson coupling

The microscopic mechanism of Josephson coupling E_J in our design differs from that of superconducting ones. In a superconductor, the Josephson coupling originates from the single-electron hopping across the junction, a mechanism inapplicable to the quantum Hall EC in the absence of disorder. This can be seen from zLL wave functions in the Landau gauge $\psi(x, y) \propto e^{ik_y y - (x - k_y \ell_B^2)^2 / 2\ell_B^2}$, where we choose y direction to run parallel to the junction. In clean samples, electrons centered at different positions x have different conserved momentum k_y , which forbids their direct hopping across a junction. What is allowed instead is the electron-hole pair (exciton) hopping generated by Coulomb interaction, which is the only source of Josephson coupling when the junction region has zero filling (Fig. 5.1(c)). However, the amplitude of this process is proportional to the overlap between Landau orbitals from two sides, which decays as a Gaussian in the width of the junction L_J , i.e. $E_J \sim e^{-L_J^2 / 2\ell_B^2}$. We thus expect such coupling to be negligible in realistic experimental setups with junction width of several tens of nm, i.e. at least a few magnetic lengths.

The Josephson coupling proposed here instead originates when the junction is kept at the same integer filling as the EC, through the dynamics of the pseudospin. Specifically, we choose appropriate gate voltages such that the pseudospin stays within the xy -plane in the two EC regions and is *almost* polarized along the z -axis inside the junction. We know from the theory of quantum-Hall ferromagnetism that the pseudospin must vary smoothly in space in order to minimize the Coulomb energy [259]. Therefore, the pseudospin inside the junction will always have a small in-plane component coupling the exciton phase to the left / right of the junction, mediating a Josephson coupling (Fig. 5.1(d)). Unlike exciton-mediated coupling, we will show that in this case $E_J \sim e^{-L_J/\xi}$, where ξ is tunable by the displacement field, and can yield an experimentally feasible Josephson effect.

To develop our intuition, we first estimate E_J with a simplified phenomenological model. This model can be derived by applying the HF approximation of the realistic system, including the details of the split-gate electrostatics, which is the focus of the next section (see Appendix D.1 for details). In the case of unit filling, the HF description is equivalent to a non-linear sigma model (NLsM) of the layer pseudospin $\mathbf{m}$, which is the only remaining degree of freedom in question. Using L_y as the length along the y direction and L_J as the junction width, and assuming translation invariance along the y direction and slow spatial

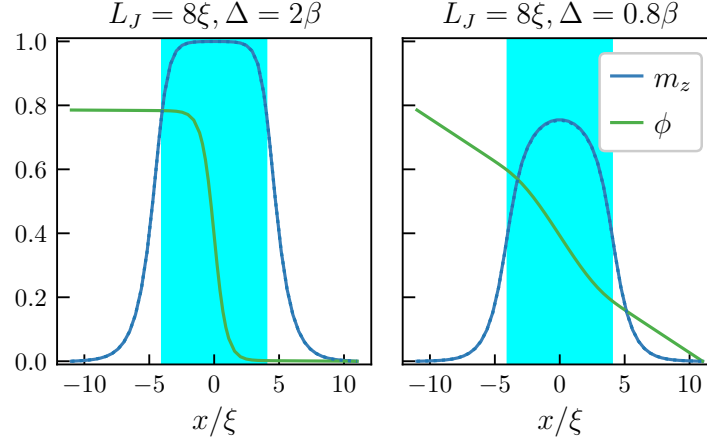


Figure 5.2: Comparison between weakly and strongly linked Josephson junction, with phase difference $(\varphi_L, \varphi_R) = (\pi/4, 0)$ controlled by the layer-polarizing potential $\Delta(x) = 0$ outside the junction and $\Delta(x) = \Delta$ within. In weakly linked junctions ($\Delta = 2\beta$ is large), $\varphi(x)$ remains constant in each island and sharply changes within the junction; In strongly linked junctions (smaller $\Delta = 0.8\beta$), $\varphi(x)$ varies smoothly from φ_L to φ_R across the junction.

variation of $\mathbf{m}$, the minimal action reads [256, 258]

$$\frac{E[\mathbf{m}]}{L_y} = \int dx \frac{\rho_{xy}}{2} [(\partial_x m_x)^2 + (\partial_x m_y)^2] + \frac{\rho_z}{2} (\partial_x m_z)^2 + \frac{\beta}{2} m_z^2 - \Delta(x) m_z. \quad (5.7)$$

Physically, ρ_{xy} and ρ_z are the stiffness of in-plane and out-of-plane pseudospin fluctuation, and β is the capacitance energy per unit area. These three terms are determined by the Coulomb interaction. Meanwhile, $\Delta(x)$ is a layer-polarizing potential applied by the displacement field, taking a nonzero value Δ inside the junction and zero outside. We comment that the NLsM reproduce the lumped-element model in Eq. (5.2), for example $C_J = \frac{e^2 A}{(4\pi\ell_B^2)^2 \beta}$ given by uniform $\mathbf{m}$ within the $\Delta(x) = 0$ region (see Appendix D.2 for details).

The performance of the Josephson junction is highly susceptible to the strength of Δ . To see that, we numerically solve for $\mathbf{m}(x)$ with fixed boundary configurations: $\mathbf{m}^L = (\cos \varphi, \sin \varphi, 0)$, $\mathbf{m}^R = (1, 0, 0)$, which represents the two EC islands with different phases. Fig. 5.2 illustrates two distinct behaviors at different Δ : For a weak polarizing potential $|\Delta| < \beta$, the junction itself remains an exciton condensate ($m_z < 1$), albeit with a smaller phase stiffness, across which the EC phase varies smoothly (Fig. 5.2(b)). In this case the Josephson coupling is too strong to identify a well-defined junction. When the polarizing potential is sufficiently large, $|\Delta| > \beta$, the pseudospin within the junction quickly polarizes to $m_z = 1$, and the EC phase exhibits a sharp jump at its center (Fig. 5.2(a)). Here the

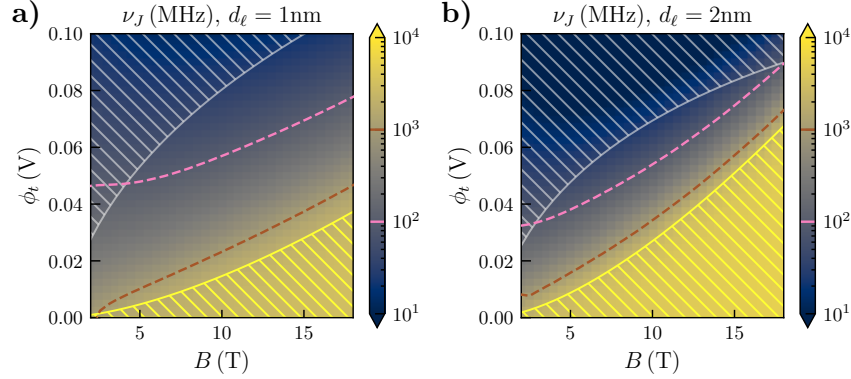


Figure 5.3: Resonant frequency $\nu_J(B, \phi_t)$ for $B \in (2, 18)$ T and $\phi_t \in (0, 0.1)$ V. Device parameters: gate distance $d_g = 25$ nm, junction width $L_J = 250$ nm, island area size $L_x = L_y = 5$ μ m, dielectric constant $\epsilon = 4\epsilon_0$, with two different layer distances: (a) $d_\ell = 1$ nm and (b) $d_\ell = 2$ nm. The white and yellow shaded regions correspond to the upper and lower bound in Eq. (5.10). The pink and red dashed lines are the contours of 100 MHz and 1000 MHz.

Josephson coupling depends exponentially on the junction length L_J (see Appendix D.1.4):

$$E_J \simeq 2\rho_{xy}L_y\xi^{-1}e^{-L_J/\xi}. \quad (5.8)$$

with an emergent coherence length $\xi = \sqrt{\frac{\rho_{xy}}{\Delta - \beta}}$. The result has two significant differences from the one of exciton hopping: (1) It decays single-exponentially regarding L_J , which can naturally be much larger than the case of a $\nu = 0$ junction. (2) ξ is not solely tied to the magnetic length, but continuously tunable by the displacement field, contributing to the high tunability of the proposed device.

5.4 Optimal regime of Josephson effect

We now compute the Josephson energy E_J for the graphene-hBN-graphene heterostructure as a concrete example, and estimate the optimal regime for observing the Josephson effect. As shown in Fig. 5.1(a) there are three tuning parameters: the bottom gate voltage ϕ_0 , the middle top gate voltage ϕ_t , and the magnetic field B . The electrons in the zLL of the graphene heterostructure have eight flavors: two layers $\pm$, two valleys K, K' , and two spins $\uparrow / \downarrow$. We assume an hBN sublattice splitting and Zeeman energy that can fully gap out the valley and spin sectors [263], thus we keep only one valley and one spin per layer in the low-energy manifold. The Hamiltonian includes gate-screened Coulomb interactions

and electrostatic potentials from ϕ_0 and ϕ_t :

$$H = \sum_{a,b} \int d\mathbf{r}_1 d\mathbf{r}_2 V_{ab}(\mathbf{r}_1 - \mathbf{r}_2) n_a(\mathbf{r}_1) n_b(\mathbf{r}_2) + \sum_a \int d\mathbf{r} U_a(\mathbf{r}) n_a(\mathbf{r}) \quad (5.9)$$

where n_a is the electron density in layer $a = \pm$. Both $V_{ab}(\mathbf{r})$ and $U_a(\mathbf{r})$ are obtained by solving the Poisson equation within the split-gate device geometry (see Appendix D.1.3), assuming translational invariance along the junction.

For each set of parameters, we solve the Hamiltonian within the HF approximation (see Appendix D.1), which at unit filling (with properly chosen ϕ_0) is approximately equivalent to solving the NLsM in Eq. (5.7). To extract E_J , we work on a torus geometry and thread $\pm\varphi/2$ flux through the x -cycle of the top/bottom layer, effectively introducing a twist in the EC phase across the junction. Using HF to obtain the resulting energy $E[\varphi]$, for weak junctions the data is well fit to the form $E_J \cos \varphi$ from which we infer E_J . Meanwhile, we determine C_J analytically from HF parameters as demonstrated in NLsM, and finally compute the resonant frequency $\nu_J = e\sqrt{E_J/C_J}/h$ featured in the proposed measurements.

Fig. 5.3 shows $\nu_J(B, \phi_t)$ as a function of ϕ_t and B with a set of realistic device parameters. The desired junction is realized only within the unshaded region, which we will clarify shortly. Regardless, this region already realizes ν_J across three orders of magnitude in frequency, and between the pink and red lines, which covers the microwave regime $\nu_J \in (100, 1000)$ MHz, is where the proposed effect is most accessible in experiments.

The yellow/white-shaded regions in the above phase diagram denote the realistic constraints on our tuning parameters: For given B , ϕ_t is lower bounded by the condition $\Delta > \beta$ of fully layer-polarizing the junction, and upper bounded by our requirement of $\nu = 1$ total filling. As is detailed in Appendix D.1.5, in the limit $d_\ell/d_g \ll 1$ we have the following range of ϕ_t for optimally chosen ϕ_0 :

$$\sqrt{\pi/2} d_\ell d_g / \ell_B^2 < e\phi_t / E_c < \sqrt{2\pi} - 2d_\ell / \ell_B, \quad (5.10)$$

where $E_c = \frac{e^2}{4\pi\epsilon\ell_B}$ is Coulomb energy scale of EC. Here we ignore the hBN potential and Zeeman energy, thus the charge gap is given only by the Coulomb interaction; including other terms only makes the conditions easier to satisfy. We conclude that small d_ℓ gives a parametrically large range of ϕ_t , but note that the HF approximation tends to overestimate the charge gap, which can lead to a smaller allowed range of ϕ_t than the simple estimate here.

5.5 Discussion

Our proposal focuses on the interlayer EC in quantum Hall graphene heterostructures at unit filling, but it can also directly apply to other bilayer vdW heterostructures [246] and cases where the junction at different electron fillings from the EC islands, e.g. between $\nu = 1$ EC and $\nu = 2$ junction. Notably, bilayer EC can potentially be realized at zero magnetic

fields [247, 248]. Despite the absence of Landau level and pseudospin description, we can consider the strength of Josephson coupling to be tunable by the exciton density inside the junction. We leave the detailed analysis of such devices to future work.

The observation of EC Josephson effect in experiments can be influenced by the presence of interlayer tunneling [249, 264–270]. It is favorable to observe the in-plane Josephson effect in the absence of tunneling events, which can be suppressed in vdW bilayers by twisting them at a finite angle to offset electron momentum. However, intrinsic disorders in vdW materials may also contribute to electron tunneling, and it will be important to understand their consequences in realistic experiments.

Beyond demonstrating macroscopic phase coherence, the EC Josephson junction could offer utility as a circuit element in quantum-Hall setups where superconductivity cannot survive. For example, it might provide a high-Q resonator for dispersive readout of the charge state of an FQH state in a layer below. To this end, it would be useful for future theoretical work to estimate the factors limiting the quality of the junction, such as the dissipative transport of gapped merons parallel to the junction and the effect of thermal fluctuation on phase coherence.

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Appendix A

Appendix to chapter 2

The Appendices to this chapter are organized as follows.

Appendix A.1 overviews insulators found in experiments at integer fillings of TBG.

Appendix A.2 shows how small strains on the graphene scale are amplified at the moiré scale.

Appendix A.3 is a self-contained description of the Hamiltonian and computational basis used in this chapter. This section also describes the “Hartree peak”.

Appendix A.4 gives numerical details of our DMRG computations, including the quantum number (τ^z, s^z) sectors used in the main text, and defines some common correlation functions.

Appendix A.5 is a brief analogy to the 1D Heisenberg model in the $s^z = 0$ sector, which highlights some features that appear in the $(0, 0)$ and $(1, 0)$ sector.

Appendix A.6 details the phases that appear at $\nu = -3$ *not* in the $(0, 0)$ sector and discusses their identification in the thin-cylinder limit.

A.6.1 the quantized anomalous Hall (QAH) phase, including its valley-polarized (QAH-VP) and intervalley-coherent (QAH-IVC) variant.

A.6.2 the compensated nematic semimetal (NSM) in the $(1, 1)$ sector.

A.6.3 the commensurate spin spiral (CSS) order in the $(1, 0)$ sector.

A.6.4 the spin-polarized IKS order in the $(0, 1)$ sector.

Appendix A.7 details the phases that appear in the $(0, 0)$ sector.

A.7.1 the symmetric Fermi liquid (FL) at intermediate strains in the $(0, 0)$ sector, both in DMRG and its manifestation within self-consistent Hartree-Fock.

A.7.2 the spinful IKS order in the $(0, 0)$ sector at $\varepsilon_{\text{Gr}} = 0.05\%$.

A.7.3 aspects of the “mixed” order at low strain in the $(0, 0)$ sector.

A.7.4 The putative phase diagram of $\nu = -3$ as a function of ε_{Gr} , including higher-strain data, and comparison with other charge sectors.

A.1 Overview of TBG Experiments at integer fillings

This appendix reviews measurements of integer filling states in TBG at zero field and without hBN-alignment. We focus on correlated insulating (CoI) states, and consider three broad classes of experimental probes:

Transport measurements Direct measurements of resistance ρ_{xx} . Correlated insulators manifest as a peak in resistance. As these measurements go across the entire sample, they are affected by sample inhomogeneity (strain, twist angle disorder, etc). This tends to suppress the signals associated with insulating states relative to local probes.

STM By measuring the local density of states above a state at a given filling as a function of bias voltage, STM can directly measure the one-electron gaps. Some experiments use point-contact spectroscopy to distinguish superconductors (SC) from correlated insulators.

SET Single electron transistors are a local probe that directly measures the inverse compressibility $\frac{d\mu}{dn}$. Insulating states appear as peaks in $\frac{d\mu}{dn}$, which may be integrated to estimate the spectral gap. SET measurements can be used to infer where flavor polarization occurs.

Table A.1 gives a non-exhaustive overview of experimental results at all integer fillings. As discussed in the introduction, the results display a strong particle-hole breaking pattern, especially at filling $\nu = \pm 3$.

A.2 Effect of Strain on the Moiré Superlattice

This appendix shows how heterostrain acts on the moiré superlattice of twisted bilayer graphene. We will conclude that its effect is enhanced by a factor of the inverse of twist angle.

Consider two layers of graphene ($\ell = \pm$) with opposite twist angle $\theta_\ell = \ell\theta/2$ and uniaxial strain $\varepsilon_\ell = \ell\varepsilon/2$. Suppose $\mathbf{R}_i$ are the lattice vectors of graphene and $\mathbf{G}_j$ are the corresponding reciprocal lattice vectors so that $\mathbf{R}_i \cdot \mathbf{G}_j = 2\pi\delta_{ij}$. The twisted lattices on each layer are then given by

$$\mathbf{R}_i^\ell = R(\theta_\ell)S(\varepsilon_\ell)\mathbf{R}_i, \quad i = 1, 2, \quad (\text{A.1})$$

where R, S are matrix representations of rotation and strain operation:

$$R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}, \quad S(\varepsilon) = \begin{pmatrix} 1 + \varepsilon & 0 \\ 0 & 1 - \nu\varepsilon \end{pmatrix}, \quad (\text{A.2})$$

Report	θ (°)	Gate type	D (nm)	-3	-2	-1	0	1	2	3	Notes
Transport											
Ref. [10]	1.10	single	10	(CoI)	CoI	(CoI)	CoI	CoI	CoI	CoI	16 mK
Ref. [11], D1	1.15	single	7				CoI				25 mK
Ref. [11], D2	1.04	single	9.8				CoI		(CoI)		25 mK
Ref. [11], D3	1.10	single	12.5		CoI		CoI	(CoI)	CoI	CoI	25 mK
Ref. [12]	1.04	single	9.5	SC			CoI		(SC)	CoI	40 mK
Ref. [13]	1.08	single	7		CoI		CoI	“ChI”	CoI	CoI	30 mK
Ref. [14], D1	1.08	single	10-30		CoI		CoI		CoI		300 mK
Ref. [14], D2	1.10	single	10-30		(CoI)		CoI		CoI		300 mK
Ref. [14], D3	1.12	single	10-30		CoI				CoI	(CoI)	100 mK
Ref. [14], D4	1.16	single	10-30		CoI		CoI		CoI	(CoI)	300 mK
Ref. [15]	~ 1.07	single	42		CoI		CoI		CoI	CoI	50 mK
Ref. [16]	1.07	dual	?		CoI		CoI	(CoI)	CoI	CoI	70 mK
Ref. [17], DA	1.09	single	50		CoI		CoI	(CoI)	CoI	CoI	70 mK
Ref. [18], D1	1.14	dual	30-60		(CoI)		CoI		CoI	CoI	10 mK
Ref. [18], D3	1.10	dual	30-60	CoI	CoI		CoI		CoI	CoI	300 mK
Ref. [18], D5	1.08	dual	30-60		CoI		CoI	(CoI)	CoI	CoI	10 mK
Ref. [19], D1	1.08	single	68		CoI		CoI	(CoI)	CoI	CoI	50 mK
Ref. [19], D2	1.09	single	6.7		CoI		CoI		CoI	CoI	50 mK
Ref. [19], D3	1.04	single	38				CoI		CoI	CoI	50 mK
Ref. [19], D4	1.18	single	7.5				CoI				50 mK
Ref. [19], D5 ([271])	1.12	single	45 (40)		CoI		CoI		CoI	CoI	10 mK
STM											
Ref. [20]([21], DB)	1.06	STM tip	-	(SC)	CoI	CoI	CoI	CoI	CoI	CoI	$\varepsilon_{\text{Gr}} = 0.1\%$
Ref. [21], DA	1.13	STM tip	-	SC	CoI		CoI		CoI	CoI	$\varepsilon_{\text{Gr}} = 0.4\%$
Ref. [21], DA'	1.01	STM tip	-	SC	CoI		CoI		CoI	CoI	$\varepsilon_{\text{Gr}} = 0.2\%$
Ref. [22]	$1.27 \rightarrow 0.97$	STM tip	-		CoI		CoI	(CoI)	CoI	CoI	$\varepsilon_{\text{Gr}} < 0.3\%$
Ref. [22] (Supp.)	$1.26 \rightarrow 0.99$	STM tip	-		CoI		CoI	CoI	CoI	CoI	
SET											
Ref. [15]	1.13	single	42	(CoI)	(CoI)	(CoI)	-	CoI	CoI	CoI	4 K
Ref. [23]	1.06	single	40		(CoI)		CoI	-	CoI	CoI	330 mK

Table A.1: An overview of integer filling states in TBG visible in selected experimental data. This list is non-exhaustive and is restricted to samples not aligned to hBN and without an applied magnetic field. Correlated insulators (CoI), superconductors (SC), and Chern insulators (ChI), are observed at the labeled integer fillings. If an insulator at filling $+\nu$ is substantially weaker than those at other fillings, in particular its particle-hole partner at $-\nu$, then it is shown in parentheses, e.g. as “(CoI)”.

where $\nu = 0.16$ is the Poisson ratio of graphene.

For $\theta, \varepsilon \ll 1$, this is approximated to leading order by

$$\mathbf{R}_i^\ell \approx M(\theta_\ell, \varepsilon_\ell) \mathbf{R}_i; \quad M(\theta, \varepsilon) = \begin{pmatrix} 1 + \varepsilon & -\theta \\ \theta & 1 - \nu\varepsilon \end{pmatrix}. \quad (\text{A.3})$$

Similarly, the reciprocal lattice vectors of each layer are

$$\mathbf{G}_i^\ell \approx [M^{-1}(\theta_\ell, -\varepsilon_\ell)]^T \mathbf{G}_i = M(\theta_\ell, -\varepsilon_\ell) \mathbf{G}_i. \quad (\text{A.4})$$

The moiré superlattice of the two layers has a reciprocal lattice

$$\mathbf{g}_i = \mathbf{G}_i^+ - \mathbf{G}_i^- = (M(\theta/2, -\varepsilon/2) - M(-\theta/2, \varepsilon/2)) \mathbf{G}_i = \begin{pmatrix} -\varepsilon & -\theta \\ \theta & \nu\varepsilon \end{pmatrix} \mathbf{G}_i. \quad (\text{A.5})$$

Note that we can view the contribution of strain separately from the twist operation:

$$\mathbf{g}_i[\theta, \varepsilon] = \underbrace{\begin{pmatrix} 1 & -\varepsilon/\theta \\ -\nu\varepsilon/\theta & 1 \end{pmatrix}}_{\tilde{M}_\theta(\varepsilon)} \begin{pmatrix} 0 & -\theta \\ \theta & 0 \end{pmatrix} \mathbf{G}_i = \tilde{M}_\theta(\varepsilon) \mathbf{g}_i[\theta, 0]. \quad (\text{A.6})$$

Diagonalizing $\tilde{M}_\theta(\varepsilon)$, we can consider the effect of strain as a dilation on the moiré scale:

$$\tilde{S}_\theta(\varepsilon) = U \tilde{M}_\theta(\varepsilon) U^\dagger = \begin{pmatrix} 1 + \sqrt{\nu}\varepsilon/\theta & 0 \\ 0 & 1 - \sqrt{\nu}\varepsilon/\theta \end{pmatrix}, \quad (\text{A.7})$$

which acts on transformed reciprocal lattice vectors $\{\tilde{\mathbf{g}}_i = U \mathbf{g}_i\}$ and the corresponding superlattice basis $\{\tilde{\mathbf{r}}_i\}$.

$$\tilde{\mathbf{g}}_i[\theta, \varepsilon] = \tilde{S}_\theta(\varepsilon) \tilde{\mathbf{g}}_i[\theta, 0], \quad (\text{A.8})$$

$$\tilde{\mathbf{r}}_i[\theta, \varepsilon] = \tilde{S}_\theta^{-1}(\varepsilon) \tilde{\mathbf{r}}_i[\theta, 0]. \quad (\text{A.9})$$

Comparing Eq. (A.3) and (A.7), we conclude that heterostrain ε_{Gr} on graphene lattice is equivalent to an amplified strain

$$\varepsilon_{\text{moiré}} \propto \frac{\varepsilon_{\text{Gr}}}{\theta} \quad (\text{A.10})$$

on the moiré superlattice. In the experimentally relevant case of $\theta \sim 1^\circ$, $\varepsilon_{\text{Gr}} \sim 0.2\%$, we have $\varepsilon_{\text{moiré}} \sim 10\%$, which is not a negligible perturbation.

A.3 Microscopic Model of Strained TBG

This appendix describes the microscopic model of strained TBG used in the main text. This model is standard; it is essentially identical to the models used in Ref. [50], which introduced our DMRG method, and Refs. [38, 39] that studied strained TBG.

A.3.1 Single Particle Hamiltonian

Strained TBG is described at the single-particle level by a generalized Bistritzer-MacDonald Hamiltonian [38, 54, 55, 96]. Strain affects the Hamiltonian in two separate ways. First, as shown above, it distorts the lattice and superlattice. Second, it changes the inter-atomic distance between carbon atoms, thereby modulating the hopping integrals and changing the energetics directly. We incorporate both effects.

Within each layer $\ell = \pm$, we use the standard model of graphene:

$$h_{\text{Gr}}(\mathbf{k}) = -t \begin{pmatrix} 0 & D(\mathbf{k}) \\ D(\mathbf{k}) & 0 \end{pmatrix}, \quad D(\mathbf{k}) = \sum_{\mu=0}^2 e^{-i\mathbf{k} \cdot \boldsymbol{\tau}_\mu}, \quad (\text{A.11})$$

where $\boldsymbol{\tau}_\mu$ are the three vectors from A to B sublattices. We use $t = 2.8 \text{ eV}$ and lattice constant $a_{\text{Gr}} = 0.236 \text{ nm}$. At low energies, this model reduces to the Dirac equation $h(\mathbf{k})_{\tau=K} = v_F \boldsymbol{\sigma} \cdot (-i\hbar \nabla)$. A long line of work (see e.g. [38, 55, 58–67]) has shown that strain on the graphene scale is incorporated into the Dirac equation as an effective vector potential $-i\nabla \rightarrow -i\nabla + \mathbf{A}$, or $\mathbf{k} \rightarrow \mathbf{k} + \mathbf{A}$ in momentum space. For the K -valley, we have

$$h_{\ell=\pm, \tau=K}(\mathbf{k}) = h_{\text{Gr}}(M(\theta_\ell, -\epsilon_\ell)[\mathbf{k} + \mathbf{A}_{\ell, \tau}]), \quad \mathbf{A}_\ell = -\frac{\ell \beta \sqrt{3}}{2} \frac{1}{2a} ([1 - \nu_P]\epsilon, 0) \quad (\text{A.12})$$

where $M(\theta, \epsilon)$ is given in Eq. (A.3), $\sigma \in \{A, B\}$ label the graphene sublattices, $a = |\mathbf{R}_i|$ is the lattice constant of graphene, $\beta \approx 3.14$ characterizes how much the carbon-carbon hopping integral changes under lattice deformations, and $\nu_P \approx 0.16$ is the Poisson ratio of graphene. Crucially C_{3z} symmetry is broken by the lattice distortion, so the Dirac points are no longer pinned to the K/K' points and are shifted by $\mathbf{A}_\ell$ [38].

We now consider the morié superlattice with reciprocal lattice vectors $\mathbf{g}_i$ defined above. We choose conventions for graphene so that $\mathbf{g}_1$ is along the x -axis of reciprocal space (up to corrections from strain). In this setting, the BM model becomes (K -valley)

$$h_K = \begin{bmatrix} h_{+,K} & T(\mathbf{r}) \\ T(\mathbf{r})^\dagger & h_{-,K} \end{bmatrix}, \quad T(\mathbf{r}) = T_0 + T_1 e^{-i\mathbf{g}_2 \cdot \mathbf{r}} + T_2 e^{i(\mathbf{g}_1 - \mathbf{g}_2) \cdot \mathbf{r}}, \quad T_n = w_{AB} \begin{pmatrix} \kappa & e^{-i2\pi n/3} \\ e^{i2\pi n/3} & \kappa \end{pmatrix} \quad (\text{A.13})$$

where $T(\mathbf{r})$ is the interlayer tunneling, whose form we assume is unchanged apart from the lattice distortion, with $w_{AB} = 110 \text{ meV}$. Due to lattice relaxation effects, the realistic range for the chiral ratio κ is thought to be $\kappa = 0.5 - 0.8$ [55–57]. As usual, the harmonics that appear in Eq. (A.13) are the lowest harmonics that connect the K -points of the two graphene layers.

The Hamiltonian for both valleys is

$$h_{\text{TBG}} = \begin{bmatrix} h_K \otimes s^0 & 0 \\ 0 & h_{K'} \otimes s^0 \end{bmatrix} \quad (\text{A.14})$$

where s^μ are the spin Pauli matrices and $h_{K'}$ is defined as the time-reversal conjugate of h_K , making h_{TBG} time-reversal symmetric. In fact, h_{TBG} inherits the C_{2z} symmetry of graphene.

However, both C_{3z} and C_{2x} symmetries are explicitly broken by strain [38]. If one makes the approximation $T(\theta_\ell, -\epsilon_\ell) \rightarrow T(0, -\epsilon_\ell)$ in the Dirac equation, then the single-particle Hamiltonian becomes particle-hole symmetric in the absence of strain [26]. Even in the presence of strain, the Hamiltonian is still largely particle-hole symmetric. We therefore expect the physics at $\pm\nu$ to be at least qualitatively similar (though this is not the case in experiments).

A.3.2 Many-Body Hamiltonian

For our many-body Hamiltonian, we take the single-particle model discussed above, add gate-screened Coulomb interactions, and integrate out the remote bands at the mean-field level. We review this procedure here; in-depth treatments are given in Refs. [26, 50, 51, 199]. Consider a basis $\hat{\mathbf{f}}_{\mathbf{k}}^\dagger = \hat{f}_{\mathbf{k}b\tau s}^\dagger$, where b labels bands of the BM model, $\tau \in \{K, K'\}$ labels valleys, and $s \in \{\uparrow, \downarrow\}$ indexes spin. We start from the microscopic Hamiltonian

$$\hat{H}_{\text{full}} = \sum_{\mathbf{k} \in \text{BZ}} \hat{\mathbf{f}}_{\mathbf{k}}^\dagger [h_{\text{TBG}}(\mathbf{k}) - h_{\text{counter}}(\mathbf{k})] \hat{\mathbf{f}}_{\mathbf{k}} + \frac{1}{2A} \sum_{\mathbf{q} \in \mathbb{R}^2} V_{\mathbf{q}} : \hat{\boldsymbol{\rho}}_{\mathbf{q}} \hat{\boldsymbol{\rho}}_{-\mathbf{q}} :, \quad V_{\mathbf{q}} = \frac{1}{2\epsilon_r \epsilon_0 q} \tanh(|\mathbf{q}| d) \quad (\text{A.15})$$

where the sums on $\mathbf{k}$ always run over the Brillouin zone, while $\mathbf{q}$ is unrestricted, $V_{\mathbf{q}}$ represents double gate-screened Coulomb interactions with gate distance $d = 25$ nm and relative permittivity $\epsilon_r = 10$, and A is the sample area. The charge density at wavevector $\mathbf{q}$ is given by $\boldsymbol{\rho}_{\mathbf{q}} = \sum_{\mathbf{k}} \hat{\mathbf{f}}_{\mathbf{k}}^\dagger \langle u_{\mathbf{k}} | u_{\mathbf{k}+\mathbf{q}} \rangle \hat{\mathbf{f}}_{\mathbf{k}+\mathbf{q}}$ in terms of the periodic part of the Bloch wavefunctions of h_{TBG} . The counterterm $h_{\text{counter}}(\mathbf{k})$ is discussed below.

We partition the Hilbert space into the space of the active band $\mathcal{A}$ and the remote bands $\mathcal{R}$. As the active bands are relatively well-separated, we make the assumption that the ground state density matrix $\hat{\rho}_{\text{full}}$ factorizes into a remote part and an active part:

$$\hat{\rho}_{\text{full}} = \hat{\rho}_{\mathcal{R}} \otimes |\Psi_{\mathcal{A}}\rangle \langle \Psi_{\mathcal{A}}|. \quad (\text{A.16})$$

We further assume that $\hat{\rho}_{\mathcal{R}}$ is a product state: fully-filled below the active bands and fully-empty above, which allows us to integrate out the remote bands at mean-field level. Up to a constant this yields

$$\hat{H}_{\mathcal{A}} = \text{tr}_{\mathcal{R}} [\hat{H}_{\text{full}} \hat{\rho}_{\mathcal{R}}] = \sum_{\mathbf{k} \in \text{BZ}} \hat{c}_{\mathbf{k}}^\dagger \left[h_{\text{TBG}}(\mathbf{k}) + h_{\text{HF}}[P_{\mathcal{R}}](\mathbf{k}) - h_{\text{counter}}(\mathbf{k}) \right] \hat{c}_{\mathbf{k}} + \frac{1}{2A} \sum_{\mathbf{q} \in \mathbb{R}^2} V_{\mathbf{q}} : \hat{\boldsymbol{\rho}}_{\mathbf{q}}^{\mathcal{A}} \hat{\boldsymbol{\rho}}_{-\mathbf{q}}^{\mathcal{A}} :, \quad (\text{A.17})$$

where $\hat{c}$ is the restriction of $\hat{\mathbf{f}}$ to the flat bands, and $\hat{\boldsymbol{\rho}}_{\mathbf{q}}^{\mathcal{A}}$ is the corresponding flat band density operator. Here $h_{\text{HF}}[P_{\mathcal{R}}]$ is the standard Hartree-Fock Hamiltonian corresponding to the correlation matrix $[P_{\mathcal{R}}(\mathbf{k})]_{bb'} = \text{Tr}[\rho_{\mathcal{R}} \hat{f}_{\mathbf{k}b'}^\dagger \hat{f}_{\mathbf{k}b}]$, which is the identity matrix on remote bands below the active band, and identically zero otherwise [26, 199]. (Spin and valley indices are left implicit.) Physically, $h_{\text{HF}}[P_{\mathcal{R}}]$ encodes a background charge density from the filled Fermi sea that affects active electrons. We use $\hat{H}_{\mathcal{A}}$ as the effective Hamiltonian for the active bands.

The final ingredient is the counterterm [26, 50, 51, 199]. A counterterm is needed because $h_{\text{HF}}[P_{\mathcal{R}}]$ diverges unphysically with the number of bands. The root of this issue is that some parameters of the BM model already take interactions into account, such as the experimentally-derived Fermi velocity, leading to an unphysical double-counting of some Coulomb interactions. In principle, “ultraviolet” Hamiltonian $h_{\text{TBG}} - h_{\text{counter}}$ should be fixed by matching to *ab initio* or experimental observations in the “infrared”. (See also [272].) We use the “decoupled” subtraction scheme: the counterterm is given by the half-filled state of two decoupled layers of graphene. Explicitly, suppose $h_K^0 = \text{diag}(h_+ \ h_-)$ [c.f. Eq. (A.13)] and is diagonalized as $h^0 U^0 = \epsilon^0 U^0$. Then define

$$h_{\text{counter}} = h_{\text{HF}}[P_{\text{counter}}]; \quad P_{\text{counter},bb'}(\mathbf{k}) = U_0^\dagger P_{\text{CNP,decoupled}} U^0 \quad (\text{A.18})$$

where $P_{\text{CNP,decoupled}}$ is the diagonal density matrix of graphene at half-filling. The Hartree-Fock correction to the Hamiltonian is therefore

$$h_{\text{HF}}[P_{\mathcal{R}}](\mathbf{k}) - h_{\text{counter}}(\mathbf{k}) = h_{\text{HF}}[P_{\mathcal{R}} - P_{\text{counter}}]. \quad (\text{A.19})$$

As $P_{\mathcal{R}}$ and P_{counter} are approximately equal far from charge neutrality, we make the approximation that bands very far from the Fermi level are irrelevant [26]. In practice we retain 5 bands above and 5 bands below charge neutrality in $P_{\mathcal{R}} - P_{\text{counter}}$ (times valley and spin), and just the two “flat” bands in $h_{\text{HF}}[P_{\mathcal{R}} - P_{\text{counter}}]$. (Another popular choice is “infinite temperature subtraction”, which leads to $h_{\text{HF}}[P_{\mathcal{R}} - P_{\text{counter}}] = h_{\text{HF}}[-I_{\mathcal{A}}/2]$, see e.g [199]). (Ref. [32] checked that the phenomenology of IKS depends only weakly on the subtraction scheme.)

Altogether, our Hamiltonian for the active bands is

$$\hat{H}_{\mathcal{A}} = \sum_{\mathbf{k} \in \text{BZ}} \hat{c}_{\mathbf{k}}^\dagger h'_0(\mathbf{k}) \hat{c}_{\mathbf{k}} + \frac{1}{2A} \sum_{\mathbf{q} \in \mathbb{R}^2} V_{\mathbf{q}} : \hat{\rho}_{\mathbf{q}}^A \hat{\rho}_{-\mathbf{q}}^A :, \quad h'_0(\mathbf{k}) = [h_{\text{TBG}}(\mathbf{k}) + h_{\text{HF}}[P_{\mathcal{R}} - \Delta]] \quad (\text{A.20})$$

As 2-fermion terms may be shuffled between the dispersion and interaction by, e.g., changing the normal ordering reference, $h'_0(\mathbf{k})$ cannot be interpreted directly as a dispersion. However, relative changes in the bandwidth of $h'_0(\mathbf{k})$ are meaningful.

We note that if one defines $\hat{\rho}_{\mathbf{q}}$ to be the charge density measured relative to (a reference density matrix at) charge neutrality, then the Hamiltonian takes the convenient “strong-coupling” form $\hat{H}_{\mathcal{A}} = \sum_{\mathbf{k} \in \text{BZ}} \hat{c}_{\mathbf{k}}^\dagger h_{\text{TBG}}(\mathbf{k}) \hat{c}_{\mathbf{k}} + \frac{1}{2A} \sum_{\mathbf{q} \in \mathbb{R}^2} V_{\mathbf{q}} : \hat{\rho}_{\mathbf{q}} \hat{\rho}_{-\mathbf{q}} :$ [26].

A.3.3 Strain-induced bandwidth and the “Hartree Peak”

A key effect of heterostrain is to greatly increase the bandwidth. We note that “bandwidth” is not a strictly well-defined concept in strongly interacting systems, as one can always shuffle 2-fermion terms between the “dispersion” and “interaction” parts of the Hamiltonian. Here we consider the “dispersion” to be $h'_0 = h_{\text{BM}} + h_{\text{HF}}[P_{\mathcal{R}} - \Delta_{\text{counter}}]$. Fig. A.1(a) shows the bandwidth of the single-particle Hamiltonians h_{TBG} and h'_0 as a function of strain. One can

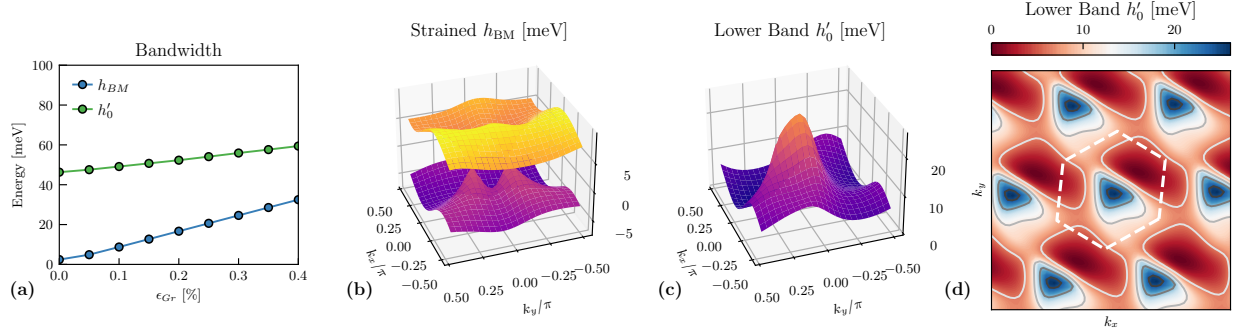


Figure A.1: Single-particle energetics of our interacting model. Here h_{BM} refers to the strained BM model and h'_0 , defined in Eq. (A.20) is related to the total dispersion. (a) The bandwidth of h_{TBM} and h'_0 as a function of strain. Note the bandwidth increase dramatically with ϵ_{Gr} . (b) The two flat bands of the BM model for $\epsilon_{Gr} = 0.2\%$ in meV (c) The lowest band of h'_0 for $\epsilon_{Gr} = 0.2\%$ showing the “Hartree peak” (the upper band is similar). (d) Same as (c), but as a contour plot. This “cat’s eye” pattern will appear below in the symmetric Fermi liquid phase. The dashed white hexagon shows the moiré Brillouin zone, which is distorted by strain. Parameters match Table A.2.

see that the bandwidth increases significantly with strain. For comparison, the interaction scale is ~ 50 meV.

Fig. A.1(b) shows h_{TBM} at $\epsilon_{Gr} = 0.2\%$. The bandwidth has increased to ~ 33 meV from ~ 2.5 meV at $\epsilon_{Gr} = 0$. As C_{3z} is broken, the Dirac nodes are no longer pinned to $K^\pm$, and instead migrate inwards to the vicinity of Γ . (Recall that the fragile topology of each valley prevents the Dirac nodes within each valley from being gapped out unless $C_2\mathcal{T}$ is broken.)

Fig. A.1(c,d) show the lower band of h'_0 at $\epsilon_{Gr} = 0.2\%$. The spectrum is dominated by the “Hartree peak” of ~ 30 meV near the Γ point. This peak is due to the spatial structure of the wavefunctions [273]. The Hartree potential can be thought of as an inhomogeneous background charge density from the filled Fermi sea, which happens to be peaked in the AA region of each unit cell. Holes (electrons) added at generic momentum will be attracted (repelled) from this charge density, thereby lowering (raising) the quasiparticle energy. However, $\psi_\Gamma(\mathbf{r})$ vanishes in the AA region at $\epsilon_{Gr} = 0$ due to C_{3z} symmetry, and is generically small in the AA region even in the presence of strain. Therefore the energies at the Γ point are essentially unaffected by the Hartree potential, causing the large Hartree peak (dip) for hole (electron) doping relative to charge neutrality.

Any order that can avoid populating electrons near Γ therefore gains a large energetic advantage. Metallic states can always do this by forming a Fermi surface partially up the peak, but we shall see below that IKS and spin spirals (Appendix A.6.3) can also take advantage of this structure.

A.3.4 Computational Basis & Numerical Details

We now specify our computational basis. We start from the band of energy bands of h_{TBG} : $\hat{c}_{\mathbf{k}b\tau s}$, where $b \in \{1, 2\}$ labels the flat bands. We apply a change of basis

$$\hat{c}_{\mathbf{k}\sigma\tau s}^\dagger = U_{\sigma b}(\mathbf{k})\hat{c}_{\mathbf{k}b\tau s}^\dagger, \quad \hat{c}_{n,k_y,\sigma\tau s}^\dagger = \int \frac{dk_x}{\sqrt{G_x}} e^{-i\mathbf{k}\cdot\mathbf{a}_1 n} \hat{c}_{\mathbf{k}\sigma\tau s}^\dagger, \quad (\text{A.21})$$

where $U(\mathbf{k})$ is a 2×2 unitary that adjusts the gauge so that $\hat{c}_{n,k_y,\sigma\tau s}^\dagger$ create hybrid Wannier orbitals: maximally localized along $\mathbf{a}_1$, but plane-waves with definite momentum k_y [50]. We have taken a rectangular moiré Brillouin zone $G_x \times G_y$, and $U(\mathbf{k})$ is complex conjugated for the K' valley so that time-reversal is preserved. At the same time, $U(\mathbf{k})$ transforms to the “sublattice” basis $\sigma \in \{A, B\}$. It has the property that the microscopic sublattice operator, defined in the band basis as $I_{bb'}(\mathbf{k}) = \langle u_{\mathbf{k}b} | \sigma^z | u_{\mathbf{k}b'} \rangle$ is diagonal with eigenvalues $\pm\gamma \approx \pm 1$, which is always possible [26]. We underscore that Eq.(A.21) is a computational basis for all eight active bands, all of which will be dynamical in our model.

Let us reiterate the symmetries of our model. Each valley has a separate $U(1)$ electric charge and $SU(2)$ spin conservation, which gives a combined $U(2) \times U(2)$ continuous symmetry (at the level of the Lie algebra). We also have time-reversal $\mathcal{T}$, C_{2z} , and the anti-unitary combination $C_{2z}\mathcal{T}$, which is k -local. Of course, we also have moiré scale translation symmetry $T_{\mathbf{a}_i}$ along $\mathbf{a}_{1,2}$. Maximal localization along $\mathbf{a}_1$ implies the Wannier orbitals are eigenstates of the projected position operator $\mathcal{P}(\mathbf{a}_1 \cdot \hat{\mathbf{r}})\mathcal{P}$, where $\mathcal{P}$ projects to the active bands. Finally, we note that the BM Hamiltonian is approximately particle-hole symmetric, but strain breaks particle-hole symmetry further. The full symmetry content of the model is discussed in Ref. [26].

A.4 Details of the DMRG Calculations

This section gives numerical details of our DMRG computations, including flavor polarization, and defines the correlation functions we study in the main text and below.

In practice we select L_y cuts through the Brillouin zone at evenly spaced momenta $k_y = \frac{2\pi m}{L_y}$ for integer m . We then resolve $\hat{H}_A$ in the computational basis as an matrix product operator (MPO). Naively, such an MPO would have bond dimension $\chi_{\text{MPO}} \approx 100,000 - 300,000$ (typical MPOs are $\chi_{\text{MPO}} \approx 60$ for short-range 2D systems). We apply MPO compression [50, 69] to reduce the MPO bond dimension to $\chi_{\text{MPO}} < 1500$, while retaining an accuracy of $\epsilon_{\text{MPO}} = 10 \times 10^{-2}$ meV or better, making the computation tractable. We note that DMRG simulations have memory requirements $O(\chi_{\text{MPO}}\chi^2)$ where χ is the bond dimension of the state (hundreds to thousands of gigabytes of memory for our largest simulations).

We use two “rings” around the cylinder as a unit cell for infinite DMRG, which allows the breaking of translation symmetry along the cylinder $T_{\mathbf{a}_1}$ down to $2T_{\mathbf{a}_1}$. Meanwhile, enforcing k_y momentum conservation prevents translation symmetry breaking around the cylinder.

Parameter	Value(s)
Twist angle θ	1.08°
Strain ε_{Gr}	$0\% - 0.2\%$
Chiral parameter κ	$0.5 - 0.8$
Interlayer tunnelling w_{AB}	110 meV
Gate distance d	25 nm
Relative permittivity ϵ_r	10
Active bands (per valley per spin)	2
Subtraction Scheme (see text)	Decoupled
Remote bands for subtraction (per valley per spin)	10
Cylinder circumference L_y	$4, 6$
MPO accuracy ϵ_{MPO}	10^{-2} meV
MPO bond dimension χ_{MPO}	$250 - 1500$
State bond dimension χ	$1024 - 24, 576$

Table A.2: Parameters our model and DMRG calculation.

A.4.1 DMRG Flavor Sectors

Our simulations explicitly conserve a $U(1)^4 \subset U(2) \times U(2)$ symmetry, corresponding to: total electric charge, valley charge, and spin- z in each valley, respectively. These are measured by $\hat{n}$, τ^z , s_K^z , and $s_{K'}^z$, respectively. As usual, the Hamiltonian is block-diagonal, with sectors labelled by the integer charges of these four symmetries. DMRG will find a ground state within each sector, based on the charge of the initial state. We consider the four “least charged” sectors, which should contain the global ground state. These are labeled by their distinct charge sectors (τ^z, s^z) . Here $s^z = s_K^z + s_{K'}^z$ is the sum of the spins in both valleys. We only consider the diagonal sectors with $s_K^z = s_{K'}^z$. We work at filling $\nu = -3$, which fully specifies the electric charge sector. Explicitly, we consider the following four sectors:

1. $(\tau^z, s^z) = (1, 1)$: electrons are populated only in the $\tau = K, s = \uparrow$ sector.
2. $(\tau^z, s^z) = (0, 1)$: electrons are equally populated between the two $\tau = K/K', s = \uparrow$ sectors.
3. $(\tau^z, s^z) = (1, 0)$: electrons are equally populated between the two $\tau = K, s = \uparrow / \downarrow$ sectors.
4. $(\tau^z, s^z) = (0, 0)$: electrons are equally populated between all four $\tau = K/K', s = \uparrow / \downarrow$ sectors.

A.4.2 2D Correlators

The key tool to identify phases in DMRG is correlation functions. In simple cases, phases have well-defined order parameters that are two-point correlation functions. However, even simple phases in 2D can be difficult to diagnose on a quasi-1D cylinder due to enforced algebraic order from the Hohenberg-Mermin-Wagner theorem. These must be characterized by the *trend* of correlators as a function of the bond dimension. This section introduces the 2D correlators whose 1D versions are evaluated in DMRG.

A key correlator is the 2-electron correlation matrix

$$P_{\alpha\beta}(\mathbf{k}) = \langle \hat{c}_{\mathbf{k},\beta}^\dagger \hat{c}_{\mathbf{k},\alpha} \rangle, \quad (\text{A.22})$$

an 8×8 matrix for each k , where $\alpha, \beta \in \{\sigma, \tau, s\}$ index sublattice, valley, and spin as above. We frequently consider the diagonal component of this correlator, such as $n_{K\uparrow}(\mathbf{k}) = \sum_{\sigma} \langle \hat{c}_{\mathbf{k},\sigma,K,\uparrow}^\dagger \hat{c}_{\mathbf{k},\sigma,K,\uparrow} \rangle$.

To detect IKS order and other phases, it is frequently useful to consider k -nondiagonal operators. Define

$$\tilde{\Delta}_{\mathbf{q}}^{ijk}(\mathbf{k}) = \hat{c}_{\mathbf{k}+\mathbf{q}}^\dagger \sigma^i \tau^j s^k \hat{c}_{\mathbf{k}}, \quad (\text{A.23})$$

which picks out a particular combination of Pauli matrices in flavor space. To convert from 2D to the quasi-1D cylinder, we apply a Fourier transform $\hat{c}_{\mathbf{k},\sigma\tau s}^\dagger := \sum_{n \in \mathbb{Z}} e^{i(\mathbf{k} \cdot n \mathbf{a}_1)} \hat{c}_{n,k_y,\sigma\tau s}^\dagger$ where $n \in \mathbb{Z}$ labels the hybrid Wannier orbital centered at $n\mathbf{a}_1$ along the cylinder. Then

$$\tilde{\Delta}_{\mathbf{q}}^{ijk}(\mathbf{k}) = \sum_{m,n \in \mathbb{Z}} e^{i\mathbf{k} \cdot m \mathbf{a}_1} \Delta_{m,q_y}^{ijk}(n, k_y); \quad \Delta_{m,q_y}^{ijk}(n, k_y) = \hat{c}_{n+m,k_y+q_y}^\dagger \sigma^i \tau^j s^k \hat{c}_{n,k_y}. \quad (\text{A.24})$$

Therefore, if a 2D order operator $\langle \tilde{\Delta}_{\mathbf{q}}(\mathbf{k}) \rangle$ is peaked at $\mathbf{q} = \mathbf{q}_0$, then we expect $\langle \Delta_{m,q_y}(n, k_y) \rangle \sim \delta(q_{0,y}) e^{-in(\mathbf{q}_0 \cdot \mathbf{a}_1)}$, and the two components of $\mathbf{q}_0$ can be extracted accordingly. When taking the quasi-1D limit, the Hohenberg-Mermin-Wagner theorem ensures that $U(1)$ symmetries (e.g.) are not spontaneously broken. So, if Δ is an order parameter for a continuous symmetry G in 2D, in the quasi-1D (thin cylinder) limit we expect either algebraic or exponential decay (depending on G) of $\langle \Delta(n) \Delta(0) \rangle$ along the cylinder. This becomes a 4-point correlation function

$$C_{\Delta}(n, q_y) = L_y^{-2} \left\langle \sum_{k_y} \Delta_{0,q_y}(0, k_y) \sum_{k'_y} \Delta_{0,q_y}^\dagger(n, k'_y) \right\rangle. \quad (\text{A.25})$$

When symmetry breaking is present, we expect $C_{\Delta}(n, q_y) \sim \delta(q_{0,y}) e^{in(\mathbf{q}_0 \cdot \mathbf{a}_1)}$, allowing us to extract the 2D $\mathbf{q}$ from DMRG data.

At finite bond dimension χ , the correlator must decay exponentially at the largest scales: $C_{\Delta}(n, q_y) \sim e^{-n/\xi_{\Delta}}$. If the correlator is algebraic, then we expect a divergence $\xi_{\Delta} \rightarrow \infty$ as $\chi \rightarrow \infty$. In fact, the subleading eigenvalues of the transfer matrix will diverge as well, which

may be used to assess scaling relations in extremely high-bond dimension data [274]. For spin-polarized IKS order, which breaks $U(1)_{\text{valley}}$ we indeed expect such algebraic decay

$$|C_{\text{IKS}}(n \gg 1, q_y)| = n^{-\eta(L_y)} \text{ as } \chi \rightarrow \infty, \quad (\text{A.26a})$$

$$\eta(L_y) \rightarrow 0 \text{ as } L_y \rightarrow \infty, \quad (\text{A.26b})$$

recovering the 2D limit. In complex systems such as the one under consideration here, one cannot reliably determine if a given correlation length ξ_Δ is truly diverging or simply approaching a finite value slowly as a function of χ . Nevertheless, we qualitatively observe that there often is a “scaling regime”: a sufficiently large χ after which the behavior $\xi_\Delta(\chi)$ either plateaus or grows regularly. We take such behavior as an indication that our bond dimension is sufficiently large to capture the “true” ground state.

A.5 1D Heisenberg model in $S^z = 0$ sector

This section briefly reviews some physics of the Heisenberg model, which will be crucial to understanding the spin correlations in DMRG. Namely, we will argue here that the following phenomena in the $S^z = 0$ sector are indicative of ferromagnetic order:

1. Because the state has in-plane long-range order, the correlation length for the sector that contains $S^+(x)S^-(0)$ diverges with χ .
2. Because the state breaks rotational symmetry, the correlation length for the $S^z(x)S^z(0)$ sector is much smaller than that of the $S^+(x)S^-(0)$ sector.
3. Because the state is ferromagnetic, the Fourier transform of the correlation function $C_{XY}(n) = \langle S^x(n)S^x(0) + S^y(n)S^y(0) \rangle$ does *not* have a dominant peak away from $q = 0$.

We corroborate this claim by showing that the 1D Heisenberg model exhibits this behavior. The Heisenberg Hamiltonian is

$$H = J \sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1}. \quad (\text{A.27})$$

When $J < 0$, the model is ferromagnetic and its ground state spontaneously breaks rotational symmetry. On the other hand, for $J > 0$, the model is antiferromagnetic. Its ground state is a rotationally invariant $S = 0$ state with gapless excitations (see e.g. [275]). We show that the above criteria are sufficient to distinguish between these two possibilities.

A.5.1 Ferromagnetic Heisenberg model

We start in the ferromagnetic case $J = -1$. A ground state of ferromagnetic Heisenberg model is a product state $|\uparrow\uparrow \cdots \uparrow\uparrow\rangle$. Other ground states can be obtained by applying the

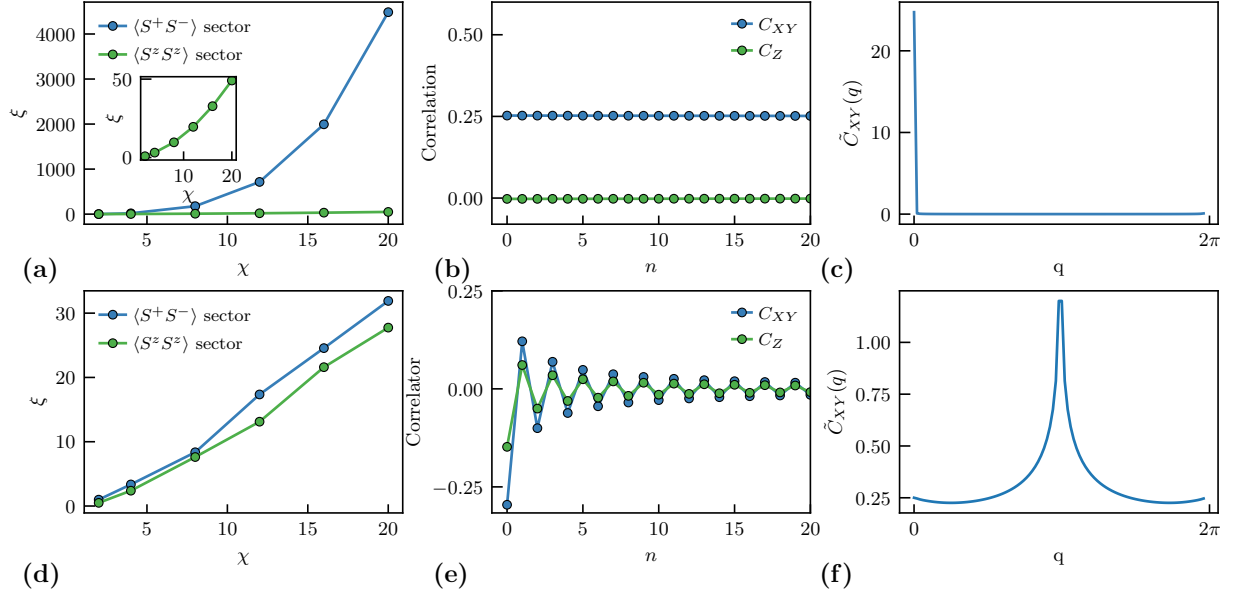


Figure A.2: Correlation length and correlation functions of the 1D Heisenberg model. (a) Correlation lengths of the ferromagnetic Heisenberg model at different values of χ . The inset shows a magnified view of the $S^z S^z$ correlation length. (b) C_{XY} and C_Z correlators of the Heisenberg model. (c) Fourier transform of the C_{XY} correlator. (d)(e)(f) Same as (a)(b)(c), except for the antiferromagnetic Heisenberg model.

lowering operator S^- to this state. For a finite system with N spins, there are $N + 1$ ground states.

We now look at the ground state in an infinite system via infinite DMRG. Numerically, it is standard to conserve quantum numbers per unit cell. In our case, we can conserve S^z quantum number. Taking a two-site unit cell, we have a choice of $S^z = 1$ or $S^z = 0$, corresponding to initial states $|\uparrow\uparrow\rangle^{\otimes\infty}$ or $|\uparrow\downarrow\rangle^{\otimes\infty}$, respectively. The former state is already a ground state. The latter state is not a ground state, of course, but is a good initial state for DMRG to find the ground state in the $S^z = 0$ sector.

We now show that the $S^z = 0$ ground state of the Heisenberg model cannot be realized at any finite bond dimension. To see this, consider the following correlator:

$$\begin{aligned}
 C_{XYZ}(n) &= \langle S^z(n)S^z(0) + S^x(n)S^x(0) + S^y(n)S^y(0) \rangle \\
 &= \langle S^z(n)S^z(0) + \frac{1}{2}(S^+(n)S^-(0) + S^-(n)S^+(0)) \rangle.
 \end{aligned}
 \tag{A.28}$$

This correlator has a constant expectation value $1/4$ for the $S^z = 1$ ferromagnet. Since the correlator is rotationally symmetric, we should also have $C_{XYZ} = 1/4$ in the $S^z = 0$ ground

state. However, at any finite bond dimension, this correlator approaches 0 exponentially fast as $n \rightarrow \infty$ (assuming the state is injective). This is because the connected component of the correlation function asymptotically goes as $e^{-n/\xi}$ where ξ is the correlation length of MPS. Since the on-site expectation values are $\langle S^z(0) \rangle = \langle S^x(0) \rangle = \langle S^y(0) \rangle$ for the $S^z = 0$ state, this means $C_{XYZ}(n)$ itself decays exponentially fast.

Therefore, in order to approximate the ground state, the correlation length ξ of the MPS found from DMRG at bond dimension χ diverges rapidly as a function of χ . In Fig. A.2(a), we show the correlation length corresponding to $\langle S^+(n)S^-(0) \rangle$ and $\langle S^z(n)S^z(0) \rangle$ extracted from transfer matrix eigenvalues. The correlation length for $\langle S^+(n)S^-(0) \rangle$ diverges rapidly as a function of χ , indicating in-plane ordering of spins. On the other hand, the correlation length for $\langle S^z(n)S^z(0) \rangle$ is much smaller, indicating a strong rotational symmetry breaking.

To confirm this interpretation, we measure the following in-plane and out-of-plane correlators:

$$C_{XY}(n) = \langle S^x(n)S^x(0) + S^y(n)S^y(0) \rangle = \frac{1}{2} \langle S^+(n)S^-(0) + S^-(n)S^+(0) \rangle, \quad (\text{A.29})$$

$$C_Z(n) = \langle S^z(n)S^z(0) \rangle. \quad (\text{A.30})$$

In Fig. A.2(b), we show the value of the correlators at $\chi = 20$ as a function of n . The in-plane correlator C_{XY} is close to constant at $1/4$, reflecting the large correlation length of 4000, while the out-of-plane correlator C_Z is close to zero. This shows that all of the spin ordering is in-plane.

Fig. A.2(c) shows $\tilde{C}_{XY}(q)$, the Fourier transform of $C_{XY}(n)$. There is a single dominant peak at $q = 0$, confirming 1D ferromagnetic Heisenberg model satisfies the three criteria laid out above.

A.5.2 Antiferromagnetic Heisenberg model

We now look at the antiferromagnetic (AFM) Heisenberg model to contrast with the ferromagnetic scenario. As the ground state of AFM Heisenberg model has $S = 0$, we can find it in the $S^z = 0$ sector with DMRG. Due to its gapless nature, there are superficial similarities in its behavior to the ferromagnetic case. In the following, we show how the criteria above can be used to distinguish it from the ferromagnetic case.

We show in Fig. A.2(d) the correlation length of AFM Heisenberg model as a function of χ . Unlike in the ferromagnetic case, $\langle S^+(n)S^-(0) \rangle$ and $\langle S^z(n)S^z(0) \rangle$ have similar correlation length, reflecting the $SO(3)$ invariance of the ground state. A similar feature can be observed in the correlators plotted in Fig. A.2(e); the C_Z correlator is roughly the half of C_{XY} correlator.

Finally, we show the Fourier transform of C_{XY} correlator in Fig. A.2(f). Reflecting the antiferromagnetic nature of spin correlation, we see the dominant peak is at $q = \pi$. These observations fully distinguish the antiferromagnetic case from the ferromagnetic case.

A.6 Phase diagram analysis at flavor-polarized sectors

In the following two sections, we will discuss the various phases found within DMRG and indicate the resulting phase diagram. This section focuses on the phases *not* in the $(\tau^z, s^z) = (0, 0)$ sector, where certain flavors are fully polarized.

A.6.1 Quantized Anomalous Hall order

This section discusses the quantized anomalous Hall (QAH) order that appears at strains close to zero in all sectors. The QAH insulator is a ground state within strong coupling theory in the chiral flat limit at $\nu = -3$ [26, 27]. The simplest example is described by the correlation matrix $P_{\text{QAH-VP}} = \left(\frac{1+\sigma^z\tau^z}{2}\right) \left(\frac{1+\tau^z}{2}\right) \left(\frac{1+s^z}{2}\right)$, which entirely fills the $(A, K, \uparrow)$ sector. This state has full polarization of the QAH order parameter

$$O_{\text{QAH}} = \frac{1}{N_k} \sum_{\mathbf{k}} \langle \hat{c}_{\mathbf{k}}^\dagger \sigma^z \tau^z \hat{c}_{\mathbf{k}} \rangle. \quad (\text{A.31})$$

As $C = \sigma^z \tau^z$ measures the Chern number, states with $O_{\text{QAH}} = \pm 1$ correspond to full polarization in Chern bands, and are thus Chern insulators with $C = \pm 1$. Even when O_{QAH} is away from polarization, we expect the state is adiabatically connected to the fully polarized Chern insulators. We therefore use $\text{sign}(O_{\text{QAH}})$ as a signature of the Hall conductance of the state. We also define

$$O_{\sigma^+} = \frac{1}{N_k} \sum_{\mathbf{k}} \langle \hat{c}_{\mathbf{k}}^\dagger \sigma^+ \hat{c}_{\mathbf{k}} \rangle, \quad (\text{A.32})$$

which is small in the QAH phase, but will appear in the semimetal discussed below.

The chiral flat limit features an emergent $U(4)_+ \times U(4)_-$ symmetry acting within each Chern sector [26]. Acting with any $U_+ \in U(4)_+$ on $P_{\text{QAH-VP}}$ gives another ground state in this limit. For instance, the state $P_{\text{QAH-IVC}} = \left(\frac{1+\sigma^z\tau^z}{2}\right) \left(\frac{1+\sigma^x\tau^x}{2}\right) \left(\frac{1+s^z}{2}\right)$ with equal occupations in $(A, K, \uparrow)$ and $(B, K', \uparrow)$. Working perturbatively in deviations from the chiral limit, one expects that $P_{\text{QAH-VP}}$ and $P_{\text{QAH-IVC}}$ are still competitive ground state candidates at $\kappa \approx 0.65$, and should still be nearly degenerate. This is borne out in our DMRG results.

We find that the ground state of each sector is a variant of QAH, adapted for that particular symmetry sector. For simplicity, we focus on the $(0, 1)$ and $(1, 1)$ sectors where spin does not play a role; the other sectors are similar. Fig. A.3 shows the value of the order parameter O_{QAH} as a function of ε_{Gr} . It is nearly unity at $\varepsilon_{\text{Gr}} = 0$ for both sectors, but strain quickly drives a transition to $O_{\text{QAH}} = 0$. For the $(1, 1)$ sector, the state we find is adiabatically connected to $P_{\text{QAH-VP}}$, similar to previous reports [50]. For $(\tau^z, s^z) = (0, 1)$, however, the requirement that occupations are balanced between valleys excludes the $P_{\text{QAH-VP}}$ state; the $(0, 1)$ state is instead descended from $P_{\text{QAH-IVC}}$. In 2D, this breaks $U(1)_{\text{valley}}$ symmetry. In 1D, however, $U(1)$ symmetry cannot be spontaneously broken; instead algebraic order will

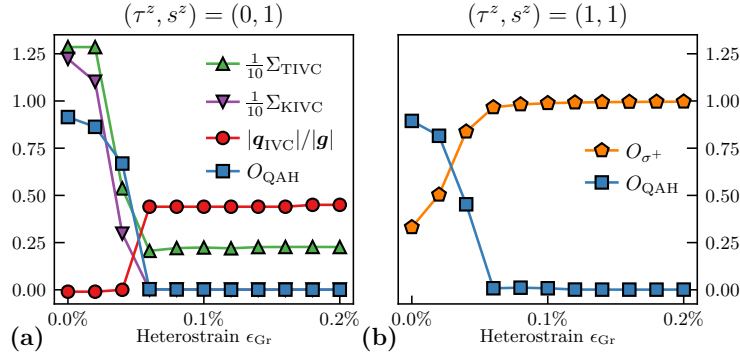


Figure A.3: (a) Correlation functions and order parameters in the $(0, 1)$ sector as a function of ϵ_{Gr} . See text for details. (b) Correlation functions in the $(1, 1)$ sector as a function of ϵ_{Gr} . Parameters: $\chi = 3072$, $\kappa = 0.7$, $L_y = 6$, otherwise matching Table A.2.

manifest in intervalley correlation functions. Define operators

$$\Delta_{TIVC}(n) = \sum_{k_y} \hat{c}_{n,k_y}^\dagger \sigma^x \tau^x \hat{c}_{n,k_y}, \quad \Delta_{KIVC}(n) = \sum_{k_y} \hat{c}_{n,k_y}^\dagger \sigma^x \tau^y \hat{c}_{n,k_y}, \quad (\text{A.33})$$

and the corresponding correlators $\Sigma_{T/KIVC} := L_y^{-2} \sum_{n \in \mathbb{Z}} |\langle \Delta_{T/KIVC}(n) \Delta_{T/KIVC}(0) \rangle|$ [39]. Fig. A.3 (a) shows both $\Sigma_{T/KIVC}$ are large in the low- ϵ_{Gr} phase. In fact, the intervalley correlation length diverges with χ , indicating the expected algebraic correlations. We note that TIVC and KIVC correlations are not distinct when only a single sublattice is occupied. However, note that after the transition, Σ_{KIVC} approaches zero while Σ_{TIVC} remains finite, a fact that will return below in our discussion of IKS order.

We therefore identify the order in the $(1, 1)$ sector as QAH-VP, and the $(0, 1)$ sector as QAH-IVC. The $(1, 0)$ sector is consistent with QAH-VP with the ferromagnetic order in xy -plane, similar to the 1D Heisenberg chain discussed in Appendix A.5. We discuss the $(0, 0)$ sector, which shows xy -ferromagnetic QAH-IVC order, in the main text and Appendix A.7.2. Fig. 4 displayed in the main text shows that all four sectors of QAH states have similar energies.

A.6.2 Nematic Semimetallic Order

This section describes the phase in the $(1, 1)$ sector away from zero strain, which we identify as a nematic semimetal (NSM), closely resembling the nematic semimetal discovered previously in the strong coupling regime [32, 50, 276]. Previous studies have shown the nematic semimetal phase to be a competitive ground state candidate favored by C_{3z} symmetry-breaking terms, in our case the uniaxial heterostrain. The nematic semimetal descends from a “parent state” within strong-coupling theory after the application of a singular gauge transformation which eliminates the Berry flux [277]. At $\epsilon_{Gr} = 0$, the gap to

the nematic soft mode decreases with κ , eventually driving a transition from QAH to the nematic semimetal [50, 277]. Adding a small amount of strain, which breaks C_{3z} explicitly, has a similar effect [32, 39].

We examine the state at $\varepsilon_{\text{Gr}} = 0.15\%$, $\kappa = 0.7$ in detail. As we are in the $(1, 1)$ sector, electrons only occupy the K -valley with spin $\uparrow$. The first observation is the state is quite close to a Slater determinant. To assess this, we define the single-particle Shannon entropy

$$S_{\text{Sh}} = -\frac{1}{N_k} \sum_k \text{Tr}[P(k) \ln P(k)], \quad (\text{A.34})$$

where $P(k)$ is the 2-body correlation matrix defined in Eq. (A.22). A state may be represented as a Slater determinant if and only if $P(k)$ is a projector i.e. $P(k)^2 = P(k)$. In this case, its eigenvalues are either 0 or 1, so $\text{Tr}[P(k) \ln P(k)] = 0$ for all k . One may therefore use S_{Sh} to assess how far a given state is from a Slater determinant. In this case, $S_{\text{Sh}} \approx 0.02$, so the state is extremely close to a Slater determinant, and we may understand the state through single-particle considerations.

To better display the physics of this phase, we employ a “superresolution” technique. Namely, we thread flux ϕ through the cylinder so that momentum cuts move to $k_y(m, \phi) = \frac{2\pi(m+\phi)}{L_y}$ for $0 \leq \phi < 1$. So long as no transitions occur as a function of ϕ (which holds here, but is non-generic), we may combine data from DMRG runs at multiple ϕ to improve our k_y resolution significantly.

Fig. A.4(c) shows the electron occupations across the Brillouin zone. Since the state is Slater-like, we can interpret this in terms of an effective Hartree-Fock band structure of two bands. The electron density is almost uniform, which indicates the state fills one of the two bands. However, there are additional features near Γ , which are due to Dirac nodes. To see this, Fig. A.4(a) shows the phase winding of

$$\arg[\sigma^+(\mathbf{k})] = \arg \langle \hat{c}_{\mathbf{k},A,K,\uparrow}^\dagger \hat{c}_{\mathbf{k},B,K,\uparrow} \rangle. \quad (\text{A.35})$$

For states close to a Slater determinant, this winds by $\pm 2\pi$ around Dirac nodes [50]. Two vortices are clearly visible near Γ , each with a $+2\pi$ winding. We note that, due to fragile topology, one cannot choose a gauge that is both smooth and periodic. We choose a periodic gauge with a discontinuity across $k_y = 0$. Fig. A.4(b) shows the electron-electron correlation length ξ_{1e} , which diverges at precisely the same k_y values as the vortex centers, indicating gapless electrons. We may conclude that we have an effective bandstructure with two Dirac nodes of the same chirality in the vicinity of Γ — quite similar to the phenomenology of the nematic semimetal, but also similar to the underlying bandstructure of TBG in the presence of strain.

In the presence of C_{3z} breaking, the Dirac nodes are not pinned to the half-filling of the two bands, and may shift in energy. The slight deviation from uniform filling in Fig. A.4(c) may thus be a consequence of such an effect, though the variation is too small to be conclusive. We note that the occupied band shows Hartree peaks feature, as seen in Fig. A.4(d): upon hole-doping, the holes enter almost entirely at Γ . In summary, this state is a semimetal with two Dirac nodes of the same chirality.

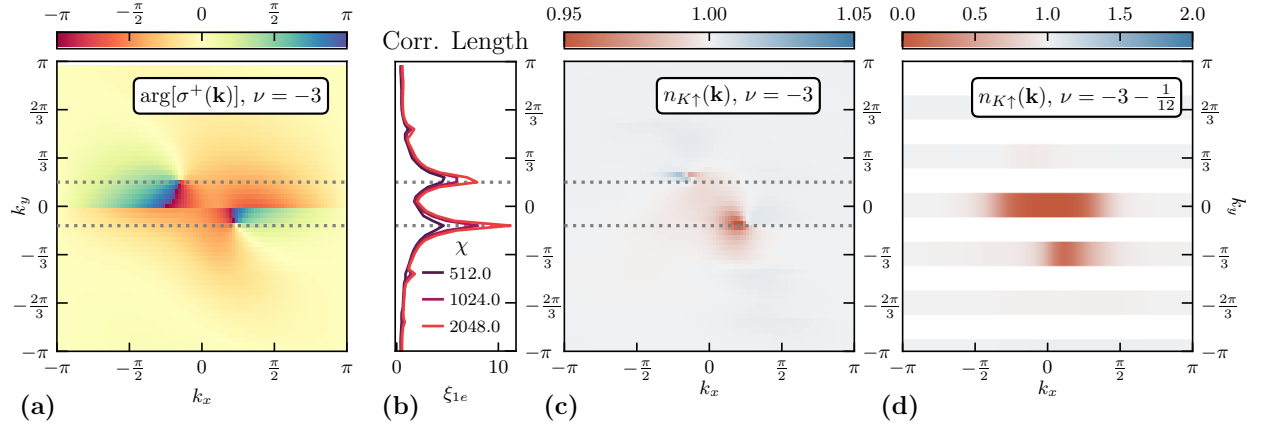


Figure A.4: Details of the CNSM phase. Panels (a,b,c) combine multiple DMRG runs with different flux threadings to produce “superresolution” plots. (a) Shows the phase of the Chern off-diagonal correlations over the Brillouin zone. The phase winds by 2π around each Dirac node. The fragile topology ensures the gauge cannot be both smooth and periodic; we adopt a periodic gauge with a discontinuity at $k_y = 0$. Dashed grey lines indicate the k_y of the Dirac nodes. (b) Single-electron correlation lengths as a function of k_y for various χ ’s, which diverge at the Dirac nodes. (c) Electron occupations in the $K \uparrow$ sector. Note small electron/hole pockets around the Dirac nodes. (d) Electron occupations in the $K \uparrow$ sector at filling $\nu = -3 - \frac{1}{12}$. The hole pocket has expanded greatly. Parameters: $\chi = 2048$, $\varepsilon_{\text{Gr}} = 0.15\%$, $\kappa = 0.7$, $L_y = 6$, $(\tau^z, s^z) = (1, 1)$ sector.

A.6.3 Commensurate Spin Spiral Order

The ground state in the $(1, 0)$ sector away from zero strains has commensurate spin spiral (CSS) order. Similar to IKS, this order breaks both $U(1)_{\text{spin}}$ and moiré translation symmetry $\hat{T}_{\mathbf{a}_i}$, but preserves a combined symmetry

$$\hat{T}_{\mathbf{a}_i}^{\text{CSS}} = \hat{T}_{\mathbf{a}_i} e^{i\mathbf{q}_{\text{CSS}} \cdot \mathbf{a}_i s^z / 2} \quad (\text{A.36})$$

for some offset vector $\mathbf{q}_{\text{CSS}}$. We will see that $\mathbf{q}_{\text{CSS}} = \mathbf{g}/2$ for some reciprocal lattice vector $\mathbf{g}$.

Fig. A.5 shows the properties of the commensurate spin spiral state [compare to Fig. 2.2 in the main text]. Panels (a,b) show the electron occupations for spin $\uparrow, \downarrow$ respectively. Note that the occupations are virtually identical; the state is symmetric under s_x -symmetry. Just like in IKS, we observe that

$$N_{\mathbf{q}_{\text{CSS}}}^{(S)}(\mathbf{k}) = n_{\uparrow}(\mathbf{k}) + n_{\downarrow}(\mathbf{k} - \mathbf{q}_{\text{CSS}}) \approx 1, \quad (\text{A.37})$$

where, in this case, $\mathbf{q}_{\text{CSS}} = \mathbf{g}_1/2$ is half of a reciprocal lattice vector.

Such commensurate spin spiral ordering will break $U(1)_{\text{spin}}$, and therefore manifest as an increasing correlation length in the appropriate correlation function. Following the main text, we define the operator

$$\hat{\Delta}_{\text{CSS}}(\mathbf{k}) = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{q}_{\text{CSS}}}^\dagger s^+ \hat{c}_{\mathbf{k}}, \quad \Delta_{\text{CSS}}(n; q_y) = \sum_{k_y} \hat{c}_{n, k_y+q_y}^\dagger s^+ \hat{c}_{n, k_y}, \quad (\text{A.38})$$

and put $C_{\text{CSS}}(n; q_y) := L_y^{-2} \langle \Delta_{\text{CSS}}(0; q_y) \Delta_{\text{CSS}}^\dagger(n; q_y) \rangle$. Fig. A.5 (d) shows the absolute value of $C_{\text{CSS}}(n, q_y = [\mathbf{g}_1/2]_y)$, whose correlation length is increasing quickly with χ , a sign of order that breaks $U(1)_{\text{spin}}$ but restores the product $\hat{T}_{\mathbf{a}_i}^{\text{CSS}}$. Fig. A.5 (e) shows the discrete Fourier transform of C_{CSS} with respect to n along the cylinder, which is strongly peaked at $q = \pi$. Therefore C_{CSS} independently finds $\mathbf{q}_{\text{CSS}} = \mathbf{g}_1/2$.

Spin-flip symmetry enforces a commensurate offset vector. Given $n_\uparrow(\mathbf{k}) = n_\downarrow(\mathbf{k})$, the same state can also be described by CSS order with $-\mathbf{q}_{\text{CSS}}$. Since $\mathbf{q}_{\text{CSS}}$ and $\mathbf{q}_{\text{CSS}} + \mathbf{g}$ are equivalent for any reciprocal lattice vector $\mathbf{g}$, we must have $\mathbf{q}_{\text{CSS}} = \mathbf{g}/2$ to ensure consistency. This is a key difference between IKS order and CSS order.

Let us note a few other properties of this state. The CSS order described here is *not* spin density wave (SDW) order (though that will appear in the (0,0) sector considered below). We have explicitly checked that the spin occupations are equal in each ring of the cylinder, as expected for a state with $\hat{T}_{\mathbf{a}_i}^{\text{CSS}}$ symmetry but not for an SDW. As only the K valley is populated, time-reversal symmetry is explicitly broken. However, there are equal occupations in both sublattices, suggesting no net Hall conductance. As noted in the main text, the phenomenology of CSS and IKS order are similar in that both depopulate the region near Γ in all sectors.

A.6.4 Spin-Polarized IKS order

This section focuses on the IKS order in the $(\tau^z, s^z) = (0, 1)$ sector, in which the spin-polarized order is enforced. As mentioned before, IKS features intervalley correlations with a momentum offset $\mathbf{q} = \mathbf{q}_{\text{IKS}}$, which is measured by the operator

$$\hat{\Delta}_{\text{IKS}}(\mathbf{k}) = \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}+\mathbf{q}_{\text{IKS}}}^\dagger \sigma^x \tau^+ \hat{c}_{\mathbf{k}}, \quad \Delta_{\text{IKS}}(n; q_y) = \sum_{k_y} \hat{c}_{n, k_y+q_y}^\dagger \sigma^x \tau^+ \hat{c}_{n, k_y}. \quad (\text{A.39})$$

Since $s^z = 1$, we ignore spin in this discussion.

To identify this 2D $U(1)$ spontaneous symmetry breaking within quasi-1D DMRG, we must perform the double scaling analysis outlined in Eq. (A.26). We define the q_y -dependent correlation function

$$C_{\text{IKS}}(n; q_y) := L_y^{-2} \langle \Delta_{\text{IKS}}(0; q_y) \Delta_{\text{IKS}}^\dagger(n; q_y) \rangle \xrightarrow{n \gg 1} e^{-n/\xi_{\text{IKS}}[q_y] + i\varphi[q_y]n}, \quad (\text{A.40})$$

where $\xi_{\text{IKS}}[q_y]$ is the IKS correlation length regarding the q_y sector, and $\varphi[q_y]$ is the corresponding phase modulation. We first consider scaling in bond dimension, then perform scaling in cylinder circumference L_y .

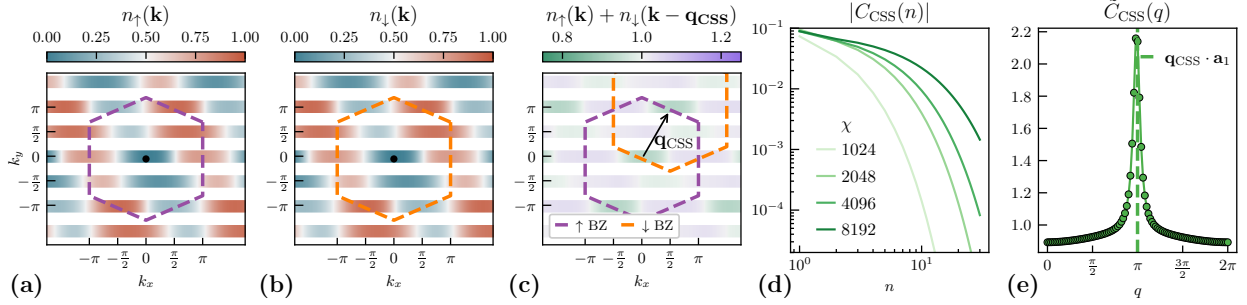


Figure A.5: Details of the CSS phase. (a) Electron occupations for spin $\uparrow$. (b) Electron occupations for spin $\downarrow$. Note these are virtually identical to the previous panel. (c) Offset occupations $n_{\uparrow}(\mathbf{k}) + n_{\downarrow}(\mathbf{k} + \mathbf{q}_{\text{CSS}}) \approx 1$. (d) The C_{CSS} correlation function, whose correlation length is growing quickly with χ . (e) The discrete Fourier transform of the same correlation function with respect to n , which is strongly peaked at $\mathbf{q}_{\text{CSS}} \cdot \mathbf{a}_1 = \pi$. Parameters: $\chi = 8192$, $\kappa = 0.65$, $\varepsilon_{\text{Gr}} = 0.2\%$, $L_y = 4$, $(\tau^z, s^z) = (1, 0)$ sector.

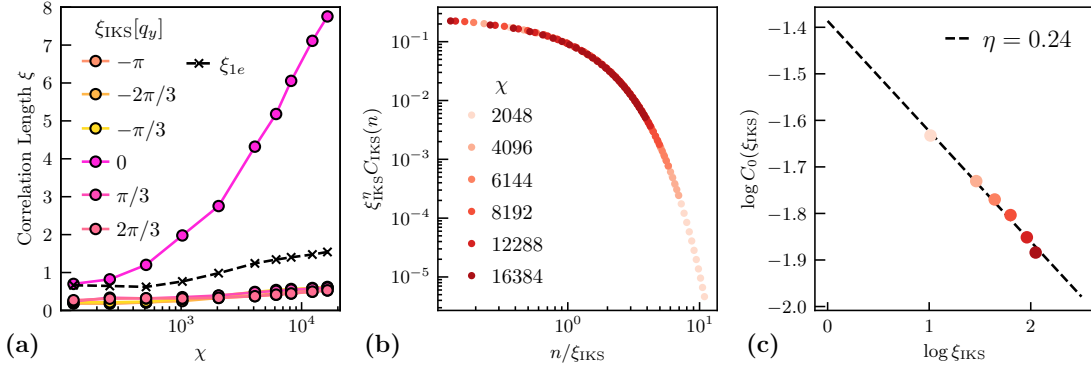


Figure A.6: (a) IKS correlation lengths as a function of χ for each momentum offset q_y . The single-electron correlation length ξ_{1e} is shown on the same scale. (b) Scaling collapse of C_{IKS} via Eq. (A.41). (c) Inference of the scaling exponent $\eta = 0.24$ as described in the text. Parameters: $\chi = 16,384$, $\kappa = 0.65$, $\varepsilon_{\text{Gr}} = 0.2\%$, $L_y = 6$, $(\tau^z, s^z) = (0, 1)$ sector.

Bond Dimension Scaling

Fig. A.6(a) shows the four-point correlation function $C_{\text{IKS}}(n; q_y)$ at all q_y , and plots the evolution of each $\xi_{\text{IKS}}[q_y]$ with χ . For $\chi > 1024$, $\xi_{\text{IKS}}[q_y = 0]$ is clearly dominant, and appears to diverge with system size. This matches the expectation that $U(1)_{\text{valley}}$ breaking in 2D manifests as algebraic order in $C_{\text{IKS}}(n; q_y)$ on the cylinder. The correlation length can

also be extracted from the eigenvalues of the MPS transfer matrix. Let λ_{IKS,q_y} be the largest eigenvalues of the MPS transfer matrix in the IKS sector $\Delta Q_{\text{IKS}} = (\Delta q_{\text{electron}} = 0, \Delta q_{\text{valley}} = 2, \Delta k_y = q_y)$. For each q_y , these obey $\lambda = e^{-1/\xi}$. Furthermore, $\lambda_{\text{IKS},q_y=0}$ is the largest eigenvalue in all sectors of the transfer matrix — and indeed the only substantial one.

We note that single-electron correlation length ξ_{1e} , shown in Fig. A.6(a), is also growing as a function of χ . In some cases, this behavior is associated with metallic order. However, ξ_{1e} may just be slowly converging to a relatively large value. If the state were metallic, one would likely expect ξ_{1e} (from $n(k) \sim [k - k_F]^\alpha$) or ξ_{0e} (gapless particle-hole modes) to be the dominant correlation length in the system, which is the case in the symmetric Fermi liquid below. This data is therefore not sufficient to determine if the state is metallic or insulating but, given that the BZ occupation is uniform after the shift by $\mathbf{q}_{\text{IKS}}$, the latter seems more plausible.

If the IKS correlators are indeed governed by a power law, then one expects to be able to perform a scaling collapse

$$|C_{\text{IKS}}(n, \xi_{\text{IKS}})| = \xi_{\text{IKS}}^{-\eta} |C_{\text{IKS}}(n/\xi_{\text{IKS}}, 1)|. \quad (\text{A.41})$$

This is done in Fig. A.6, with the fitting procedure from Ref. [39]. Given that all correlations functions must decay exponentially at finite bond dimensions, we perform fits on $|C_{\text{IKS}}(n \gg 1, \xi_{\text{IKS}})| \equiv C_0(\xi_{\text{IKS}})e^{-n/\xi_{\text{IKS}}}$ to extract the n -independent prefactor. If the scaling collapse holds true, we will expect $C_0(\xi_{\text{IKS}}) \sim \xi_{\text{IKS}}^{-\eta}$, from which the exponent η is extracted. Fig. A.6(b-c) shows the fitting results for all correlation functions among $\chi = 2048 - 16384$, where an excellent scaling collapse is established at $\eta = 0.24$. This scaling collapse verifies the bond dimension scaling we expected, firm evidence for quasi-1D IKS order at this cylinder size.

Cylinder Circumference Scaling

We perform cylinder circumference scaling for $L_y = 4, 5, 6$. This small maximum size is limited by computational resources. To see why, recall that for a gapped state that obeys the area law, the entanglement entropy scales as $S \propto N_F L_y = 8L_y$ and the expected bond dimension to describe such a state scales as $\chi \sim e^S \sim e^{8aL_y}$ (a is some constant). Compounding the difficulty, the fact that the IKS state has no many-body gap (despite being gapped to 1-electron excitations) means the state's entanglement increases faster than area law, so we may roughly estimate the required bond dimension to resolve the IKS ground state as $\chi \gtrsim e^{8aL_y}$. In practice, this would be bond dimensions of hundreds of thousands to go past $L_y = 4$. Here we restrict to the $(\tau^z, s^z) = (0, 1)$ sector to reduce the number of active flavors from 8 to 4, making it possible to compute well-converged ground states up to $L_y = 6$ with the supercomputing resources at our disposal.

Fig. A.7 shows the scaling of the ground state in the $(0, 1)$ sector at $\epsilon = 0.1\%$ at $L_y = 4, 5, 6$. We show later in Appendix A.7.4 that this sector likely has the global ground state at these parameters, justifying our restriction to this sector. At each circumference, the charge densities in the K and K' valleys (first and second columns) are almost perfectly nested:

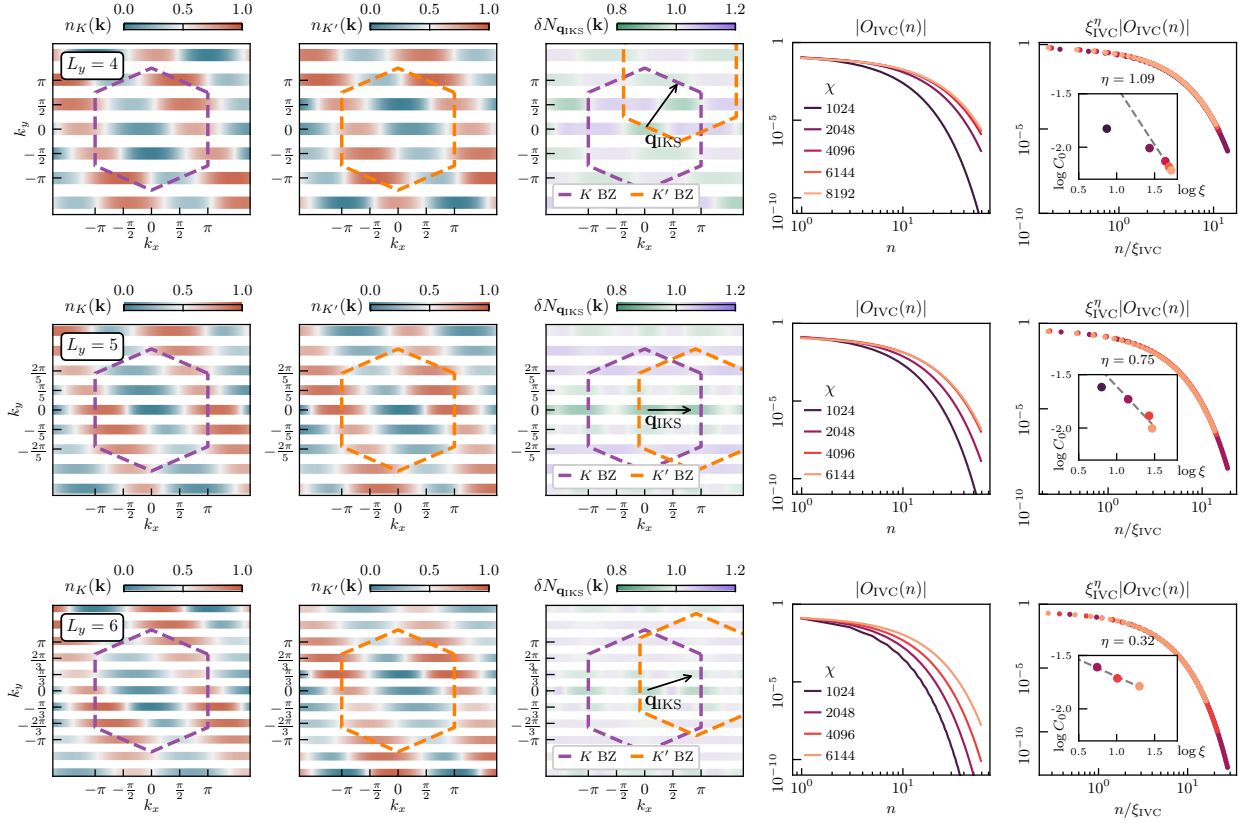


Figure A.7: Circumference scaling of the IKS state, as described in the text. Parameters: $\chi = 1024 - 8192$, $\kappa = 0.65$, $\varepsilon_{\text{Gr}} = 0.1\%$, $L_y = 4 - 6$, $(\tau^z, s^z) = (0, 1)$ sector.

their offset sum $\delta N_{\mathbf{q}_{\text{IKS}}}(\mathbf{k})$ only deviates slightly from 1 across the whole Brillouin zone (third column) — a strong heuristic piece of evidence for IKS order.

We then consider the correlators $|C_{\text{IKS}}(n)|$ (fourth column of Fig. A.7), which can be seen by eye to approach a power law as χ increases over about a decade of scaling at the largest χ . We perform a scaling collapse (Fig. A.7, fifth column) with χ for each set of correlators to extract the power-law exponent. As above, this is done by a linear fit $C_0(\xi_{\text{IKS}}) \sim \xi_{\text{IKS}}^{-\eta}$ to the three largest bond dimensions available at each size. The exponents thus extracted, $\eta(4) = 1.09$, $\eta(5) = 0.75$, $\eta(6) = 0.32$, are indeed decreasing to zero as expected. However, we note that the behavior of $\log C_0$ is not particularly linear with $\log \xi_{\text{IKS}}$ except at the largest bond dimensions. Our estimates of η may therefore be quite inaccurate. Nevertheless, the correlators do clearly decay as power laws that appear to be getting flatter with L_y . All the system sizes we may access therefore support the finding of IKS order.

We comment briefly on $\mathbf{q}_{\text{IKS}}$. Fig. A.7 shows a large jump in $\mathbf{q}_{\text{IKS}}$ between $L_y = 4$ and

$L_y = 5$, and a moderate jump from 5 to 6. We attribute this behavior to the phenomena of the fact that the energy landscape of IKS states with respect to $\mathbf{q}_{\text{IKS}}$ is quite flat [32]. Even dramatic changes of $\mathbf{q}_{\text{IKS}}$ — across half the Brillouin zone, say — may change the overall energy by much less than 1 meV/electron, with several broad pockets of low energy. We therefore interpret these jumps in $\mathbf{q}_{\text{IKS}}$ as slightly different global minima appearing in the IKS landscape as the number and location of the k_y cuts change. We further note that the $n_{\text{K/K'}}(\mathbf{k})$ is quite qualitatively similar between all three plots, with a stripe-like feature at the same angle. Between $L_y = 5$ and $L_y = 6$, the maxima of those stripes appear to change location only slightly. For all L_y , the Γ point and its vicinity are nearly depleted, a fact we return to below.

A.7 Phase diagram analysis at the neutral sector

This final appendix details the phases found in the $(\tau^z, s^z) = (0, 0)$ sector. This is the only sector where flavor polarization is not enforced by quantum numbers, allowing a rich array of phases to appear. As a result, two challenges arise in the numerical simulation: 1) With more active degrees of freedom, the strongly correlated state cannot be represented or characterized until reaching sufficiently large bond dimensions. 2) With close competition between different low-energy states, including flavor-polarized and unpolarized ones, DMRG ground states are more likely to exhibit a mixture of several orders at finite bond dimensions.

As an overview, Fig. A.8 displays the correlation lengths categorized by charge sectors for each state at different strains ε_{Gr} and bond dimensions χ . Accordingly, we will break down our phase diagram discussion into three non-disjoint regions:

1. At $\varepsilon_{\text{Gr}} \geq 0.2\%$, the states feature leading correlations in both neutral ($0e$) and one-electron ($1e$) charge sector, signaling a **symmetric Fermi liquid**. We will take $\varepsilon_{\text{Gr}} = 0.2\%$ as an example to illustrate the characteristics of this order.
2. At $\varepsilon_{\text{Gr}} \leq 0.05\%$, the states feature leading correlations in inter-valley and inter-spin sectors, much stronger than neutral/one-electron correlation at large χ , signaling **spontaneous flavor polarization**. We will confirm that the states at $\varepsilon_{\text{Gr}} = (0, 0.05)\%$ are each consistent with the spin-polarized QAH-IVC and IKS order discussed in previous sections.
3. At $\varepsilon_{\text{Gr}} = (0.1, 0.15)\%$, the states also feature a VDW/SDW order coexisting with the metallic order, signaling a **mixed order** (unlike the case at $\varepsilon_{\text{Gr}} = 0.2\%$). This indicates close competition between different orders in the regime of intermediate strain.

We note that the states in this sector are the unambiguous overall ground state of the system only for $\varepsilon_{\text{Gr}} > 0.2\%$, a fact we return to at the end of this appendix.

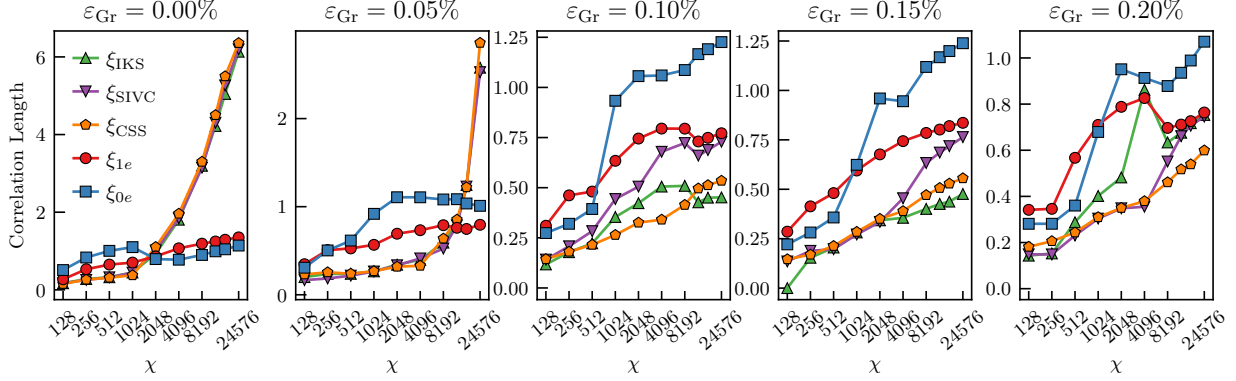


Figure A.8: The correlation lengths in the $(\tau^z, s^z) = (0, 0)$ sector as a function of bond dimension χ . Here ξ_{0e} corresponds to neutral (density-density) correlations, ξ_{1e} is the maximum electron-electron correlation length among all momentum sectors, and ξ_{IVC} , ξ_{SIVC} , and ξ_{CSS} correspond to $\hat{\Delta}_{IKS}$, $\hat{\Delta}_{SIVC}$, and $\hat{\Delta}_{CSS}$ correlations respectively (defined in the text).

A.7.1 Symmetric Fermi liquid at high ε_{Gr}

We start our discussion of the phases with the symmetric Fermi liquid (FL) state: a metallic state where all discrete and continuous symmetries are preserved, with Fermi surfaces in all four Fermion flavors. This phase is the natural ground state in the limit of weak interactions; it is what results from the non-interacting band structure to filling $\nu = -3$. Fermi liquid theory tells us that metals are relatively stable in the presence of interactions. The symmetric Fermi liquid is therefore a reasonable phase to appear in the intermediate coupling regime. Unfortunately, we shall see that it is inherently difficult to resolve in DMRG.

The zeroth order expectation is that one starts with non-interacting dispersion in Eq.(A.20) and fills the lower band to 1/4 filling. Due to the large Hartree peak near Γ as shown in Fig.A.1(c), one expects Fermi surface(s) which do *not* enclose Γ , i.e. the symmetric Fermi liquid depletes the Γ point just as the IKS and CSS phases do.

To incorporate the effect of interactions, we first work at the mean-field level to understand the phenomenology. We performed self-consistent Hartree-Fock (SCHF) at $\nu = -3$ at size 16×16 with all 8 active bands. By enforcing all symmetries, we stabilize a self-consistent FL state. Fig. A.9(d,e) shows the Hartree-Fock bandstructure of the lowest (partially filled) band in both valleys, as well as the sharp Fermi surfaces within SCHF. As expected, the region near Γ is unoccupied in both valleys.

We now turn to DMRG. As gapless systems, metals are inherently difficult to capture within DMRG, and a 2D Fermi surface with four Fermion species is even harder. Fig. A.9 shows the electron occupations in both valleys at $\chi = 24576$, the largest accessible bond

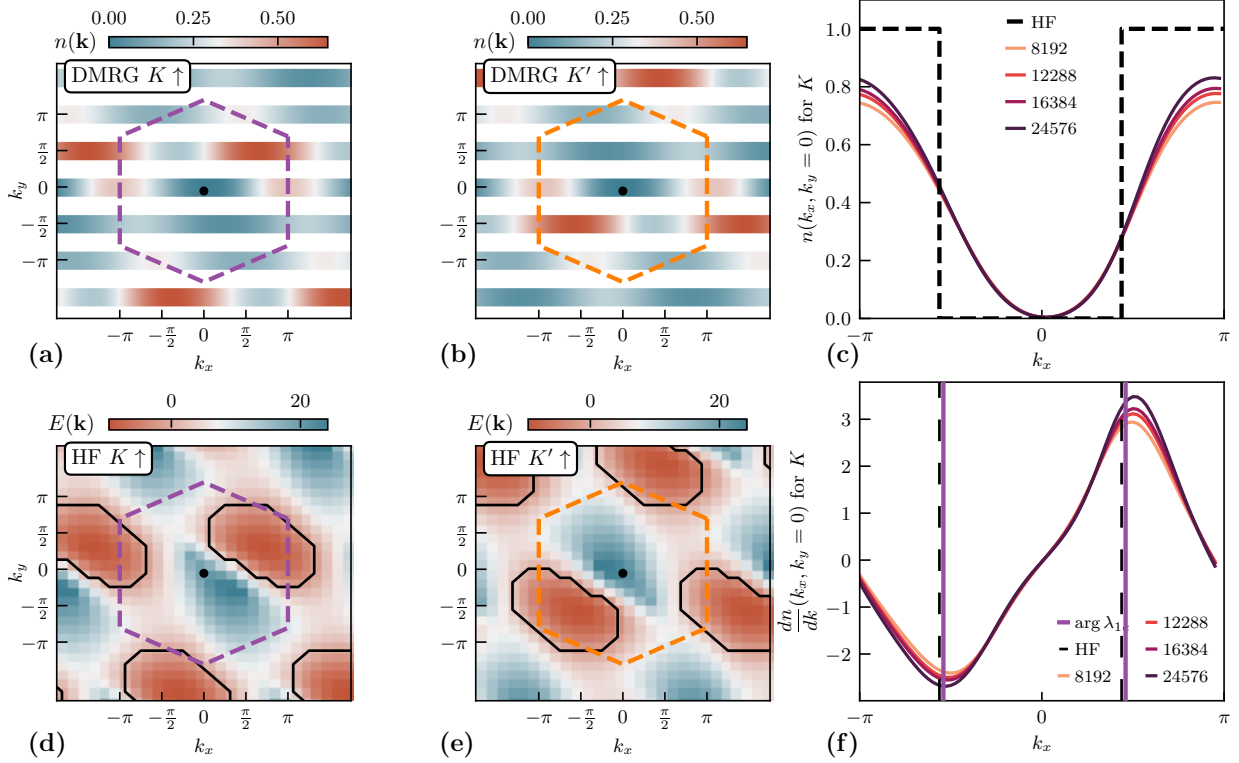


Figure A.9: FL in the $(0,0)$ sector at $\varepsilon_{\text{Gr}} = 0.2\%$. (a,b) Electron occupations within DMRG in the (K, K') valleys respectively. The state has spin flip s^x symmetry, so the $\downarrow$ occupations are identical. Note that the region around Γ (black dot) is fully depleted. (c) The DMRG electron occupations in the K valley along the $k_y = \frac{\pi}{2}$ wire at various bond dimensions. Dashed black lines give the corresponding occupations in SCHF. One can see the DMRG occupations are slowly increasing outside of the nascent “Fermi pocket”. (d, e) Energies of the FL within fully-symmetric Hartree-Fock. Dotted line indicates the location of the Fermi surface. (f) Derivatives of the electron occupations dn/dk . One can see the occupations are increasing most quickly near the “Fermi surfaces”. Also shown are $q_x = \arg \lambda_{1e}$, the momentum associated to the $1e$ correlation channel in the system. Note that it matches the SCHF Fermi surfaces extremely well. Parameters: $\kappa = 0.65$, $\varepsilon_{\text{Gr}} = 0.2\%$, $L_y = 4$, $\chi = 24576$ for (a-b).

dimension. The electron occupations manifestly respect time-reversal and spin-flip s^x symmetry. Furthermore, electrons are fully depleted near Γ in both valleys, and Fermi (electron) pockets closely match the Fermi surfaces from SCHF. We can even identify nascent “Fermi surfaces” forming in the electron occupations, where the derivative dn/dk is peaked and increases with χ [Fig. A.9(c,f)]. The location of the Fermi surfaces agrees well with the ones predicted by SCHF, and also coincides with the corresponding eigenvalues λ_{1e} of the one-electron sector of the transfer matrix [Fig. A.9(f)]. Therefore the occupations and general phenomenology are consistent with the expectation for a symmetric Fermi liquid.

The observed correlation lengths are also consistent with a symmetric Fermi liquid, albeit not wholly conclusive. Recall that interacting Fermi liquids in 1d are described by $c = 1$ Luttinger liquids via bosonization. Both particle-hole excitations and charge $\pm$ excitations are gapless, and the occupations near the “Fermi surface” are power-law rather than a step function like in higher dimensions. A quasi-1D cylinder can be thought of as a coupled wire construction with L_y wires, each containing N_f flavors. In our case, this gives a model of $c = N_f L_y = 16$ coupled Luttinger liquids. Recall that the entanglement entropy divergences with the correlation length as [278]

$$S = \frac{c}{6} \log \xi = \frac{1}{\sqrt{\frac{12}{c} + 1}} \log \chi \quad (\text{A.42})$$

when representing gapless systems. This large central charge means the symmetric Fermi liquid is extremely challenging to capture within DMRG. We indeed see apparently-diverging correlation lengths in both the $0e$ and $1e$ sectors (Fig. A.8). We identify the source of the correlations (q_x, q_y) in the Brillouin zone using the phase information and symmetry sector as in the IKS phase described above. We see that the $1e$ correlations come from the vicinity of the SCHF Fermi surface, and the $0e$ correlations come from the vectors *between* the nascent Fermi surfaces. Using the alternative form $S \propto \log \chi$, we find that the correlations are consistent with $c = 16$, but even the largest accessible bond dimension of $\chi = 24576$ is insufficient to determine the scaling behavior precisely. Meanwhile, the intervalley and interspin correlations are subleading but still substantial in the state, which can be viewed as particle-hole excitation between different sectors. Therefore the DMRG state at $\varepsilon_{\text{Gr}} = 0.2\%$ is consistent with a symmetric Fermi liquid in a variety of non-trivial ways. We suggest the symmetric Fermi liquid is indeed the ground state order at $\varepsilon_{\text{Gr}} = 0.2\%$.

A.7.2 Ferromagnetic QAH-IVC & IKS order at low ε_{Gr}

This section will establish that the state at $\varepsilon_{\text{Gr}} = 0\%$ has QAH-IVC order and the state at $\varepsilon_{\text{Gr}} = 0.05\%$ is consistent with ferromagnetic IKS order. The nature of the two states is summarized in Fig. A.10.

As mentioned in the main text, we identify the $\varepsilon_{\text{Gr}} = 0$ state as a flavor-rotation of the QAH state discussed above. The first piece of evidence is time-reversal symmetry breaking:

the order parameter $C_{\text{QAH}} = 0.87$. Together with the near-uniform occupation of the Brillouin zone, Fig A.10(a), we can identify this as an anomalous Hall insulator. From A.10(c,e) one can see the intervalley correlations are substantial, but the state has $\mathbf{q}_{\text{IVC}} = 0$ (i.e. no IKS ordering). Since we are in the $\tau^z = 0$ sector, we identify this as the intervalley coherent version of the Hall insulator, QAH-IVC. Both this state and the $\varepsilon_{\text{Gr}} = 0.05\%$ state are consistent with ferromagnetic spin ordering, as we describe below.

For $\varepsilon_{\text{Gr}} = 0.05\%$, $C_{\text{QAH}} = 0.003$ so time-reversal symmetry is unbroken. Fig. A.10(d) show that intervalley correlations are increasing quickly with χ . As before, both the shifted BZ occupations in Fig. A.10(a) and the Fourier transform of the IKS correlation function Fig. A.10(d) give $\mathbf{q}_{\text{IKS}} \approx (0.277, 0.25)$. We therefore identify this state as having IKS order.

Finally, we use spin-spin correlations to establish the ferromagnetic ordering of the spins. As a starting note, the simplest ferromagnetic order — spins aligned in the $+z$ direction — is incompatible with the $(\tau^z, s^z) = (0, 0)$ sector. Given that we only conserve $U(1) \subset SU(2)$, we must deduce ferromagnetism in a slightly indirect way. As discussed in Appendix A.5, the hallmarks of ferromagnetic states in the $s^z = 0$ sector are:

1. The correlation length for $\langle s^+(n)s^-(0) \rangle$ diverges with χ .
2. The correlation length $\xi_{S^z S^z}$ for $\langle s^z(n)s^z(0) \rangle$ is much smaller than $\xi_{S^x S^x}$ for $\langle s^+(n)s^-(0) \rangle$.
3. The correlation function doesn't have peaks at nonzero momenta.

The first condition establishes spin ordering, the second shows rotational symmetry breaking, and the final condition rules out antiferromagnetic order. In Figs. A.10(c,d), we see that the correlation length $\xi_{S^x S^x}$ are increasing rapidly with χ , establishing the first property. (This correlation length corresponds to C_{CSS} , which is defined below Eq. (A.38).) We see there is no corresponding increase in $\xi_{S^z S^z} = \xi_{0e}$, establishing property 2. Finally the Fourier transform of C_{CSS} shows a single peak at $q = 0$ in Fig. A.10(g,h), establishing condition 3. Combining these observations, we identify both $\varepsilon_{\text{Gr}} = 0, 0.05\%$ as having ferromagnetic order alongside their QAH-IVC and IKS orders in the sublattice/valley flavors.

A.7.3 “Mixed” order at intermediate ε_{Gr}

The $\varepsilon_{\text{Gr}} = (0.1, 0.15)\%$ states of the $(\tau^z, s^z) = (0, 0)$ sector feature what we will term “mixed” order, with features of both symmetric Fermi liquid and flavor-polarized states, complicated by possibly-transient translation-breaking order. We start with Fig. A.8 showing the correlation lengths at these strain values. One can see their leading correlations in $0e$ and $1e$ sectors, consistent with a symmetric Fermi liquid. However, they also manifest strong spin asymmetry in intervalley correlations, namely with ξ_{SIVC} (between opposite spins) much larger than ξ_{IVC} (between the same spins) in both states. This behavior deviates from the observation in either the symmetric Fermi liquid or the ferromagnetic orders, which we hypothesize to result from “partial” spin polarization to be further examined.

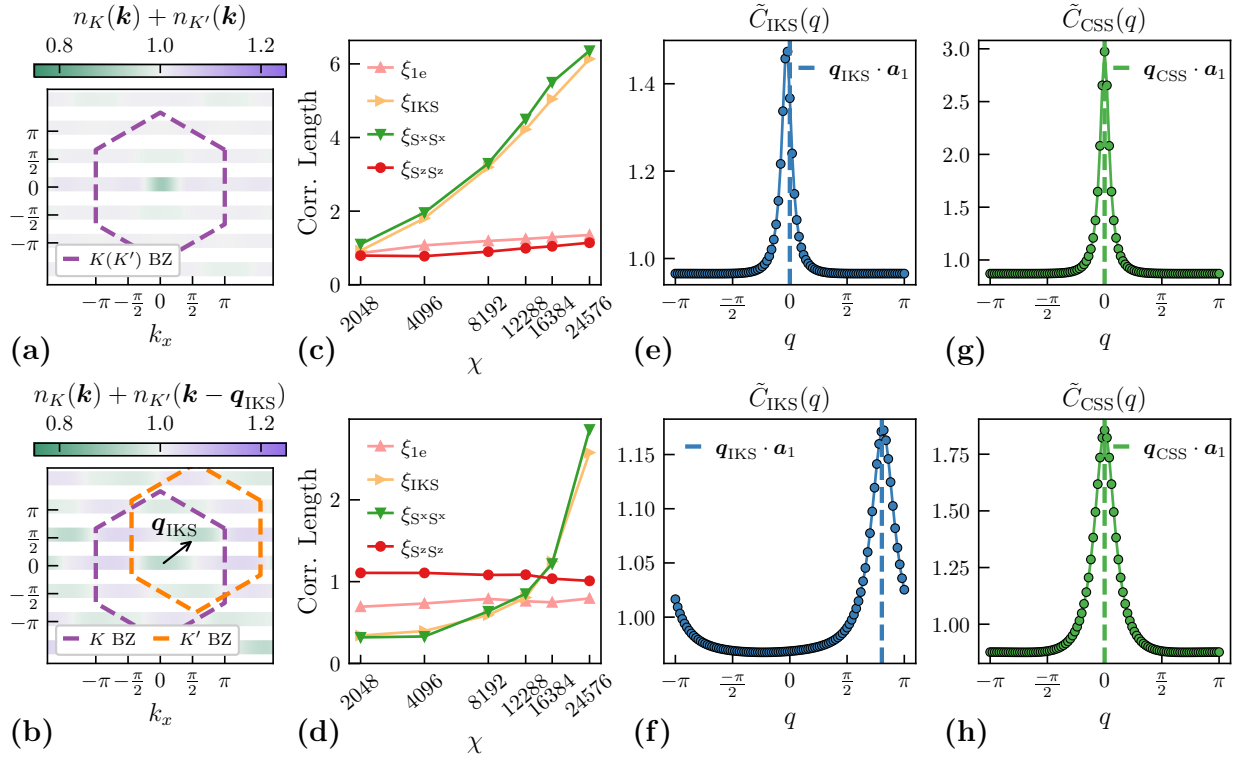


Figure A.10: The spinful QAH-IVC (a,c,e,g) and IKS (b,d,f,h) phases. (a-b) The total electron density of each phase in Eq.(2.12), where (b) undergoes a relative boost by $\mathbf{q}_{\text{IKS}}$. (c-d) Correlation lengths of various sectors as a function of χ . The IVC correlation length, ξ_{IKS} , and spin-flip correlation length, $\xi_{S \times S^x}$, are larger than other sectors. (e-f) The Fourier transform of $C_{\text{IKS}}(n)$. The peak at $\mathbf{q}_{\text{IKS}} \cdot \mathbf{a}_1$ agrees with $\mathbf{q}_{\text{IKS}}$ obtained from occupations $n(\mathbf{k})$. (g-h) The Fourier transform of $C_{\text{CSS}}(n)$ signaling spin-flip correlations, which shows a peak at $q = 0$. (Unlike previous figures, $q = 0$ is positioned at the center in (e-h) for a better view.)

Next, we take a closer look at the pattern of flavor polarization in these states, which reveals a strong spin density wave (SDW) order and a transient valley density wave (VDW) order. These orders break translation $T_{\mathbf{a}_1}$ along the cylinder down to $2T_{\mathbf{a}_1}$, and are detected by order parameters that probe flavor-resolved charge imbalances between adjacent rings on the cylinder: Let $-1/2 \leq P(k_y)_{\sigma,\tau} < 1/2$ be the polarization (center of charge) of the hybrid Wannier orbitals [50], then the order parameters are defined as

$$N_{\text{VDW}}(\pi) = \frac{1}{L_x} \sum_{n, k_y, \sigma \tau s} e^{i\pi(n+P(k_y, \sigma, \tau))} \langle \hat{c}_{n, k_y, \sigma \tau s}^\dagger [\tau^z]_{\tau \tau} \hat{c}_{n, k_y, \sigma \tau s} \rangle, \quad (\text{A.43})$$

$$N_{\text{SDW}}(\pi) = \frac{1}{L_x} \sum_{n, k_y, \sigma \tau s} e^{i\pi(n+P(k_y, \sigma, \tau))} \langle \hat{c}_{n, k_y, \sigma \tau s}^\dagger [s^z]_{ss} \hat{c}_{n, k_y, \sigma \tau s} \rangle. \quad (\text{A.44})$$

The sum is taken over some segments with unit cells $n = 1, 2, \dots, L_x$, and here we choose L_x even since the density waves double the unit cell.

Fig. A.11(a-b) show the behavior of VDW and SDW orders in the ground states at all strain values. In all cases, the VDW order is present at smaller bond dimensions χ but disappears at the largest $\chi = 24576$. Note that they share a common trend of “finite- χ phase transition”: N_{VDW} has a substantial value, perhaps decreasingly slightly, until it abruptly vanishes. As for the SDW order, at $\varepsilon_{\text{Gr}} = (0, 0.05, 0.2)\%$ it has vanished by $\chi = 16384$, but at $\varepsilon_{\text{Gr}} = (0.1, 0.15)\%$ it persists even at the largest χ . This is consistent the hypothesis of “partial polarization” from correlation lengths: the SDW order results in nonzero s^z polarization alternating in each unit cell (thus not violating the net $s^z = 0$), arguably leading to the spin asymmetry found in intervalley correlations. Meanwhile, unlike ferromagnetic orders, there is no net spin polarization either in the z direction or in the xy plane, which agrees with the weak spin-spin correlations. Nevertheless, we caution that the SDW order could also be a finite- χ effect, which may disappear suddenly if one access even larger bond dimensions.

For completeness, we also comment on some other characteristics of the “mixed” order. Fig. A.11(c) includes the entanglement entropy of the ground states at different ε_{Gr} , where the states with “mixed” order show similar growth in entanglement as other phases. We also find that no choice of $\mathbf{q}_{\text{IKS}}$ makes their electron occupations entirely uniform across the Brillouin zone, though certain choices that offset the Hartree peaks work somewhat well.

Given the mix of signals for $\varepsilon_{\text{Gr}} = (0.1, 0.15)\%$ states — metallic order, spin-asymmetric correlations, and possibly transient spin density waves — we do not make a definitive claim of the phase at intermediate ε_{Gr} , and instead refer to these states as “mixed” order on phenomenological grounds. We note that these states has very close energy to the spin-polarized IKS states in the (0,1) sector (as shown in Fig. 4(a)), suggesting the close competition between different orders in this regime.

A.7.4 Higher Strain and the Phase Diagram at $\nu = -3$

We conclude with some data on higher strain values above 0.2% and speculation on the true phase diagram. Fig. A.12 gives DMRG ground state energies in all four sectors up to $\varepsilon_{\text{Gr}} = 0.5\%$. Due to numerical expense, we restrict to $\chi = 8192$ or less. Recall in Fig. 4(a) that (0,0) [FL] is the global ground state at $\varepsilon_{\text{Gr}} = 0.2\%$, with an energy difference of < 0.01 meV from the (0,1) [IKS] state. For even larger strains, we see the (0,0) sector is the clear energetic winner. As more strain continues to increase the bandwidth of the flat

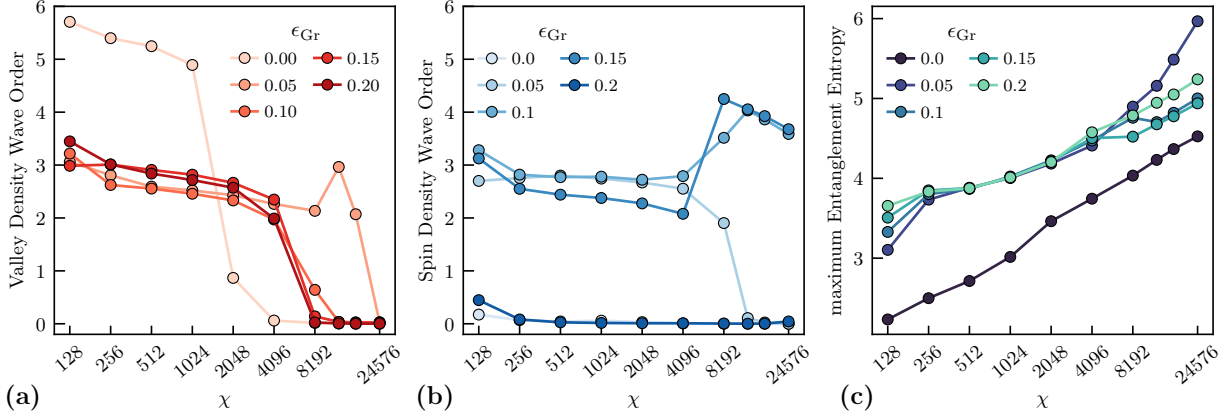


Figure A.11: Other characteristics of $(\tau^z, s^z) = (0, 0)$ states at different ϵ_{Gr} as a function of bond dimension χ . (a) Valley density wave measured by N_{VDW} ; (b) Spin density wave measured by N_{SDW} ; (c) Entanglement entropy.

bands, this is physically reasonable. We note, however, that our assumptions that the active bands are relatively well-isolated from the remote bands likely break down for sufficiently large strain.

Taking the identifications of states in our model at face value and incorporating all sectors, we arrive at the following possible phase diagram of $\nu = -3$.

1. Quantized anomalous hall order at $\epsilon_{Gr} \leq 0.05\%$.
2. IKS order at $0.05\% < \epsilon_{Gr} < 0.1\%$.
3. Crossover region between 0.1% and 0.2% .
4. A symmetric Fermi liquid at $0.2\% \leq \epsilon_{Gr}$.

This is shown in Fig. 2.1(c). We note that the exact phase boundaries are expected to change somewhat depending on finite-size effects and other parameters such as κ . For instance, using $L_y = 6$ stabilizes QAH at a larger strain value, as does decreasing κ to approach the chiral limit. Furthermore, the energy differences between these phases are only slightly larger than the numerical precision of our Hamiltonian and ground state — and much larger than the physical uncertainty in our model. Nevertheless, we expect the basic picture of the three phases to be robust.

Finally, we comment on the phase transitions. As QAH and IKS order lie in different quantum number sectors, we expect a first-order phase transition between them. For the $(0, 0)$ sector, the ferromagnetic IKS order breaks symmetries, whereas the FL does not. The transition between them may in principle be second-order (though we do not rule out a

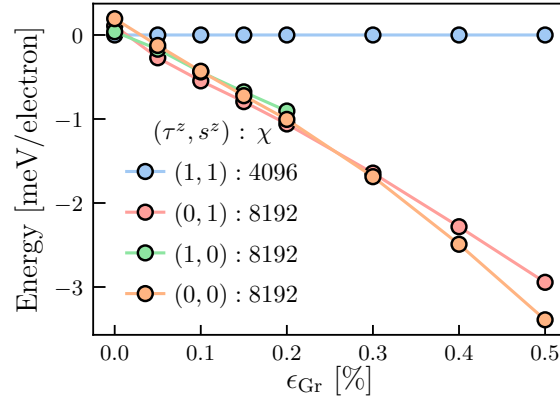


Figure A.12: DMRG energies in all four sectors as a function of heterostrain ϵ_{Gr} . Due to computational expense, we use $\chi = 8192$ except in the $(1,1)$ which is already well-converged by $\chi = 4096$. The $(1,0)$ sector was not computed beyond $\epsilon_{\text{Gr}} = 0.2\%$, but is expected to be above $(0,0)$ and $(0,1)$ in energy. Note that the $(0,0)$ is clearly the lowest energy for $\epsilon_{\text{Gr}} > 0.2\%$. The phases and transitions are discussed in the text in detail.

first-order transition). If this is the case, any quantum critical behavior would manifest in the region where we have found the “mixed” order.

Appendix B

Appendix to chapter 3

B.1 Dirac points in the flat bands

To illustrate how the multiple Dirac points in Fig. 3.1 (b) and (c) emerge when we turn on SOC strength λ_R , in Fig. B.1 we show the energy difference between the flat bands in the first mBZ, which also reveal the 2D positions of these Dirac points. The emergent Dirac points are already noticeable for λ_R as small as 2 meV: In the originally degenerate upper bands, four Dirac cones show up at Γ point and on the $\Gamma - M$ lines. Between the middle bands also appear extra Dirac cones, which are located at lower-symmetry points between the Γ and $K^\pm$ points. Upon increasing λ_R , all these Dirac points move closer to the Γ point, and are located very close to Γ at the physical value $\lambda_R = 16$ meV.

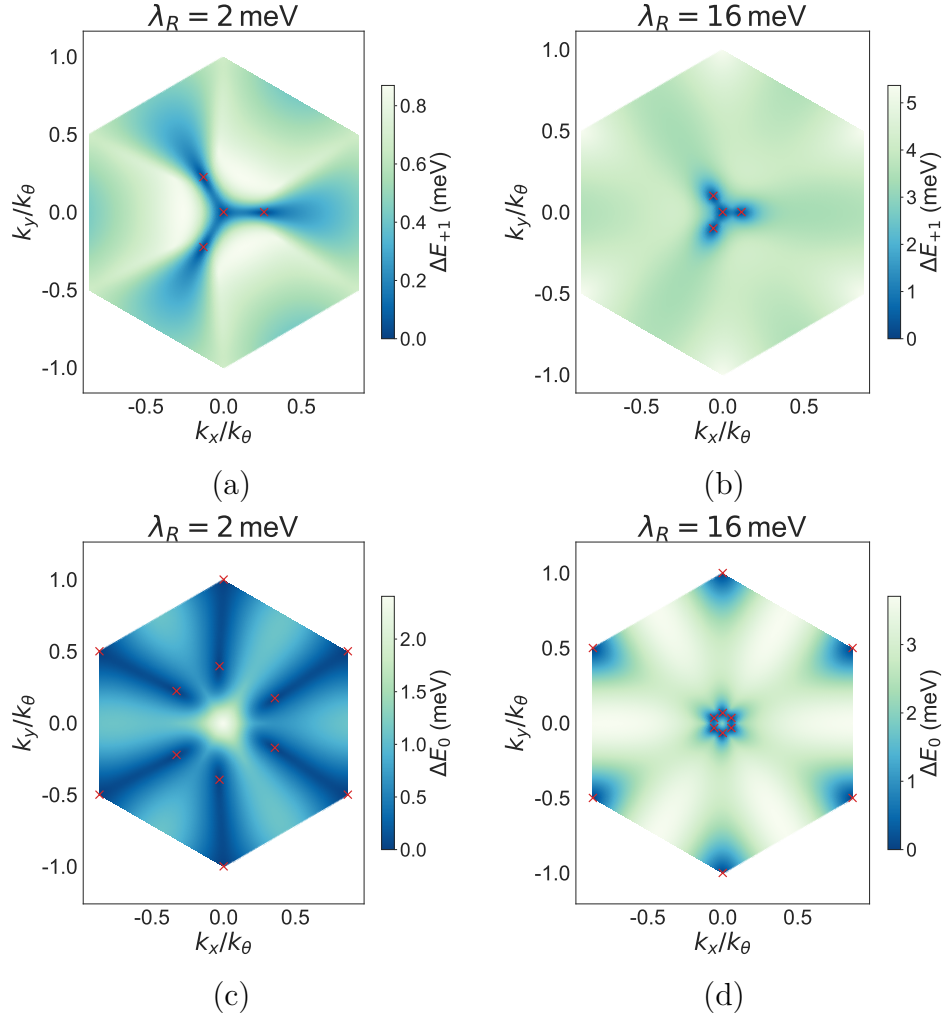


Figure B.1: Energy difference ΔE between the flat bands from Eq.(3.13) with $\lambda_R^+ = 0$. (a)-(b): ΔE_{+1} between the two upper bands for (a) $\lambda_R^- = 2 \text{ meV}$ and (b) $\lambda_R^- = 16 \text{ meV}$. (c)-(d): ΔE_0 between the two middle bands for (c) $\lambda_R^- = 2 \text{ meV}$ and (d) $\lambda_R^- = 16 \text{ meV}$. The energy difference between the lower two bands is similar to that of the upper two bands. The positions of the Dirac points, where $\Delta E = 0$, are highlighted by red crosses.

Appendix C

Appendix to chapter 4

C.1 Details of the Microscopic Model

This appendix fully specifies the models discussed in the main text.

C.1.1 Rhombohedral Graphene

Let $a \approx 2.46\text{\AA}$ be the lattice constant of graphene and consider real space and reciprocal lattices spanned by

$$\mathbf{R}_1 = (a, 0), \quad \mathbf{R}_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right), \quad (\text{C.1})$$

$$\mathbf{G}_1 = \frac{2\pi}{a} \left(1, -\frac{1}{\sqrt{3}}\right), \quad \mathbf{G}_2 = \frac{2\pi}{a} \left(0, \frac{2}{\sqrt{3}}\right). \quad (\text{C.2})$$

For N -layer Rhombohedral graphene [204, 205] (see also: [169, 177, 206, 207, 279] and references therein), consider p_z orbitals of carbon at positions

$$\mathbf{r}_{A,\ell} = \left(0, \frac{\ell-1}{\sqrt{3}}a, c\right), \quad \mathbf{r}_{B,\ell} = \left(0, \frac{\ell}{\sqrt{3}}a, c\right) \quad (\text{C.3})$$

for layer $\ell \in [1, N_L]$ with inter-layer spacing c . Let the nearest neighbor vectors be $\boldsymbol{\delta}_n = R_{n2\pi/3}(0, \frac{1}{\sqrt{3}}a)^T$ for $n = 0, 1, 2$ where R_θ is the counterclockwise rotation matrix by angle θ . Below we index sublattice by $\sigma \in \{A, B\} = \{-1, 1\}$. We define standard high-symmetry points $\mathbf{K} = \frac{2}{3}\mathbf{G}_1 + \frac{1}{3}\mathbf{G}_2$ and $\mathbf{K}' = \frac{1}{3}\mathbf{G}_1 + \frac{2}{3}\mathbf{G}_2$.

For each orbital, we have a corresponding second-quantized Fermion operator $\hat{c}_{\mathbf{R},\sigma,\ell}^\dagger = \hat{c}^\dagger(\mathbf{R} + \mathbf{r}_{\sigma,\ell})$. Its Fourier transform is $\hat{c}_{\mathbf{k}\sigma\ell}^\dagger = N^{-\frac{1}{2}} \sum_{\mathbf{R}} e^{+i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_{\sigma,j})} \hat{c}^\dagger(\mathbf{R} + \mathbf{r}_{\sigma,\ell})$, with normalization so that it obeys canonical commutation relations $\{\hat{c}_{\mathbf{k}\sigma\ell}, \hat{c}_{\mathbf{k}\sigma'\ell'}^\dagger\} = \delta_{\sigma\sigma'}\delta_{\ell\ell'}$. The Hamiltonian for N -layer rhombohedral graphene is $\hat{h}_{RG}^{(N_L)} = \sum_{\mathbf{k} \in \text{BZ}} \hat{c}_{\mathbf{k}\sigma j}^\dagger \left[h_{RG}^{(N_L)}(\mathbf{k}) \right]_{\sigma j, \sigma' j'} \hat{c}_{\mathbf{k}\sigma' j'}$

where

$$h_{RG}^{(N_L)}(\mathbf{k}) = \begin{bmatrix} h_\ell^{(0)} & h^{(1)} & h^{(2)} & & & \\ h^{(1)\dagger} & h_\ell^{(0)} & h^{(1)} & h^{(2)} & & \\ h^{(2)\dagger} & h^{(1)\dagger} & h_\ell^{(0)} & \ddots & \ddots & \\ & h^{(2)\dagger} & \ddots & \ddots & h^{(1)} & h^{(2)} \\ & & \ddots & h^{(1)\dagger} & h_\ell^{(0)} & h^{(1)} \\ & & & h^{(2)\dagger} & h^{(1)\dagger} & h_\ell^{(0)} \end{bmatrix} \quad (\text{C.4})$$

which is a matrix in layer space with entries in sublattice space

$$h_\ell^{(0)}(\mathbf{k}) = \begin{pmatrix} u_{A\ell} & -t_0 f_{\mathbf{k}} \\ -t_0 \bar{f}_{\mathbf{k}} & u_{B\ell} \end{pmatrix} \quad (\text{C.5a})$$

$$h^{(1)}(\mathbf{k}) = \begin{pmatrix} t_4 f_{\mathbf{k}} & t_3 \bar{f}_{\mathbf{k}} \\ t_1 & t_4 f_{\mathbf{k}} \end{pmatrix} \quad (\text{C.5b})$$

$$h^{(2)}(\mathbf{k}) = \begin{pmatrix} 0 & \frac{t_2}{2} \\ 0 & 0 \end{pmatrix} \quad (\text{C.5c})$$

$$f_{\mathbf{k}} = \sum_{i=0}^2 e^{i\mathbf{k} \cdot \boldsymbol{\delta}_i}. \quad (\text{C.5d})$$

We take graphene hopping $t_0 = 3.1$ eV and vertical interlayer hopping $t_1 = 380$ meV. Following e.g. [280] we take higher hopping parameters $(t_2, t_3, t_4) = (-21, 290, 141)$ meV. Finally, $u_{\sigma\ell}$ are on-site potentials that reflect internal and external displacement fields. Although their value varies with layer [279] to partially screen applied electric fields, for simplicity we consider fields with a uniform potential difference per layer u_D :

$$u_{\sigma,\ell} = u_D \left(\ell + 1 - \frac{N_L - 1}{2} \right). \quad (\text{C.6})$$

Aside from lattice translation, the model enjoys the following symmetries

$$\overline{h(\mathbf{k})} = h(-\mathbf{k}) \quad (\text{Time reversal}) \quad (\text{C.7a})$$

$$h(\mathbf{k}) = h(C_{3z}\mathbf{k}) \quad (\text{Three fold rotation}) \quad (\text{C.7b})$$

$$M_{C_{2x}} h(\mathbf{k}) M_{C_{2x}}^{-1} = h(C_{2x}\mathbf{k}) \quad (\text{Two-fold } x\text{-rotation}) \quad (\text{C.7c})$$

$$h(\mathbf{k}) = h(M_x \mathbf{k}) \quad (\text{Mirror}) \quad (\text{C.7d})$$

$$V_{\mathbf{G}} h(\mathbf{k}) V_{\mathbf{G}}^\dagger = h(\mathbf{k} + \mathbf{G}) \quad (\mathbf{G}\text{-translation}) \quad (\text{C.7e})$$

where time-reversal acts anti-unitarily, C_{2x} reverses layers as $[M_{C_{2x}}]_{\sigma\ell,\sigma'\ell'} = \delta_{\sigma,-\sigma'}\delta_{\ell,N-(\ell'+1)}$, and other symmetries have trivial orbital part. We note that the last equation is not a symmetry per se, but simply a constraint on the Hamiltonian with $[V_{\mathbf{G}}]_{\sigma'\ell',\sigma\ell} = \delta_{\sigma\sigma'}\delta_{\ell\ell'}e^{i\mathbf{G}\cdot\mathbf{r}_{\sigma,\ell}}$, reflecting the unit cell embedding.

C.1.2 Moiré Rhombohedral Graphene Hamiltonian

The direct lattice of the hBN substrate is generated by

$$\mathbf{R}'_j = M R_\theta \mathbf{R}_j; \quad M = (1 + \varepsilon)I \quad (\text{C.8})$$

where R_θ is counterclockwise rotation by θ and $\varepsilon = a_{\text{hBN}}/a_{\text{Gr}} \approx 1.018$. We take $\mathbf{G}'_j$ such that $\mathbf{R}'_j \cdot \mathbf{G}'_k = 2\pi\delta_{jk}$ as usual.

Define moiré reciprocal lattice vectors

$$\mathbf{g}_j = \mathbf{G}_j - \mathbf{G}'_j = [I - M^{-1}R_\theta]\mathbf{G}_j, \quad (\text{C.9})$$

with corresponding direct vectors $\mathbf{a}_j \cdot \mathbf{g}_k = 2\pi\delta_{jk}$ whose moiré superlattice period is

$$L_M = |\mathbf{a}_j| = a \frac{1 + \varepsilon}{\sqrt{\varepsilon^2 + 2(1 + \varepsilon)(1 - \cos\theta)}} \quad (\text{C.10})$$

and where the lattice scale mismatch rotates the moiré-Brillouin zone so that $\mathbf{a}_1$ is rotated clockwise from the x axis by an angle

$$\phi = \arctan\left(\frac{-\sin\theta}{1 + \varepsilon - \cos\varepsilon}\right). \quad (\text{C.11})$$

As θ changes from 0 to 1, the superlattice scale changes only gradually, but ϕ rotates quickly, as shown in Fig. C.1.

To conveniently express C_3 -symmetric quantities, further define $\mathbf{g}_3 = -\mathbf{g}_1 - \mathbf{g}_2$ and likewise for $\mathbf{G}_3, \mathbf{G}'_3$. We then have high-symmetry points at

$$\begin{aligned} \boldsymbol{\gamma} &= \mathbf{K}_{\text{Gr}}, \quad \boldsymbol{\kappa}^+ = \boldsymbol{\gamma} - \frac{1}{3}\mathbf{g}_1 + \frac{1}{3}\mathbf{g}_2, \\ \boldsymbol{\kappa}^+ &= \boldsymbol{\gamma} - \frac{2}{3}\mathbf{g}_1 - \frac{1}{3}\mathbf{g}_2, \quad \boldsymbol{\mu} = \boldsymbol{\gamma} - \frac{1}{2}\mathbf{g}_1. \end{aligned} \quad (\text{C.12})$$

Crucially, we have taken the center of the moiré Brillouin zone $\boldsymbol{\gamma}$ to be at the $\mathbf{K}$ -point of graphene.

We may now express the moiré potential generated by the hBN substrate. We assume that the moiré potential of the hBN substrate only affects the closest layer. We follow [187] (which uses an opposite valley convention), we have

$$V_{\text{hBN}}(\mathbf{r}) = V_0\sigma^0 + V_1\mathbf{f}(\mathbf{r}, \psi) \cdot \boldsymbol{\sigma}, \quad (\text{C.13})$$

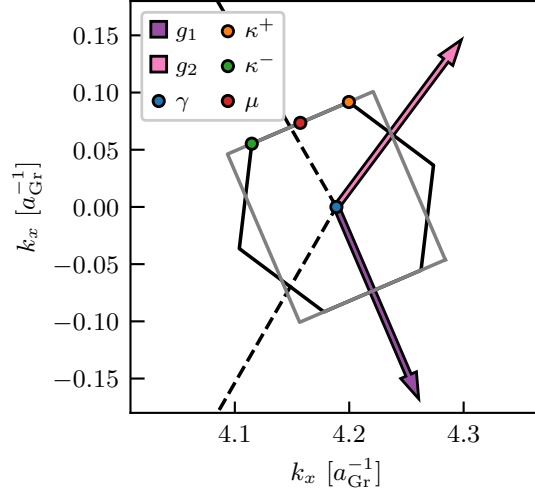


Figure C.1: Geometry of the moiré Brillouin zone at $\theta = 0.77^\circ$. The dashed line is the Brillouin zone of (unrotated) graphene, and the gray rectangle is the Brillouin zone used for DMRG (see text).

where

$$\begin{aligned} \mathbf{f}(\mathbf{r}, \psi) \cdot \boldsymbol{\sigma} = & e^{-i\psi} \left[e^{i\mathbf{g}_1 \cdot \mathbf{r}} \begin{pmatrix} 1 & 1 \\ \omega & \omega \end{pmatrix} + e^{i\mathbf{g}_2 \cdot \mathbf{r}} \begin{pmatrix} 1 & \omega^2 \\ \omega^2 & \omega \end{pmatrix} \right. \\ & \left. + e^{-i(\mathbf{g}_1 + \mathbf{g}_2) \cdot \mathbf{r}} \begin{pmatrix} 1 & \omega \\ 1 & \omega \end{pmatrix} \right] + \text{H.c.} \end{aligned} \quad (\text{C.14})$$

Unless otherwise stated we take values $(V_0, V_1, \psi) = (28.9 \text{ meV}, 21 \text{ meV}, -0.29)$ following [187]. The Hamiltonian in the K' valley is defined via time-reversal symmetry.

C.1.3 Many-Body Hamiltonian

Let the single-particle eigenstates be given by

$$\hat{h}_{kin} |\psi_{\mathbf{k}\tau sb}\rangle = \epsilon_{\mathbf{k}\tau sb} |\psi_{\mathbf{k}\tau sb}\rangle \quad (\text{C.15})$$

where $\tau \in \{K, K'\} = \{-1, 1\}$ labels valley, $s \in \{\uparrow, \downarrow\} = \{-1, 1\}$ labels spin, and b labels bands. Consider creation operators

$$c_{\mathbf{k}\tau sb}^\dagger |0\rangle = |\psi_{\mathbf{k}\tau sb}\rangle, \quad \{c_{\mathbf{k}\tau sb}, c_{\mathbf{k}'\tau's'b'}\} = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\tau\tau'} \delta_{ss'} \delta_{bb'}. \quad (\text{C.16})$$

We consider the interacting model

$$\hat{H} = \hat{h}_{kin} + \frac{1}{2A} \sum_{\mathbf{q}} U_{|\mathbf{q}|} : \hat{\rho}_{\mathbf{q}} \hat{\rho}_{-\mathbf{q}} :, U_{\mathbf{q}} = \frac{2\pi \tanh(qd)}{\epsilon_r \epsilon_0 q} \quad (\text{C.17})$$

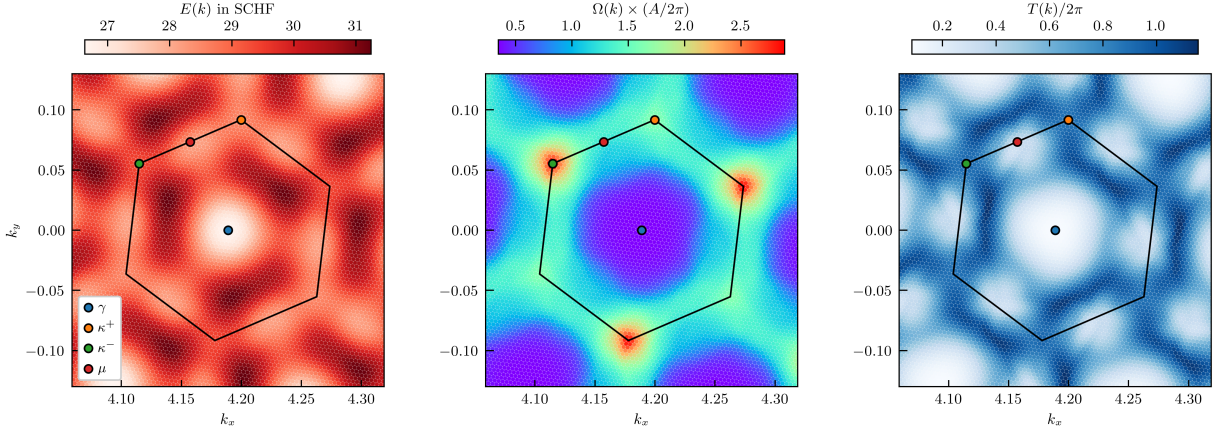


Figure C.2: Details of the SCHF state at $\nu = 1$. (Left) Dispersion. (Middle) Berry curvature. (Right) trace condition violation. Parameters: $(u_D, \theta) = (50 \text{ meV}, 0.77^\circ)$, 48×48 unit cells.

where U_q represents Coulomb interactions screened by both top and bottom gates at a distance of $d = 250 \text{ \AA}$.

To make the Hilbert space tractable, we restrict to a limited number of bands N_b above charge neutrality. (Alternatively one could use a plane-wave basis and use some number of shells of Brillouin zones around the first.) More explicitly, we work with the projected density operator,

$$\hat{\rho}_{\mathbf{q}} = \sum_{\mathbf{k}} \sum_{\alpha, \beta} \sum_{b, b' < N_b} \hat{c}_{\mathbf{k}\alpha b}^\dagger \langle \psi_{\mathbf{k}\alpha b} | e^{-i\mathbf{q} \cdot \mathbf{r}} | \psi_{\mathbf{k}+\mathbf{q}, \beta, b'} \rangle \hat{c}_{\mathbf{k}+\mathbf{q}, \beta, b'} \quad (\text{C.18})$$

where α, β index valley, spin, and b, b' labels band. In some contexts such as twisted bilayer graphene, the operation of restricting to low-energy bands is fraught with difficulties due to double-counting of interaction effects, necessitating procedures such as “Hartree-Fock subtraction” [26, 199] or more sophisticated renormalization-group treatments [272]. Happily, here these issues are ameliorated in the limit where the displacement field opens a gap comparable to or larger than the interaction strength. In that case, the insulating state at charge neutrality is a natural choice of vacuum. The operation of integrating out the “remote” higher-energy conduction bands $N_b + 1, N_b + 2, \dots$, and valence bands at mean-field level is equivalent to simply *restricting* the band indices in all sums in Eq. (C.17). We note, however, that beyond-mean-field effects like RPA-level screening from remote bands could substantially influence the system. This is often captured at a phenomenological level by increasing the relative dielectric constant ϵ_r .

C.2 Details of the Hartree-Fock calculation

We use standard self-consistent Hartree-Fock calculations to obtain the SCHF ground state of the electronic system.

C.2.1 Numerical Setup

As usual, we consider single-particle density matrices $P(\mathbf{k})_{\alpha\beta} = \langle c_{\mathbf{k}\beta}^\dagger c_{\mathbf{k}\alpha} \rangle$, where α and β are collective indices for valley, spin, and band. These density matrices are in one-to-one correspondence with Slater determinant states. We define the Hartree and Fock Hamiltonians as

$$h_H[P](\mathbf{k}) = \frac{1}{A} \sum_{\mathbf{g}} V_{\mathbf{g}} \Lambda_{\mathbf{g}}(\mathbf{k}) \left(\sum_{\mathbf{k}} \text{Tr}[P(\mathbf{k}) \Lambda_{\mathbf{g}}(\mathbf{k})^\dagger] \right) \quad (\text{C.19a})$$

$$h_F[P](\mathbf{k}) = -\frac{1}{A} \sum_{\mathbf{q}} V_{\mathbf{q}} \Lambda_{\mathbf{q}}(\mathbf{k}) P([\mathbf{k} + \mathbf{q}]) \Lambda_{\mathbf{q}}(\mathbf{k})^\dagger \quad (\text{C.19b})$$

where $[\Lambda_{\mathbf{q}}(\mathbf{k})]_{\alpha\beta} = \langle \psi_{\mathbf{k}\alpha} | e^{-i\mathbf{q}\cdot\mathbf{r}} | \psi_{\mathbf{k}+\mathbf{q}\beta} \rangle$ are form factors, and are treated as matrices whose labels are identical to the single-particle ones. The sum over $\mathbf{g}$ runs over reciprocal vectors while $\mathbf{q}$ runs over all momentum transfers. Via Wick's theorem, the energy of the Slater-determinant state is

$$E[P] = \frac{1}{2} \text{Tr}[P(2h_{\text{kin}} + h_H[P] + h_F[P])] \quad (\text{C.20})$$

where the trace is over momentum and all other band labels.

To differentiate different ground states obtained in HF, we compute the Chern number and the HF gap. We regard any states with gap $\Delta_{\text{HF}} < 5 \text{ meV}$ as a metal. For insulators, we show their Chern number in the phase diagram. We note that AHC and WLI have identical symmetry and therefore cannot be probed individually within HF by fixing symmetry. Instead, we use 50 random seeds and a few physically motivated seeds to ensure a global minimum is found and the phase boundary between AHC and WLI is better resolved.

C.2.2 Hartree-Fock Convergence

We comment briefly on the stringent criteria we have used to ensure convergence of our SCHF numerics.

We use the optimal-damping algorithm (ODA) to converge to states satisfying the self-consistency condition

$$[P, h_{\text{kin}} + h_H[P] + h_F[P]] = 0 \quad (\text{C.21})$$

to tolerances approaching the square root of machine precision (i.e. machine precision in $E[P]$). We use both rectangular and Monkhorst-Pack grids with 24×24 , 30×30 , 36×36 , or

48×48 unit cells, depending on the sensitivity of the state to finite-size effects. We impose C_3 symmetry explicitly in the Monkhorst-Pack case, but find comparable results in both cases for sufficiently large system sizes. We ensure that the range of momentum transfers $\mathbf{q}$ considered is sufficiently large to converge the energy of the state, out to several Brillouin zone distances. To avoid non-global minima, we initialize SCHF in a variety of states for each parameter point, often using a mix of physical ansatzes as well as random initial states. We also assume electrons are spin- and valley-polarized.

We now detail the convergence of our SCHF calculations as a function of the number of k -points and the number of single-particle bands. Fig. C.3(a) shows the ground state energy per electron within SCHF on a system of $N_k \times N_k$ unit cells with a Monkhorst-Pack lattice with the number of bands $N_b=7$. One can see that the energy is decreasing monotonically with the system size, and 1% relative accuracy is achieved by 24×24 unit cells. Furthermore, we note that the Berry curvature and energetic details of the isolated Chern band are qualitatively stable with system size (with the notable exception of 18×18 which is often qualitatively different, yielding different phase boundaries). We therefore conclude that 24×24 unit cells is sufficient to capture quantitative details of phase boundaries to reasonably good fidelity.

Our SCHF is carried out in a Hilbert space spanned by the projector into the lowest N_b conduction bands. We take $N_b = 7$ bands throughout the main text, a choice we now justify. At an initial qualitative level, we note that the conduction band wavefunctions come from folding the bands of rhombohedral graphene into the moiré Brillouin zone, then mixing them between $\mathbf{k}$ and $\mathbf{k} + \mathbf{g}$ under the moiré potential. We note that the first seven bands are largely supported on the first moiré Brillouin zone together with the first shell of six higher Brillouin zones. Indeed, the first seven bands span a range of kinetic energy much greater than the interaction scale. This suggests the first 7 bands span an adequately large Hilbert space to understand the physics at filling $\nu = 1$. We now investigate this claim quantitatively. Fig. C.3(b) show the SCHF energy as a function of N_b (with values chosen to match centered hexagon numbers, i.e. complete shells of Brillouin zones). One can see that the energy is converged to better than 0.5% relative error by $N_b = 7$. Furthermore, we investigate the participation of the higher bands in the Chern band that appears in SCHF at $\nu = 1$. Explicitly, we compute the participation $P_n = \frac{1}{N} (\sum_{\mathbf{k}} |\langle \phi_{\mathbf{k},1}^{\text{HF}} | \psi_{\mathbf{k},n} \rangle|^2)$ of the single-particle bands in the wavefunction of the isolated Chern band $\phi_{\mathbf{k},1}^{\text{HF}}$ at $\nu = 1$ with normalization so that $\sum_n |P_n|^2 = 1$. We find these overlaps decrease precipitously after $n = 3$ and, furthermore, we find the participations are essentially stable after $N_b = 7$. In conclusion, the SCHF ground state of our model is captured to good quantitative accuracy by 24×24 systems with $N_b = 7$.

As a final note, we emphasize that the errors from experimental and modelling uncertainties are likely to be vastly larger than numerical errors in this work.

C.2.3 Metal versus Anomalous Hall Crystal Competition

To examine the competition between the metallic “quarter metal” state and the anomalous Hall crystal shown in Fig. 1(b), we must determine the ground state energy both

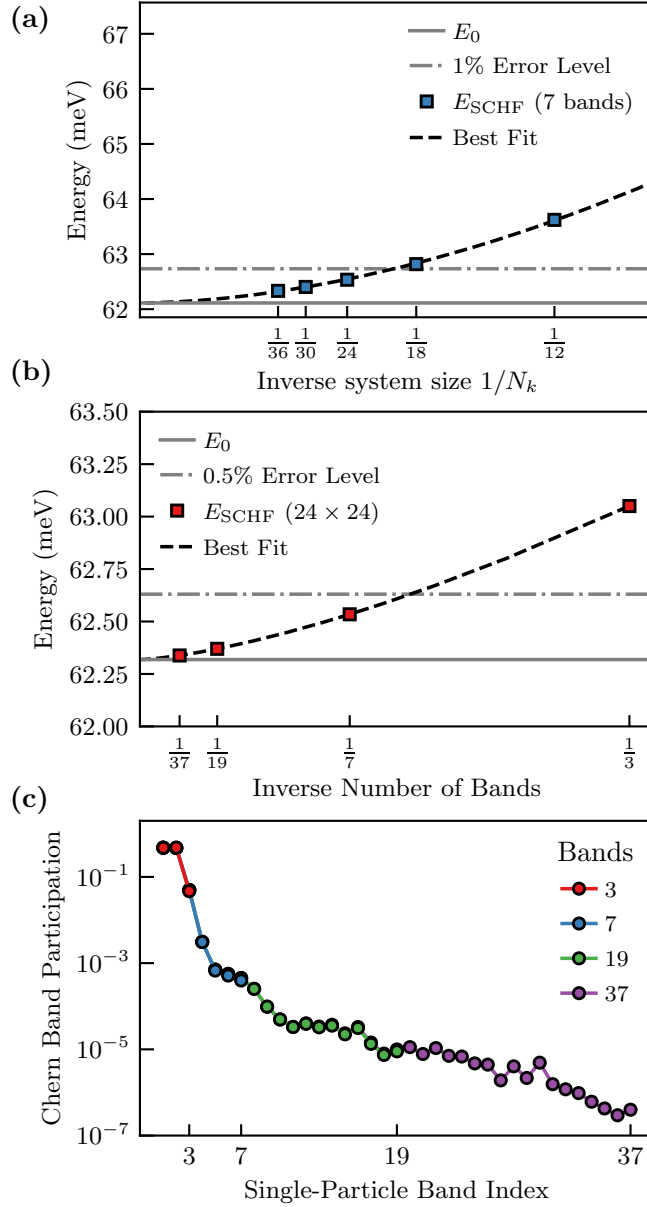


Figure C.3: Convergence details of SCHF computations. (a) SCHF Ground state energy convergence as a function of system size $N_k \times N_k$ with $N_b = 7$ bands. (b) SCHF ground state energy convergence as a function of the number of bands. (c) Participation of the single-particle bands in the isolated Chern band found within SCHF. Note that only the first three bands contribute significantly, and contributions are negligible after $N_b = 7$. Parameters: $(u_D, \theta) = (50 \text{ meV}, 0.77^\circ)$ unless specified.

with and without continuous translation symmetry. To do this, we first compute the SCHF ground state of standalone rhombohedral graphene in a patch near the K point that is much bigger than the moiré Brillouin zone, finding a metallic state with enforced continuous translation symmetry. We then compute another SCHF ground state with a folded Brillouin zone, which gives the possibility of breaking continuous translation symmetry. No hBN moiré potential is added. At small u_D , the energies from both methods agree to extremely high precision and indeed describe the same quarter-metal state. At a critical u_D , however, the translation-breaking ansatz finds a ground state with an interaction induced gap that is lower energy than the metal — the anomalous Hall crystal described in the main text.

C.2.4 Isospin symmetry breaking

A universal feature of RMG at high displacement field D and low filling ν is isospin symmetry breaking, regardless of the moiré potential. A plethora of evidence, including quantum oscillation experiments [169, 174, 175, 181] and SCHF numerics [206, 280], support a fully spin and valley polarized state around filling $n \sim 10^{11} \text{ cm}^{-2}$ (unity moiré filling at twist angle $\theta < 1^\circ$). Therefore, we assume full spin and valley polarization in the SCHF calculation presented in the main text. In this section, we justify this choice by performing SCHF with both spin and valley degrees of freedom in the parameter regime where we have observed AHC.

Group	flavor order	Symmetry		
		$SU(2)_s$	$\tilde{\mathcal{T}}$	$U(1)_v$
(i)	SP	×	✓	✓
	VP	✓	×	✓
	SVL	×	×	✓
(ii)	SVP	×	×	✓
(iii)	SIVC	×	✓	×

Table C.1: Symmetry of various magnetic orders, including the spin $SU(2)_s$ symmetry, spinless time-reversal $\tilde{\mathcal{T}}$ symmetry, and valley $U(1)_v$ symmetry.

If we neglect charge orders for the moment, different flavor orders can be classified by the isospin symmetry breaking pattern (Table C.1). We consider states in the following groups: (i) an $N_F = 2$ state, where two out of four possible spin-valley flavors are occupied evenly. This includes a spin polarized (SP) state, a valley polarized (VP) state, and a spin-valley locked (SVL) state. These are candidate states for experimentally observed “half metal” states. (ii) a spin-valley polarized (SVP) $N_F = 1$ state, where only one spin-valley species is

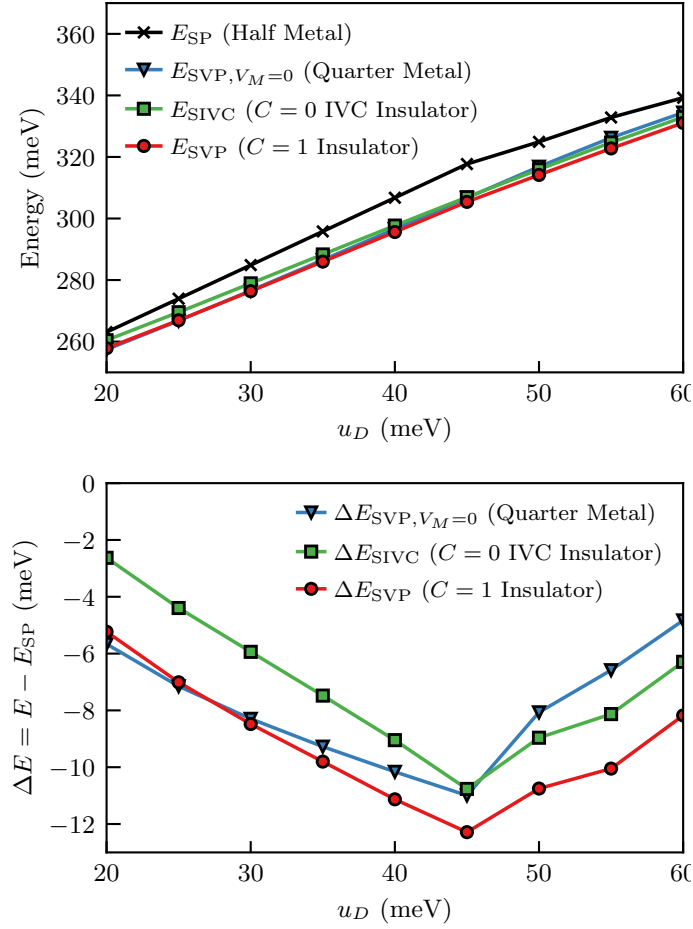


Figure C.4: Energy per electron of states with different flavor ordering patterns. (top panel) The energy per electron of four competing ground state candidate states. (bottom panel) The energy per electron of three competing candidate states relative to the $N_f = 2$ spin polarized state.

occupied, and (iii) a spin polarized IVC $N_F = 1$ state (SIVC) that breaks $U(1)_v$. The latter two groups include the “quarter metal” states seen in experiment.

Since the aforementioned states have different symmetries/quantum numbers Table C.1, we can enforce symmetries in the HF calculation and compare the energy among these states. On top of the magnetic order, we also allow translation symmetry breaking at moiré lattice vectors. Our Hamiltonian does not include any spin-orbit coupling or Hund’s term, so the system has an enlarged $SU(2)_K \times SU(2)_{K'}$ symmetry. At HF level, candidate ground states within the group (i) are degenerate, whether it be SP, VP, or SVL. We therefore choose an SP state to represent the group (i).

In the top panel of Fig. C.4, we show the energy per electron of $N_f = 2$ SP states, $N_f = 1$ SIVC states, $N_f = 2$ SVP states. For comparison, we also show SVP metallic states that do not break translation symmetry computed with $V_M = 0$.

At $\nu = 1$, we always find the $N_F = 2$ SP state to have the highest energy, so we plot the energy of the other states relative to the SP state in the bottom panel of Fig. C.4. We note that the SP states are always metallic since they correspond to $\nu = 0.5$ per flavor. We find that the isospin symmetry breaking happens at an energy scale at least 5 times bigger than the formation of an insulating state within the SVP phase (see also Fig. 1(b)).

In terms of flavor order, The closest competing state of the SVP AHC is an SIVC AHC. We find that SVP always have lower energy than SIVC, likely due to the winding energy penalty of SIVC hybridizing two Chern bands with opposite Chern number [200]. The energy splitting, however, is comparable to the energy splitting between the metallic state and the AHC state.

Finally, we make a few comments based on the SCHF data. In RMG, the energy splitting due to different mechanisms form the following hierarchy,

$$\Delta_{\text{Stoner}} \gg \Delta_{\text{AHC}} \approx \Delta_{\text{IVC}} \gg \Delta_{\text{moiré}} \quad (\text{C.22})$$

The system first forms a flavor order due to Stoner ferromagnetism, and then interaction drives the ‘quarter metal’ to an insulator with finite Chern number, while disfavoring the IVC state by Δ_{IVC} . The moiré potential is not strong enough to alter the energy competition at $\nu = 1$.

C.2.5 Identification of moiré-proximate side from $\nu = 4$ SCHF

To confirm whether our setup of moiré-proximate/distant side corresponds to that in experiments, we identify the experiment observation of correlated insulator at $N_L = 5, \nu = 4$ [117]: At low displacement field $|D| < 0.5 \text{ V/nm}$, corresponding to $u_D \sim 30 \text{ meV}$, an insulator is found at $D < 0$ side up to $|D| = 0.4 \text{ V/nm}$, but not at $D > 0$. We now will show that this agrees with our numerical observation at similar u_D , establishing a matching between the two works.

We perform self-consistent Hartree-Fock (SCHF) with both spin and valley degrees of freedom. We only include the conduction band as in the main text, and restrict ourselves

to $u_D \geq 15$ meV where the valence bands are sufficiently separated. At $\nu = 4$, we search for the ground state in the manifold without intervalley coupling, which excludes intervalley coherent (IVC) orders.

We examine the resulting charge gap Δ at different u_D , as shown in Fig. C.5, which shows a clear asymmetry between $u_D > 0$ and $u_D < 0$: a charge gap is only identified for $u_D < 0$ but not for $u_D > 0$, which agrees with the experiment described above. This suggests that the experiment identifies $\nu = 4$ insulator only on the moiré-proximate regime. Although there could be other competing orders unconsidered here, the identification of the gapless phase is expected to be robust even beyond Hartree-Fock approximations.

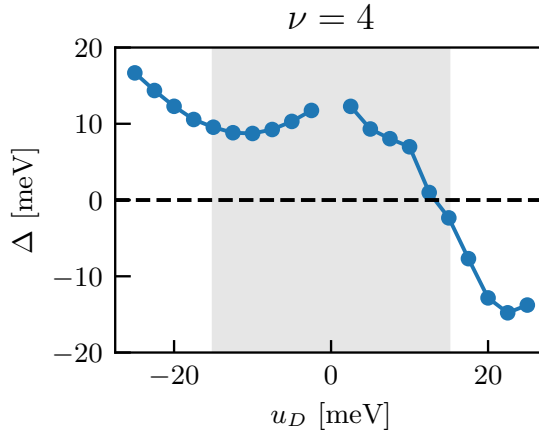


Figure C.5: Charge gap of SCHF ground state at $\nu = 4$ for $N_L = 5$. Model parameters follow Appendix C.2.1, but include both spins and valleys. $|u_D| < 15$ meV results are shaded since they are less reliable in SCHF. Parameters: $\theta = 0.77^\circ$, 30×30 unit cells.

C.2.6 Details of N_L - u_D phase diagram

Fig. C.6 shows the extended N_L - u_D phase diagram in Fig. 1(c) which we extend up to $u_D = 160$ meV. Each N_L shows similar patterns as $N_L = 5$ discussed in Fig. 2(a). First, a broad regime of $C = -1$ AHC phase is stabilized at moderate u_D . The lower critical u_D , referred to as u_D^* in the main text, decreases with N_L , indicating the stronger relevance of AHC in higher- N_L rhombohedral graphenes. Meanwhile, the higher critical u_D is controlled by the development of an indirect band gap between $C = -1$ band and higher bands, which leads to a first-order transition into metal (and occasionally the “reentrance” of $C = -1$ state at $N_L = 4$.) At even higher u_D , other phases such as the $C = 0$ insulator take over, but given the stronger band mixing it is necessary to include more bands in SCHF to accurately resolve the phase competition. We therefore caution against trusting the phase diagram at large u_D .

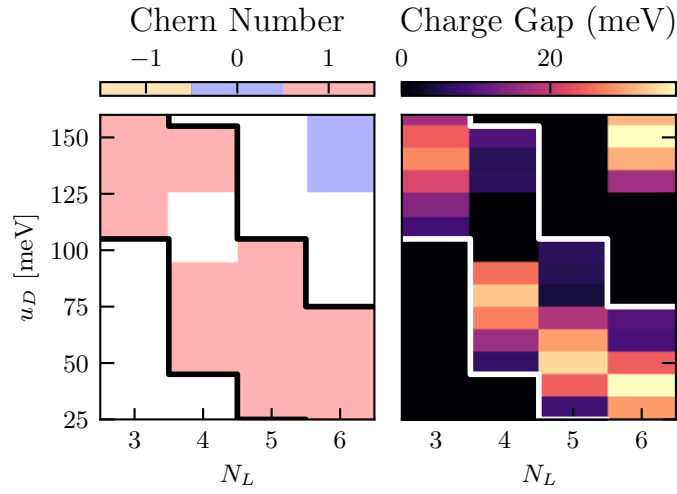


Figure C.6: (a) Chern-number and (b) charge-gap phase diagram at $\nu = 1$ for rhombohedral graphene with $N_L = 3 - 6$ and $u_D = 0 - 160$ meV, with fixed $\theta = 0.77^\circ$ and $\epsilon_r = 5$ at each N_L . The boundary of $C = -1$ AHC phase is highlighted. The white region in the Chern-number plot denotes metal with a direct or indirect band gap. Parameters: $\theta = 0.77^\circ$, 36×36 unit cells.

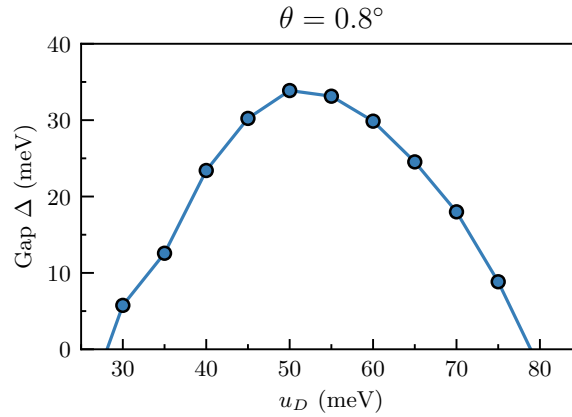


Figure C.7: Dependence of charge gap on u_D at $N_L = 5$, $\theta = 0.8^\circ$ and $\epsilon_r = 5$. We take a 30×30 unit cell. A clear non-monotonic dependence of the charge gap on u_D is observed.

We note that the charge gap, shown in Figs. C.6 and C.7, has sensitive and non-monotonic dependence on displacement u_D . However, it is not directly proportional to the moiré potential, shown in Fig. 3(a) of the main text. Here we also comment on the observable effects

of the charge gap. In addition to the thermal activation behavior expected in transport measurements, the width of the plateau with quantized Hall conductance also depends on the charge gap [281, 282]. If we assume that impurities induce subgap localized states with a constant density of states, the Hall conductance will remain quantized until the doped charge fully fills all subgap states, whose total density is proportional to the charge gap. In Ref. [117], the plateau width of the $\nu = 1$ Chern insulator also behaves non-monotonically with the displacement field, possibly related to this behavior of the charge gap.

C.2.7 Effect of Graphene-Scale Parameters

This section considers the effect of the graphene-scale parameters on our results. An important phenomenon in graphene and its related systems is the renormalization of the Fermi velocity by Coulomb interactions, which has been observed experimentally [2, 283, 284]. Namely, the effective velocity (i.e. t_0) increases as the energy scale or filling approaches charge neutrality. When discussing phenomena such as those here that depend on both a small moiré scale and a much larger displacement field scale, it is unclear which Fermi velocity to employ. Estimates in the literature for $u_D = 0$ vary between $t_0 \approx 2.6$ eV and $t_0 \approx 3.1$ eV, depending on the relevant energy scales, number of layers, and other details [169, 204]. Moreover, this problem is exacerbated by the fact that one must use a “bare” Fermi velocity in models to which interactions are added, but renormalization of the velocity is a beyond-mean-field effect.

We now show changing the Fermi velocity dramatically shifts the phase boundaries but not the phases present. Fig. C.8 shows phase diagrams at $\nu = 1$ within SCHF for $t_0 = 2.6$ eV and 3.1 eV, respectively. The latter option is used in the main text and throughout the rest of this work. Given that the various ground states candidates are separated on the $O(1)$ meV scale, this 500 meV perturbation has a remarkably small effect. Comparing Fig. C.8 (a) and (b), one sees that the smaller t_0 favors $C = 0$ over $C = 1$. This remarkable resilience of the Chern band to these parameter changes suggests a much smaller number of hidden parameters that control the phase diagram. Future work will explicate this phenomenon.

In addition, it turns out that even large differences in the graphene-scale parameters do not strongly affect our results at $\nu = 1$. Fig. C.9 demonstrates the robustness of AHC as the higher hopping terms are varied. Explicitly, we replace hopping terms $t_{2,3,4}$ in Eq. (C.4) with $\lambda t_{2,3,4}$, where $\lambda = 1$ correspond to realistic RMG and $\lambda = 0$ correspond to simplified RMG with only nearest-neighbor hoppings. We then compute its ground state at $\lambda \in (0, 1)$, which all result in AHC phases with $C = -1$. The charge gap of the ground state remains large through the tuning, suggesting the stability of the phase. The bandwidth of the $C = -1$ band gradually increases at lower λ , which indicates its deviation from the optimal condition realizing FQAH.

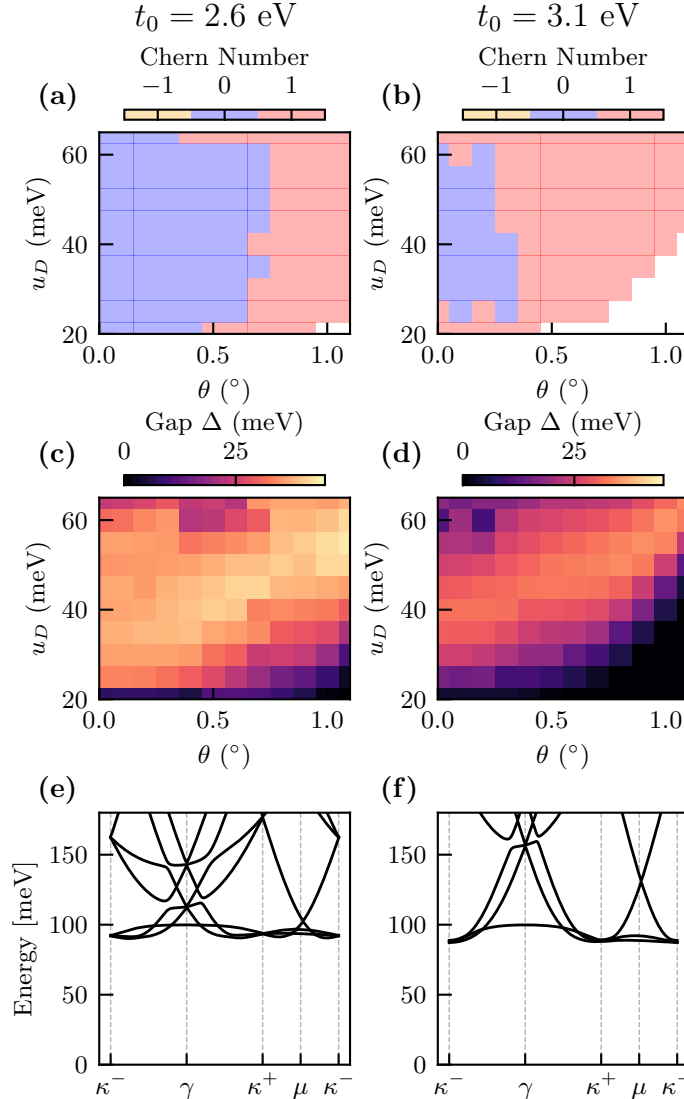


Figure C.8: The effect of large versus small Fermi velocity is minimal. (a,b) SCHF phase diagrams at $\nu = 1$ as a function of twist angle θ and vertical displacement field u_D , showing the difference between large Fermi velocity, corresponding to $t_0 = 3100$ meV, versus small Fermi velocity with $t_0 = 2600$ meV. Here colors show the Chern number of insulators, and gray data points have gaps of 2 meV or less. (c,d) Charge gaps above $\nu = 1$ within SCHF. (e,f) Single-particle ($\nu = 0$) bandstructures at large and small Fermi velocity. Note that the gap to the second band at γ increases dramatically at large t_0 .

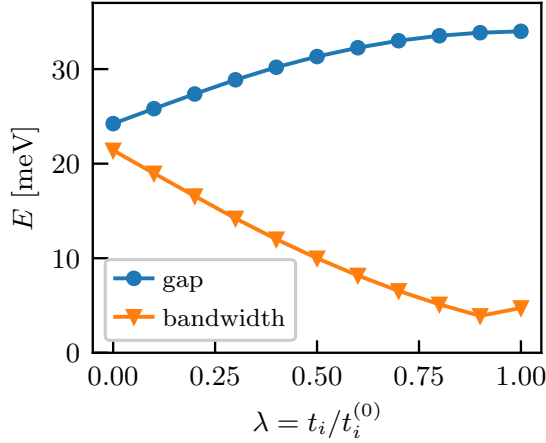


Figure C.9: Charge gap and bandwidth of RMG ground states with modified hopping strength $\lambda t_{2,3,4}$, $\lambda \in (0, 1)$. All ground states are found to be AHC phase with $C = -1$. Parameters: $(u_D, \theta) = (50 \text{ meV}, 0.77^\circ)$, 30×30 unit cells.

C.3 Details of the Many-Body Numerics at Fractional Filling

To determine the many-body ground state at fractional filling, we undertake a two-step procedure: (1) solve for the SCHF ground state at filling $\nu = 1$ and then (2) solve the many-body problem restricted to the lowest SCHF band (which is spin and valley-polarized) at fractional filling using either exact-diagonalization or the density-matrix renormalization group numerics.

An explicit assumption of such numerics is spin- and valley-polarization within the whole range $0 \leq \nu \leq 1$. When should this procedure be valid? It is first helpful to review the experimental phenomena. Ref [117] reported Laughlin and Jain sequence states at fillings $\nu = 2/5, 3/7, 4/9, 4/7, 3/5$ as well as $\nu = 2/3$. Crucially, they also reported that the region of large Hall conductance only extends down to $\nu = 0.2 - 0.4$ (depending on u_D), whereupon it transitions to a “speckled” region that may be due to Wigner crystallization. Our assumption that the many-body ground state is within the many-body Hilbert space of the $\nu = 1$ Chern band is clearly violated at this point, rendering our model inapplicable for sufficiently low fillings. It is also helpful to note the simpler case of the lowest Landau level, where the fractional state at $\nu = 2/3$ can be spin unpolarized [227–229] despite a spin-polarized LL being favored at $\nu = 1$.

It is unclear how to perform the corresponding computation without spin polarization, as it is unclear what the 2-band low-energy (i.e. 1 band with spin) Hilbert space should be considered. One *cannot* simply add spin to the $\nu = 1$ Chern band; instead one must restrict to a spinful Hilbert space from the full Hilbert space. Determining such a minimal model

may require a four-flavor many-body calculation with many-band and is beyond the scope of the current work. Nevertheless, we expect that spin- and valley-polarized states are at least low-energy candidate ground states through most of the range. We therefore work within the one-band model to examine the presence of Jain sequence states in the simplest scenario.

Explicitly, this is done as follows. Consider the SCHF Hamiltonian $h_{HF}[P]$ at $\nu = 1$, which may be diagonalized as

$$h_{HF}[P]_{\alpha\beta}(\mathbf{k})U_{\beta\gamma}(\mathbf{k}) = U_{\alpha\gamma}(\mathbf{k})E_{\gamma}(\mathbf{k}). \quad (\text{C.23})$$

We may then pass to the basis of Hartree-Fock bands

$$|\phi_{\mathbf{k}\alpha}\rangle = |\psi_{\mathbf{k}\beta}\rangle U_{\beta\alpha}(\mathbf{k}), \quad (\text{C.24})$$

which constitutes a unitary rotation of our set of N_b low-energy bands. We may then integrate out the $N_b - 1$ bands above the $\nu = 1$ gap at mean-field level — which again is simply an index restriction — to arrive at a one-band Hamiltonian

$$\hat{H} = \sum_{\mathbf{k}} t_{\mathbf{k}} \hat{n}_{\mathbf{k}} + \frac{1}{2A} \sum_{\mathbf{q}, \mathbf{k}, \mathbf{k}'} U_{\mathbf{q}} \lambda_{\mathbf{q}}(\mathbf{k}) \lambda_{-\mathbf{q}}(\mathbf{k}') \hat{d}_{\mathbf{k}}^{\dagger} \hat{d}_{\mathbf{k}'}^{\dagger} \hat{d}_{\mathbf{k}'-\mathbf{q}} \hat{d}_{\mathbf{k}+\mathbf{q}}, \quad (\text{C.25})$$

where $\hat{d}_{\mathbf{k}}|0\rangle = |\phi_{\mathbf{k}0}\rangle$ is a creation operator for the lowest SCHF band, a band with form factors $\lambda_{\mathbf{q}}(\mathbf{k}) = \langle \phi_{\mathbf{k}0} | e^{-i\mathbf{q}\cdot\mathbf{r}} | \phi_{\mathbf{k}+\mathbf{q}0} \rangle$, and $\hat{n}_{\mathbf{k}} = \hat{d}_{\mathbf{k}}^{\dagger} \hat{d}_{\mathbf{k}}$. Note that while we have projected into the Hilbert space of the first SCHF band, the kinetic energy of the band is determined relative to $\hat{H}_{\text{RMG}}$ at $\nu = 0$ to avoid double-counting interactions.

C.3.1 Exact Diagonalization at Fractional Filling

To perform exact diagonalization, we compute Eq. (C.25) on a momentum space Monkhorst-Pack grid $\mathbf{k}[n_1, n_2]$ of size $N_{k_1} \times N_{k_2}$. We then subsample that grid on points

$$\{\mathbf{k}[s_1 m_1 + \phi_1, s_2 m_2] : 0 \leq m_1 < M_1, 0 \leq m_2 < M_2\}, \quad (\text{C.26})$$

to produce a grid of size $M_1 \times M_2$ where the integer ratios s_i obey $s_1 M_1 = N_{k_1}$ and $s_2 M_2 = N_{k_2}$. Here $0 \leq \phi_1 < s_1$ is an offset in the subsampling to enable flux threading. For the main text, we take $N_{k_1} \times N_{k_2} = 36 \times 36$ and $M_1 \times M_2 = 4 \times 6$.

Exact diagonalization was performed at a range of fractional fillings to determine their suitability for fractional quantum Hall states: $\nu = 1/3, 2/5, 3/5, 4/7, 3/5, 2/3$. At each filling we computed spectrum over a range of system sizes and performed flux threading along k_x for the largest system size available, with $N_k = N_{k_1} \times N_{k_2}$ up to 30. The results are shown in Fig. C.10.

The top row of Fig. C.10 shows the low-lying spectrum at all center of mass momenta for each system size. In each case, we observe a quasi-degenerate ground states with degeneracy q at filling $\nu = p/q$, with a gap of 1 meV to 3 meV, depending on filling. This suggests that the ground states here are all fractional Chern insulators of Laughlin and Jain type.

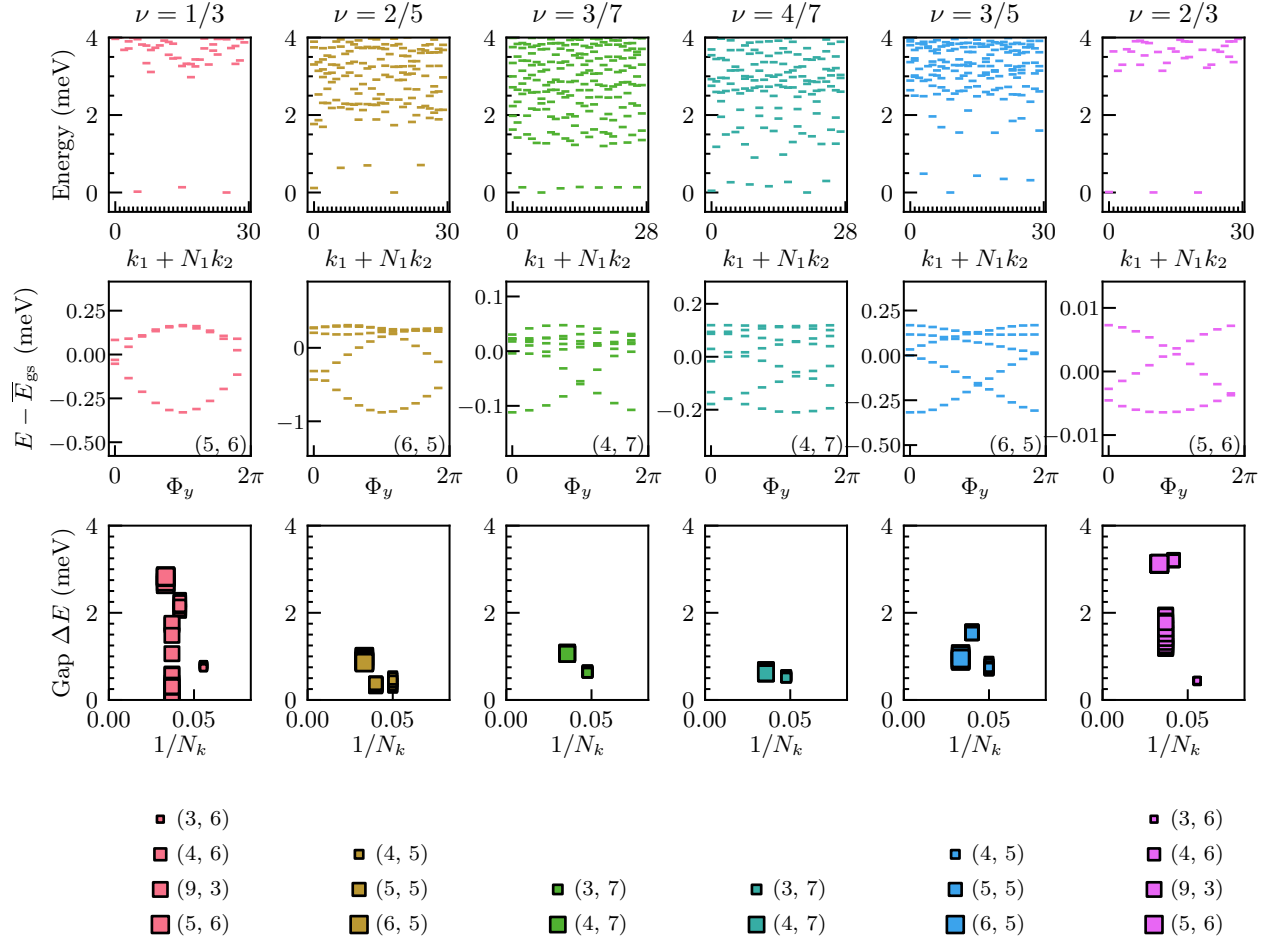


Figure C.10: Exact diagonalization at various fractional fillings over the lowest $\nu = 1$ band of RMG. Top row: spectra at the largest system sizes available at each filling. Second row: spectral flow under flux threading. Third row: system size dependence, showing the gap between the quasidegenerate ground states and the first excited state for all fluxes at each available system size. Details in text. Parameters: $\theta = 0.77^\circ$, $u_D = 50$ meV, other parameters match Fig. 2 of the main text

To support this inference, the second row of Fig. C.10 shows the spectral flow under flux threading for each filling. To make the permutation of states clear, we plot energies $E - \bar{E}_{\text{gs}}$, where $\bar{E}_{\text{gs}}(\Phi_y)$ is the average energy of the quasidegenerate ground states at each flux Φ_y . For instance $\nu = 2/3$, the spectral flow clearly permutes the ground states on a 5×6 site cluster (see main text on 4×6 sites). Indeed, we see a permutation of the quasidegenerate ground states for each filling for at least some system sizes. Explicitly, we see such a spectral flow for 5×6 at $\nu = 1/3$, but the 9×3 cluster is gapless at the same filling. This flux pumping evidence supports the inference that FCIs of Laughlin and Jain types are ground state competitors at each filling we consider. However, they may not be the true ground state at all fillings in the thermodynamic limits.

Finally, the bottom row of Fig. C.10 shows the system size dependence of the gaps. For each system size, we show the gap between the top quasidegenerate ground state and the next state in the spectrum at the same filling with any momentum. Each box represents that gap at one value of the flux, and the sizes of the boxes increase with system size. We note that the system size dependence is highly non-monotonic and far from the scaling regime, suggesting that finite size effects dominate the results — as expected for a system with such concentrated Berry curvature pockets and other quantum geometric features. Of particular note is the system sizes 9×3 at $\nu = 1/3$ filling, where we observe gap closings under spectral flow. This suggests a qualitatively different state is stabilize at these oblong aspect ratios, whose energy per electron is slightly less than the competing FCI state (at these small system sizes).

Overall we may conclude that FCIs are low-energy ground state *candidates* at all fillings $\nu = 1/3, 2/5, 3/7, 4/7, 3/5, 2/3$. However, the many-body gaps for these states are small at $\nu = 2/5$, and can vanish entirely at $\nu = 1/3$, depending on the cluster considered. Moreover, the gaps have not stabilized on even the largest sizes we could consider, and we find small changes in parameters such as u_D often favor CDW orders or Fermi liquids. Finally, modelling uncertainty greatly exceeds finite-size effects here. The balance of the evidence supports the following conclusions: filling $1/3$ is inconclusive; $2/5$ and $4/7$ are likely FCIs with small gaps, and $3/7, 3/5, 2/3$ have FCI ground states within our model.

C.3.2 DMRG at Fractional Filling

To apply the density-matrix renormalization group, we follow previous work on moiré DMRG systems [6, 39, 50, 199] to place the system onto an infinite cylinder geometry. We start with a rectangular moiré Brillouin zone, shown in Fig. C.1, with side lengths $B_1 = |\mathbf{g}_1|, B_2 = \frac{\sqrt{3}}{2} |\mathbf{g}_2|$. We impose periodic boundary conditions in the “2” direction corresponding to momentum discretization

$$k_2[n] = B_2 \times \begin{cases} -\frac{1}{2} + \frac{n + \frac{\Phi_2}{2\pi}}{N_2} & \text{if } N_2 \equiv 0 \pmod{2} \\ -\frac{1}{2} + \frac{n + \frac{\Phi_2}{2\pi} + \frac{1}{2}}{N_2} & \text{if } N_2 \equiv 1 \pmod{2} \end{cases}, \quad (\text{C.27})$$

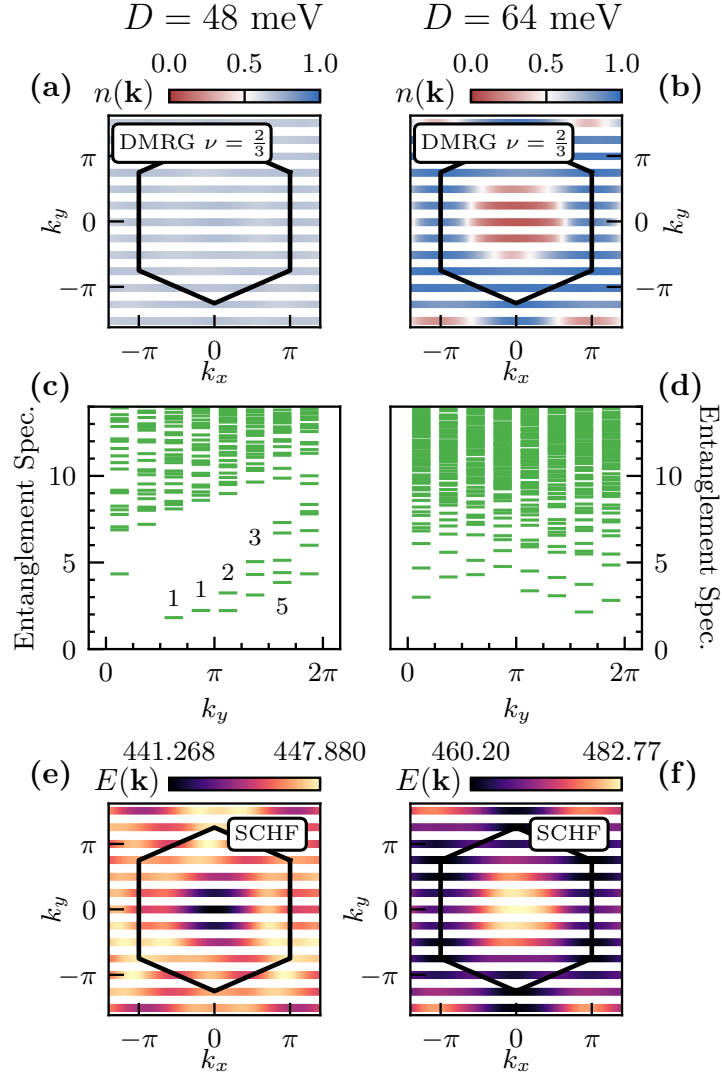


Figure C.11: DMRG results at $u_D = 48$ meV (left) and 64 meV (right). Here (a,b) give occupations over the Brillouin zone, (c,d) give entanglement spectra, and (e,f) show the dispersion of the corresponding lowest SCHF Chern band at $\nu = 1$. See text for details.

relative to an origin at moiré- γ . This gives N_2 evenly spaced “wires” across the Brillouin zone, which intersect the γ point for flux $\Phi_2 = 0$.

We then take a basis of hybrid Wannier functions along each wire, i.e. maximally localized along $\mathbf{a}_1$ and periodic along $\mathbf{a}_2$:

$$|w_{n,k_2}\rangle = \frac{1}{\sqrt{N_1}} \sum_{\mathbf{k}_1} |\varphi_{\mathbf{k}}\rangle e^{-i\mathbf{n}\mathbf{k}\cdot\mathbf{a}_1}; \quad |\varphi_{\mathbf{k}}\rangle = |\phi_{\mathbf{k}0}\rangle e^{i\zeta(\mathbf{k})}. \quad (\text{C.28})$$

Here the gauge choice $\zeta(\mathbf{k})$ is chosen such that

$$\hat{T}_1 |w^{n,k_2}\rangle = |w^{n-1,k_2}\rangle \quad (\text{C.29a})$$

$$\hat{T}_2 |w^{n,k_2}\rangle = e^{i2\pi k_2/B_2} |w^{n,k_2}\rangle \quad (\text{C.29b})$$

$$\hat{P} e^{-i\hat{r}_1 B_1} \hat{P} |w^{n,k_2}\rangle = e^{i2\pi P_1(k_2)} |w^{n,k_2}\rangle \quad (\text{C.29c})$$

where the polarizations $P_1(k_2) = \frac{B_1}{2\pi} \langle w^{0,k_2} | \hat{r}_1 | w^{0,k_2} \rangle$ are the centers of the Wannier orbitals in the first unit cell, in accordance with the modern theory of polarization [285]. The Hamiltonian (C.25) can be straightforwardly expressed in terms of fermion operators $\hat{f}_{n,k_2}^\dagger |0\rangle = |w_{n,k_2}\rangle$ on an infinite cylinder geometry. As this is a long-ranged, two-dimensional Hamiltonian, working with it efficiently as a matrix product operator (MPO) requires the technique of “MPO Compression” developed by some of us [50, 69], which creates a faithful low-rank approximation of the Hamiltonian with errors below the 10^{-2} meV level.

We then apply standard DMRG using the open-source tenpy [286] library. We work at cylinder circumference $L_y = 8$. For FCI states, we converge the ground state to norm error below 10^{-13} on bond dimensions up to $\chi = 1536$ — since the state is fully gapped, only moderate bond dimensions are required. To diagnose the fractional Chern insulator we use the entanglement spectrum technique first proposed by [208], finding the characteristic degeneracy counting matching partition numbers 1, 1, 2, 3, 5, 7, ... for each bond. We have also verified this holds for $L_y = 5, 6$.

Fig. C.11 compares the results of DMRG at two difference displacement fields, $u_D = 48$ meV and $u_D = 64$ meV. The first is selected as the location where the FCI gap is maximized in ED. The second is in a regime where the $\nu = 1$ state is still a Chern band, but whose bandwidth is now ~ 20 meV and trace condition violation is ≈ 1 . Both systems are at $\theta = 0.77^\circ$ and all other parameters are identical.

Fig C.11(a,b) shows the occupation numbers $n(\mathbf{k}) = \langle \hat{c}_{\mathbf{k}}^\dagger \hat{c}_{\mathbf{k}} \rangle$ across the Brillouin zone for both displacement fields. For $u_D = 48$ meV, $n(\mathbf{k}) = \frac{2}{3} \pm 0.04$ over the whole Brillouin zone, whereas for $u_D = 64$ meV the occupations $n(\mathbf{k})$ vary from 0.08 to 0.95 at $\chi = 1536$. Moreover, the occupations are almost entirely depleted near γ , precisely where the SCHF bandstructure, Fig C.11(f), is peaked. We further check that the charge 0 and charge 1 correlation lengths are increasing with bond dimension, which gives further confirmation of gapless modes in these channels as expected from a Fermi liquid. The entanglement spectrum Fig C.11(d) does not have a clear low-lying branch separated from the rest of

the spectrum, and is clearly not chiral with the expected CFT degeneracies. The large displacement field system at $u_D = 64 \text{ meV}$ is therefore a Fermi liquid. However, we caution that this Fermi liquid from doping the $\nu = 1$ Chern band may not correspond to the experimentally-observed Fermi liquid at larger displacement fields.

Appendix D

Appendix to chapter 5

The Appendices to this chapter are organized as follows.

Appendix D.1 discussion on the non-linear sigma model (NLsM) under Hartree-Fock (HF) approximation.

D.1.1 general formulation of Hartree-Fock in the lowest Landau level.

D.1.2 derivation of the NLsM from the HF Hamiltonian.

D.1.3 parameters in the NLsM obtained from gate-screened Coulomb interaction.

D.1.4 analytical solution of the NLsM in weak junction and the corresponding Josephson energy.

D.1.5 estimation of charge gap of the exciton condensate and layer-polarized state and the resulting restrictions.

Appendix D.2 discussion on the validity of the lumped element model and its connection to the NLsM.

D.1 Non-linear sigma model under Hartree-Fock approximation

In this section, we derive the non-linear sigma model (NLsM) by using the HF approximation [256]. It also provides an estimate of the coefficients in the NLsM in terms of microscopic parameters, which is useful for calculating the Josephson coupling in realistic devices. We begin with writing down the HF Hamiltonian in most general situations, multi-flavor electrons in the lowest Landau level (LLL). Then, we derive the NLsM for the specific case, the bilayer quantum Hall problem with spinless fermion.

D.1.1 General formulation of Hartree-Fock in the lowest Landau level

Consider a two-dimensional electron gas with various flavors labeled by a , which can be layers, spins, etc. We assume a generic two-body interaction $V_{ab}(\mathbf{r})$ and an external potential $U_a(\mathbf{r})$. The Hamiltonian after the LLL projection is

$$H = \frac{1}{2} \sum_{a,b} \int V_{ab}(\mathbf{r}_1 - \mathbf{r}_2) c_a^\dagger(\mathbf{r}_1) c_b^\dagger(\mathbf{r}_2) c_b(\mathbf{r}_2) c_a(\mathbf{r}_1) d\mathbf{r}_1 d\mathbf{r}_2 + \sum_a \int U_a(\mathbf{r}) c_a^\dagger(\mathbf{r}) c_a(\mathbf{r}) d\mathbf{r}, \quad (\text{D.1})$$

where $c_a(\mathbf{r})$ is the fermion annihilation operator projected onto the LLL. We choose a periodic boundary condition along the y direction and adopt the Landau gauge $A_x = 0$, $A_y = -Bx$, and have

$$c_a(\mathbf{r}) = \frac{1}{\sqrt{L_y}} \sum_k \varphi_k(x) e^{iky} c_{k,a}, \quad \varphi_k(x) = \left(\frac{1}{\pi \ell_B^2} \right)^{1/4} e^{-\frac{(x - k\ell_B^2)^2}{2\ell_B^2}} \quad (\text{D.2})$$

where k is the momentum in the y direction and also controls the center of the wave function $\varphi_k(x)$ in the x direction. It is more convenient to work in the momentum space. Therefore, let us introduce $A = L_x L_y$ as the area of the 2D system and $V_{ab}(\mathbf{r}) = \frac{1}{A} \sum_{\mathbf{q}} \tilde{V}_{ab}(\mathbf{q}) e^{-i\mathbf{q} \cdot \mathbf{r}}$ as the two-body interaction in the momentum space. The interacting Hamiltonian can be then rewritten as

$$H_{\text{int}} = \frac{1}{2A} \sum_{a,b} \sum_{\mathbf{q}, k, k'} \tilde{V}_{ab}(\mathbf{q}) F(\mathbf{q}) F(-\mathbf{q}) e^{iq_x(k' - k)\ell_B^2} c_{k - \frac{q_y}{2}, a}^\dagger c_{k' + \frac{q_y}{2}, b}^\dagger c_{k' - \frac{q_y}{2}, b} c_{k + \frac{q_y}{2}, a} \quad (\text{D.3})$$

where $F(\mathbf{q}) = e^{-|\mathbf{q}|^2 \ell_B^2 / 4}$ is the LLL form factor.

In the HF approximation, we assume that the ground state and the low-energy excited states can be well approximated by Slater determinants. Within this variational manifold, the interacting Hamiltonian is decoupled into a Hartree and Fock term $H_{\text{int}} = H_{\text{Hartree}} + H_{\text{Fock}}$. The Hartree term comes from the direct interaction

$$H_{\text{Hartree}} = \frac{1}{A} \sum_{a,b} \sum_{\mathbf{q}, k, k'} \tilde{V}_{ab}(\mathbf{q}) F(\mathbf{q}) F(-\mathbf{q}) e^{iq_x(k' - k)\ell_B^2} c_{k - \frac{q_y}{2}, a}^\dagger c_{k + \frac{q_y}{2}, a} \langle c_{k' + \frac{q_y}{2}, b}^\dagger c_{k' - \frac{q_y}{2}, b} \rangle \quad (\text{D.4})$$

The Fock term comes from the exchange interaction

$$H_{\text{Fock}} = -\frac{1}{A} \sum_{a,b} \sum_{\mathbf{q}, k, k'} \tilde{V}_{ab}(\mathbf{q}) F(\mathbf{q}) F(-\mathbf{q}) e^{iq_x(k' - k)\ell_B^2} c_{k - \frac{q_y}{2}, a}^\dagger c_{k' - \frac{q_y}{2}, b} c_{k' + \frac{q_y}{2}, b}^\dagger c_{k + \frac{q_y}{2}, a} \quad (\text{D.5})$$

where the minus sign comes from the fermi statistics.

It will help both the analytical and numerical manipulation if we can write the Hartree and Fock term in a similar form and treat them on an equal footing. Let us introduce

$$n_{ab}(\mathbf{q}) = \sum_k e^{-iq_x k \ell_B^2} c_{k - q_y/2, a}^\dagger c_{k + q_y/2, b}, \quad (\text{D.6})$$

which characterizes the charge fluctuation in the momentum space. Note that so-defined $n_{ab}(\mathbf{q})$ is different from the naive Fourier transformation of the projected density operator $c_a^\dagger(\mathbf{r})c_b(\mathbf{r})$. The Hartree term becomes

$$H_{\text{Hartree}} = \frac{1}{A} \sum_{a,b} \sum_{\mathbf{q}} \tilde{V}_{ab}^{\text{Hartree}}(\mathbf{q}) n_{aa}(\mathbf{q}) \langle n_{bb}(-\mathbf{q}) \rangle, \quad \tilde{V}_{ab}^{\text{Hartree}}(\mathbf{q}) = \tilde{V}_{ab}(\mathbf{q}) F(\mathbf{q}) F(-\mathbf{q}). \quad (\text{D.7})$$

For the Fock term, we first realize that the four fermion operators can be rewritten via n_{ab} by manipulating the momenta as follows

$$\begin{aligned} & \sum_{k,k'} e^{iq_x(k'-k)\ell_B^2} c_{k-\frac{q_y}{2},a}^\dagger c_{k'+\frac{q_y}{2},b} \langle c_{k'+\frac{q_y}{2},b}^\dagger c_{k+\frac{q_y}{2},a} \rangle \\ &= \sum_{k_1,p_y} e^{iq_x p_y \ell_B^2} c_{k_1-\frac{p_y}{2}-q_y,a}^\dagger c_{k_1+\frac{p_y}{2}-q_y,b} \langle c_{k_1+\frac{p_y}{2},b}^\dagger c_{k_1-\frac{p_y}{2},a} \rangle, \quad (k = k_1 - \frac{p_y}{2} - \frac{q_y}{2}, k' = k_1 + \frac{p_y}{2} - \frac{q_y}{2}) \\ &= \frac{1}{N_\phi} \sum_{k_1,k_2,\mathbf{p}} e^{iq_x p_y \ell_B^2 - i(k_1-k_2)p_x \ell_B^2} c_{k_1-\frac{p_y}{2}-q_y,a}^\dagger c_{k_1+\frac{p_y}{2}-q_y,b} \langle c_{k_2+\frac{p_y}{2},b}^\dagger c_{k_2-\frac{p_y}{2},a} \rangle, \quad (N_\phi = A/2\pi\ell_B^2) \\ &= \frac{1}{N_\phi} \sum_{\mathbf{p}} e^{i(q_x p_y - q_y p_x) \ell_B^2} n_{ab}(\mathbf{p}) \langle n_{ba}(-\mathbf{p}) \rangle \end{aligned}$$

After renaming the dummy variables we have

$$\begin{aligned} H_{\text{Fock}} &= -\frac{1}{A} \sum_{a,b} \sum_{\mathbf{q}} \tilde{V}_{ab}^{\text{Fock}}(\mathbf{q}) n_{ab}(\mathbf{q}) \langle n_{ba}(-\mathbf{q}) \rangle, \\ \tilde{V}_{ab}^{\text{Fock}}(\mathbf{q}) &= \frac{1}{N_\phi} \sum_{\mathbf{q}'} \tilde{V}_{ab}(\mathbf{q}') F(\mathbf{q}') F(-\mathbf{q}') e^{i(q'_x q_y - q'_y q_x) \ell_B^2} \end{aligned} \quad (\text{D.8})$$

This way the Hartree (D.7) and Fock Hamiltonian (D.8) are in the same form and we can write the total HF Hamiltonian as

$$\begin{aligned} H_{\text{HF}} &= \frac{1}{A} \sum_{a,b} \sum_{\mathbf{q}} \tilde{V}_{ab}^{\text{HF}}(\mathbf{q}) n_{ab}(\mathbf{q}), \\ \tilde{V}_{ab}^{\text{HF}}(\mathbf{q}) &= \delta_{a,b} \sum_c \tilde{V}_{ac}^{\text{Hartree}}(\mathbf{q}) \langle n_{cc}(-\mathbf{q}) \rangle - \tilde{V}_{ab}^{\text{Fock}}(\mathbf{q}) \langle n_{ba}(-\mathbf{q}) \rangle \end{aligned} \quad (\text{D.9})$$

with which one can have a more efficient numerical implementation than using their original form (D.4) and (D.5).

We assume that the ground state is translationally invariant along the y direction but not necessarily along the x direction. Then the fermion two-point function is

$$\langle c_{k,b}^\dagger c_{k',a} \rangle = \delta_{k,k'} P_{ab}(k) \quad (\text{D.10})$$

where $P(k)^2 = P(k)$ is a Hermitian spectral projector. In the Landau gauge $P_{ab}(k)$ captures the charge fluctuation around $x = k\ell_B^2$. Accordingly, we can define the real-space interaction as

$$V_{ab}^X(x) = \frac{1}{L_x} \sum_{q_x} \tilde{V}_{ab}^X(q_x) e^{ixq_x}, \quad X = \text{Hartree or Fock} \quad (\text{D.11})$$

and write the Hartree and Fock energy as (note the extra factor of 2 comparing with the expression of the Hartree Fock Hamiltonians)

$$\begin{aligned} E_{\text{Hartree}}[P] &= \frac{1}{2L_y} \sum_{a,b} \sum_{x,x'} V_{ab}^{\text{Hartree}}(x-x') P_{aa}(x) P_{bb}(x') \\ E_{\text{Fock}}[P] &= \frac{1}{2L_y} \sum_{a,b} \sum_{x,x'} V_{ab}^{\text{Fock}}(x-x') P_{ab}(x) P_{ba}(x') \end{aligned} \quad (\text{D.12})$$

where we write $P_{ab}(x)$ in place of $P_{ab}(k = x\ell_B^{-2})$ for the clarity of the expression. Equivalently, we can define the charge fluctuation in the momentum space $\tilde{P}(q_x) = \sum_k e^{-ikq_x\ell_B^2} P(k)$ and have

$$\begin{aligned} E_{\text{Hartree}}[\tilde{P}] &= \frac{1}{2A} \sum_{a,b} \sum_{q_x} \tilde{V}_{ab}^{\text{Hartree}}(q_x) \tilde{P}_{aa}(q_x) \tilde{P}_{bb}(-q_x) \\ E_{\text{Fock}}[\tilde{P}] &= -\frac{1}{2A} \sum_{a,b} \sum_{q_x} \tilde{V}_{ab}^{\text{Fock}}(q_x) \tilde{P}_{ab}(q_x) \tilde{P}_{ba}(-q_x) \end{aligned} \quad (\text{D.13})$$

When analyzing situations where the configuration is slowly varying along the x -direction, Eq. (D.12) or (D.13) will be a convenient starting point for approximations.

D.1.2 Derivation of non-linear sigma model

In this section, we derive the non-linear sigma model (NLsM) used in the main text. Our derivation shares the same spirit as the Sec. IV C in Ref. [256] and has the advantage of being easily generalizable.

Consider the bilayer quantum Hall problem where the fermions have two flavors $a = \pm$ corresponding to the two layers. One can consider a global $SU(2)$ transformation that rotates the layer-pseudospin of the electrons, which will become a symmetry of the Hamiltonian when the interaction is fully isotropic. Here we only assume a symmetric interaction, i.e., $V_{++} = V_{--}$ and $V_{+-} = V_{-+}$ and organize the HF energy (D.13) by the $SU(2)$ symmetry. The Hartree energy can be decomposed into an $SU(2)$ -symmetric part depending only on the total density and another $SU(2)$ -symmetry-breaking part that comes from layer charge polarization and the anisotropy of the interaction

$$\begin{aligned} E_{\text{Hartree}}[\tilde{P}] &= \frac{1}{2A} \sum_{q_x} \frac{\tilde{V}_{++}^{\text{Hartree}}(q_x) + \tilde{V}_{+-}^{\text{Hartree}}(q_x)}{2} \text{Tr}(\tilde{P}(q_x)) \text{Tr}(\tilde{P}(-q_x)) \\ &\quad + \frac{\tilde{V}_{++}^{\text{Hartree}}(q_x) - \tilde{V}_{+-}^{\text{Hartree}}(q_x)}{2} \text{Tr}(\tilde{P}(q_x)\sigma_z) \text{Tr}(\tilde{P}(-q_x)\sigma_z) \end{aligned} \quad (\text{D.14})$$

The Fock energy has a similar decomposition that reads

$$E_{\text{Fock}}[\tilde{P}] = -\frac{1}{2A} \sum_{q_x} \frac{\tilde{V}_{++}^{\text{Fock}}(q_x) + \tilde{V}_{+-}^{\text{Fock}}(q_x)}{2} \text{Tr}(\tilde{P}(q_x)\tilde{P}(-q_x)) \\ + \frac{\tilde{V}_{++}^{\text{Fock}}(q_x) - \tilde{V}_{+-}^{\text{Fock}}(q_x)}{2} \text{Tr}(\tilde{P}(q_x)\sigma_z\tilde{P}(-q_x)\sigma_z) \quad (\text{D.15})$$

At the unit total filling $\nu = 1$, it is convenient to adopt the pseudospin parameterization

$$P(k) = \frac{1 + \mathbf{m}(k) \cdot \boldsymbol{\sigma}}{2}, \quad |\mathbf{m}(k)| = 1, \quad (\text{D.16})$$

and we have (up to additive constants)

$$E_{\text{HF}}[\tilde{\mathbf{m}}] = \frac{1}{2A} \sum_{q_x} \frac{\tilde{V}_{++}^{\text{Hartree}}(q_x) - \tilde{V}_{+-}^{\text{Hartree}}(q_x) - \tilde{V}_{++}^{\text{Fock}}(q_x)}{2} \tilde{m}_z(q_x)\tilde{m}_z(-q_x) \\ - \frac{\tilde{V}_{+-}^{\text{Fock}}(q_x)}{2} (\tilde{m}_x(q_x)\tilde{m}_x(-q_x) + \tilde{m}_y(q_x)\tilde{m}_y(-q_x)). \quad (\text{D.17})$$

Here m_z measures the charge polarization and is affected by both the Hartree and Fock term, and m_x, m_y characterizes the interlayer coherence which comes only from the Fock term.

Assuming that the wave function varies slowly along the x direction we can approximate the HF energy by expanding the interactions at the small momenta $q_x \ell_B \ll 1$. It suffices for our purpose to keep the expansion up to the second order (Note that the linear order of q_x vanishes owing to the reflection symmetry $x \rightarrow -x$):

$$\tilde{V}_{ab}^{\text{Hartree}}(q_x) = \tilde{V}_{ab}(q_x)e^{-q_x^2 \ell_B^2/2} \approx \tilde{V}_{ab}(0) + \left(\frac{\tilde{V}_{ab}''(0)}{2\ell_B^2} - \frac{\tilde{V}_{ab}(0)}{2} \right) q_x^2 \ell_B^2 \quad (\text{D.18})$$

$$\tilde{V}_{ab}^{\text{Fock}}(q_x) = \frac{1}{N_\phi} \sum_{\mathbf{q}'} \tilde{V}_{ab}(\mathbf{q}') e^{-|\mathbf{q}'|^2 \ell_B^2/2} e^{-iq_x q'_y \ell_B^2} \\ \approx \frac{1}{N_\phi} \sum_{\mathbf{q}'} \tilde{V}_{ab}(\mathbf{q}') e^{-|\mathbf{q}'|^2 \ell_B^2/2} \left(1 - \frac{q_y'^2 \ell_B^4}{2} q_x^2 \right) \\ = \tilde{V}_{ab}^{\text{Fock}}(0) - \left(\frac{1}{N_\phi} \sum_{\mathbf{q}'} \tilde{V}_{ab}(\mathbf{q}') e^{-|\mathbf{q}'|^2 \ell_B^2/2} \frac{|\mathbf{q}'|^2 \ell_B^2}{4} \right) q_x^2 \ell_B^2 \quad (\text{D.19})$$

The leading term penalizes the charge polarization

$$\frac{\tilde{\beta}}{2} \sum_x m_z^2(x), \quad \tilde{\beta} = \frac{\tilde{V}_{++}^{\text{Hartree}}(0) - \tilde{V}_{+-}^{\text{Hartree}}(0) - \tilde{V}_{++}^{\text{Fock}}(0) + \tilde{V}_{+-}^{\text{Fock}}(0)}{2 \times 2\pi \ell_B^2}, \quad (\text{D.20})$$

and the next non-vanishing term produces stiffness

$$E_{\text{HF}}^{(2)}[\mathbf{m}] = \frac{\tilde{\rho}_z}{2} \sum_x (\partial_x m_z(x))^2 + \frac{\tilde{\rho}_{xy}}{2} \sum_x (\partial_x m_x(x))^2 + (\partial_x m_y(x))^2 \quad (\text{D.21})$$

where

$$\begin{aligned} \tilde{\rho}_z &= \frac{\tilde{V}_{++}''(0) - \tilde{V}_{+-}''(0)}{4 \times 2\pi\ell_B^2} - \frac{\tilde{V}_{++}(0) - \tilde{V}_{+-}(0)}{4 \times 2\pi\ell_B^2} \ell_B^2 + \frac{1}{8A} \sum_{\mathbf{q}'} \tilde{V}_{++}(\mathbf{q}') e^{-|\mathbf{q}'|^2 \ell_B^2/2} |\mathbf{q}'|^2 \ell_B^2 \\ \tilde{\rho}_{xy} &= \frac{1}{8A} \sum_{\mathbf{q}'} \tilde{V}_{+-}(\mathbf{q}') e^{-|\mathbf{q}'|^2 \ell_B^2/2} |\mathbf{q}'|^2 \ell_B^2 \end{aligned} \quad (\text{D.22})$$

Note that $\tilde{\rho}_z$ here differs from that in Ref. [256] but should be the correct one to use. Let us also provide details of the Fourier transformation,

$$\begin{aligned} \sum_{q_x} q_x^2 \tilde{m}_\alpha(q_x) \tilde{m}_\alpha(-q_x) &= \sum_{q_x} \sum_{k, k'} q_x^2 e^{-iq_x(k-k')\ell_B^2} m_\alpha(k) m_\alpha(k') \\ &= \frac{L_x L_y}{(2\pi)^2} \sum_{k'} \int dq_x dk q_x^2 e^{-iq_x(k-k')\ell_B^2} m_\alpha(k) m_\alpha(k') \\ &= \frac{L_x L_y}{(2\pi)^2} \sum_{x'} \int dq_x \frac{dx}{\ell_B^2} q_x^2 e^{-iq_x(x-x')\ell_B^2} m_\alpha(x) m_\alpha(x') \quad (k = x/\ell_B^2, k' = x'/\ell_B^2) \end{aligned}$$

Note that we define $m_\alpha(x) = m_\alpha(k)$ in the last step so that we still have the normalization $m^2(x) = 1$. Then we have

$$\begin{aligned} \sum_{q_x} q_x^2 \tilde{m}_\alpha(q_x) \tilde{m}_\alpha(-q_x) &= \frac{L_x L_y}{(2\pi)^2 \ell_B^2} \sum_{x'} \int dq_x dx (\partial_x^2 e^{-iq_x(x-x')\ell_B^2}) m_\alpha(x) m_\alpha(x') \\ &= \frac{L_x L_y}{2\pi \ell_B^2} \sum_x (\partial_x^2 m_\alpha(x)) m_\alpha(x) \end{aligned}$$

When taking the continuum limit we do

$$\sum_x \rightarrow \frac{L_y}{2\pi \ell_B^2} \int dx$$

Thus we have

$$E_{\text{HF}}[\mathbf{m}] \approx \frac{L_y}{2\pi \ell_B^2} \int dx \frac{\tilde{\rho}_{xy}}{2} \left((\partial_x m_x)^2 + (\partial_x m_y)^2 \right) + \frac{\tilde{\rho}_z}{2} (\partial_x m_z)^2 + \frac{\tilde{\beta}}{2} m_z^2. \quad (\text{D.23})$$

We then arrive at the NLsM in main text with $(\beta, \rho_{xy}, \rho_z) = (\tilde{\beta}, \tilde{\rho}_{xy}, \tilde{\rho}_z)/2\pi \ell_B^2$. Note that this factor equals the flux density $n_0 = N_\phi/A = (2\pi \ell_B^2)^{-1}$.

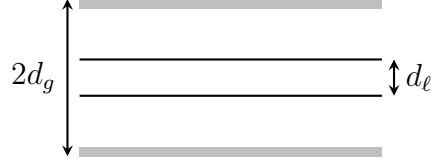


Figure D.1: Geometry of the device that realizes the bilayer quantum Hall system.

Finally, we add the single-particle potential $U_a(\mathbf{r})$ to our non-linear sigma model, which is more convenient to represent in real space

$$E_p[\mathbf{m}] = L_y n_0 \int dx (U_+(x)m_+ + U_-(x)m_-) = L_y \int dx (\mu(x) - \Delta(x)m_z) \quad (\text{D.24})$$

with

$$\mu(x) = n_0 \frac{U_+(x) + U_-(x)}{2}, \Delta(x) = -n_0 \frac{U_+(x) - U_-(x)}{2} \quad (\text{D.25})$$

We then arrive at the NLsM that we used in the main text: $E[\mathbf{m}] = E_{\text{HF}}[\mathbf{m}] + E_p[\mathbf{m}]$.

D.1.3 Parameters in non-linear sigma model

Now we specify interaction $V(q)$ and potential $U(q)$ according to our device and discuss how the NLsM parameters β , ρ_{xy} , ρ_z , and Δ depend on the device geometry. For convenience we will set $\ell_B = 1$ and $E_c = e^2/(4\pi\epsilon\ell_B) = 1$, and omit the tilde marks tied to q -quantities below.

As depicted in Fig. D.1, we place the active electron in bilayers at $z = \pm d_\ell/2$ and apply electrostatic potentials $\phi_\pm(q)$ to two graphite gates at $z = \pm d_g$. The gates have two effects: they imprint external potentials in each layer

$$U_\pm(q) = \sum_{a=\pm} e\phi_a(q) \frac{\sinh(q(d_g \pm \frac{ad_\ell}{2}))}{\sinh(qd_g)} \frac{1}{2 \cosh(qd_g)}, \quad (\text{D.26})$$

and partially screen the Coulomb interaction between electrons

$$V_{+\pm}(q) = \frac{4\pi}{q} \frac{\sinh(q(d_g \pm \frac{d_\ell}{2})) \sinh(q(d_g - \frac{d_\ell}{2}))}{\sinh(2qd_g)}. \quad (\text{D.27})$$

As seen in the previous section, the interaction often appears in the following linear combinations

$$\begin{aligned} V_0(q) &= \frac{V_{++}(q) + V_{+-}(q)}{2} = \frac{2\pi}{q} \frac{\cosh(qd_\ell/2) \sinh(q(d_g - d_\ell/2))}{\cosh(qd_g)} \\ V_z(q) &= \frac{V_{++}(q) - V_{+-}(q)}{2} = \frac{2\pi}{q} \frac{\sinh(qd_\ell/2) \sinh(q(d_g - d_\ell/2))}{\sinh(qd_g)} \end{aligned} \quad (\text{D.28})$$

Below we will derive the NLsM parameters from these analytic expressions and focus on the experimentally relevant regime $d_g \gg 1, d_\ell \ll 1$.

We first analyze the capacitance energy parameter

$$\beta = \frac{1}{2\pi} \int_0^\infty \frac{dq}{2\pi} q e^{-q^2/2} (V_z(0) - V_z(q)) \approx \frac{V_z(0)}{4\pi^2} + \frac{1}{4\pi} \int_0^\infty dq e^{-q^2/2} (1 - e^{-qd_\ell}),$$

where we have used the approximation $V_z(q) \approx \frac{2\pi}{q} \sinh(qd_\ell/2) e^{-qd_\ell/2} = \frac{\pi}{q} (1 - e^{-qd_\ell})$. Assuming a small interlayer distance $d_\ell \rightarrow 0$, we can expand the integrand with respect to d_ℓ and have

$$\begin{aligned} \beta &\approx \frac{V_z(0)}{4\pi^2} + \frac{1}{4\pi} \int_0^\infty dq e^{-q^2/2} \left(-qd_\ell + \frac{q^2 d_\ell^2}{2} + \dots \right) \\ &= \frac{d_\ell}{4\pi} \left(1 - \frac{d_\ell}{2d_g} \right) + \frac{1}{4\pi} \left(-d_\ell + \sqrt{\frac{\pi}{8}} d_\ell^2 + \dots \right) \end{aligned}$$

We thus find the leading order expansion of β in terms of d_ℓ and d_g :

$$\beta \approx \frac{d_\ell^2}{8\sqrt{2\pi}} \left(1 - \sqrt{\frac{2}{\pi}} d_g^{-1} \right) \quad (\text{D.29})$$

The fact that β has a quadratic dependence on the interlayer distance d_ℓ is important for the single split gate to work in a large parameter regime.

Then we analyze the stiffness parameter ρ_z and ρ_{xy} . We first compute

$$\rho_z = \frac{1}{8\pi^2} (V_z''(0) - V_z(0)) + \frac{1}{16\pi} \int_0^\infty \frac{dq}{2\pi} e^{-q^2/2} q^3 V_{++}(q).$$

The first term is determined by $V_z(0)$ and $V_z''(0) \approx \frac{\pi}{3} d_\ell^3$. (Note that $d_g \rightarrow \infty$ is taken before computing $q \rightarrow 0$) The second term can be approximated given $V_{++}(q) \approx \frac{2\pi}{q} (1 - 2e^{-2qd_g} + 2e^{-4qd_g} + \dots)$:

$$\begin{aligned} &\int_0^\infty dq e^{-q^2/2} q^2 (1 - 2e^{-2qd_g} + 2e^{-4qd_g} + \dots) \\ &\xrightarrow{d_g \rightarrow \infty} \sqrt{\frac{\pi}{2}} - 2 \int_0^\infty dq q^2 (e^{-2qd_g} - e^{-4qd_g} + \dots) = \sqrt{\frac{\pi}{2}} + O(d_g^{-3}) \end{aligned}$$

Therefore to the leading order we have

$$\rho_z \approx \frac{1}{16\sqrt{2\pi}} - \frac{1}{8\pi} d_\ell \left(1 - \frac{d_\ell}{2d_g} \right) + \frac{1}{24\pi} d_\ell^3, \quad (\text{D.30})$$

which is valid as long as we take $d_\ell \rightarrow 0$ before $d_g \rightarrow \infty$. We can similarly compute

$$\rho_{xy} = \frac{1}{16\pi} \int_0^\infty \frac{dq}{2\pi} e^{-q^2/2} q^3 V_{+-}(q).$$

Given $V_{+-}(q) \approx \frac{2\pi}{q}(e^{-qd_\ell} - 2e^{-2qd_g} + 2e^{-4qd_g} \cosh(qd_\ell) + \dots)$, we have

$$\begin{aligned} \rho_{xy} &\xrightarrow{d_g \rightarrow \infty} \frac{1}{16\pi} \int_0^\infty dq e^{-q^2/2} q^2 e^{-qd_\ell} + O(d_g^{-3}) \\ &\xrightarrow{d_\ell \rightarrow 0} \frac{1}{16\pi} \int_0^\infty dq e^{-q^2/2} q^2 (1 - qd_\ell + \dots) + O(d_g^{-3}) \\ &\approx \frac{1}{16\sqrt{2}\pi} - \frac{1}{8\pi} d_\ell \end{aligned} \quad (\text{D.31})$$

Thus, we conclude that $\rho_{xy} = \rho_z = \frac{E_c}{16\sqrt{2}\pi}$ at $d_\ell = 0$ and is reduced at the order of $O(d_\ell)$ for $d_\ell \neq 0$.

Finally, we analyze the displacement potential

$$\Delta(q) = -n_0 \frac{U_+(q) - U_-(q)}{2} = -e(\phi_+(q) - \phi_-(q)) \frac{\sinh(qd_\ell/2)}{4\pi \sinh(qd_g)}. \quad (\text{D.32})$$

For our single split gate setup: $\phi_+(|x| < L_J/2) = \mu/e + \phi_t$ and $\phi_+(|x| > L_J/2) = \phi_-(x) = \mu/e$, we have $\phi_+(x) - \phi_-(x) = \phi_t(\Theta(x + L_J/2) - \Theta(x - L_J/2))$, leading to

$$\phi_+(q) - \phi_-(q) = \int_{-L_J/2}^{L_J/2} dx e^{iqx} \phi_t = \phi_t \frac{\sin(qL_J)}{qL_J} \quad (\text{D.33})$$

Therefore

$$\Delta(q) = -e\phi_t \frac{\sin(qL_J)}{qL_J} \frac{\sinh(qd_\ell/2)}{4\pi \sinh(qd_g)} \quad (\text{D.34})$$

We can then evaluate $\Delta(x)$ using the convolution formula, with $\mathcal{F}^{-1}$ denoting the inverse Fourier transform:

$$\Delta(x) = -\frac{e\phi_t}{4\pi} \int_{-L_J/2}^{L_J/2} dx' \mathcal{F}^{-1} \left[\frac{\sinh(qd_\ell/2)}{\sinh(qd_g)} \right] (x - x') \quad (\text{D.35})$$

If we approximate $d_\ell \ll 1$, we have

$$\mathcal{F}^{-1} \left[\frac{\sinh(qd_\ell/2)}{\sinh(qd_g)} \right] \approx \mathcal{F}^{-1} \left[\frac{qd_\ell/2}{\sinh(qd_g)} \right] = \frac{\pi d_\ell}{8d_g^2 \cosh^2 \left(\frac{\pi x}{2d_g} \right)} \quad (\text{D.36})$$

then we have

$$\Delta(x) = -\frac{e\phi_t d_\ell}{4\pi} \int_{-L_J/2+x}^{L_J/2+x} dx' \frac{\pi}{8d_g^2 \cosh^2 \left(\frac{\pi x'}{2d_g} \right)} = -\frac{e\phi_t d_\ell}{16\pi d_g} \tanh \left(\frac{\pi x}{2d_g} \right) \Big|_{-L_J/2+x}^{L_J/2+x} \quad (\text{D.37})$$

For $|x \pm L_J/2| \ll d_g$, we obtain the result consistent with the uniform potential $\Delta(x) \approx \Delta_0 = \frac{d_\ell}{4d_g} \frac{e\phi_t}{2\pi}$.

D.1.4 Analytical solution of non-linear sigma model and Josephson energy in weak junction

We have shown the numerical solution of the non-linear sigma model in the main text. This section gives an analytical solution for weak junctions with $\Delta > \beta$ and estimates its Josephson energy E_J . In this case, we expect an almost polarized pseudospin $\mathbf{m} \simeq (0, 0, 1)$ deep inside the junction, where we can expand Eq. (7) to the leading order of $\vec{m}_{\parallel} = (m_x, m_y)$:

$$\frac{E[\vec{m}_{\parallel}]}{L_y} \simeq \int_{-L_J/2}^{L_J/2} dx \frac{\rho_{xy}}{2} ((\partial_x m_x)^2 + (\partial_x m_y)^2) + \frac{\Delta - \beta}{2} (m_x^2 + m_y^2) \quad (\text{D.38})$$

where the ρ_z term appears at the quartic order and is ignored. Although the approximation is no longer accurate near the junction boundary, we argue that the boundary effect is negligible if $L_J \gg \xi$. The corresponding equations of motion are

$$\partial_x^2 m_{\alpha} = \frac{\Delta - \beta}{\rho_{xy}} m_{\alpha}, \quad \alpha = x, y. \quad (\text{D.39})$$

which introduce the emergent length scale $\xi = \sqrt{\frac{\rho_{xy}}{\Delta - \beta}}$ governing the fluctuation of the pseudospin. It is then straightforward to solve $\vec{m}_{\parallel}(x)$ for the given boundary condition:

$$\vec{m}_{\parallel}(x) = \vec{m}_{\parallel}^L e^{-\frac{L_J/2+x}{\xi}} + \vec{m}_{\parallel}^R e^{-\frac{L_J/2-x}{\xi}}, \quad (\text{D.40})$$

where

$$\vec{m}_{\parallel}^L \simeq (\cos \varphi - e^{-L_J/\xi}, \sin \varphi), \quad \vec{m}_{\parallel}^R \simeq (1 - e^{-L_J/\xi} \cos \varphi, -e^{-L_J/\xi} \sin \varphi). \quad (\text{D.41})$$

satisfy $\vec{m}_{\parallel}(-L_J/2) = (\cos \varphi, \sin \varphi)$, $\vec{m}_{\parallel}(L_J/2) = (1, 0)$.

As a result, we can estimate the energy of the Josephson junction at phase difference φ :

$$E[\varphi] = \rho_{xy} L_y \xi^{-2} \int_0^{L_J} dx' e^{-2x'/\xi} (|\vec{m}_{\parallel}^L|^2 + |\vec{m}_{\parallel}^R|^2) = -E_J \cos \varphi + \text{const.} \quad (\text{D.42})$$

where the Josephson energy reads

$$E_J \simeq 2\rho_{xy} L_y \xi^{-1} e^{-L_J/\xi} \quad (\text{D.43})$$

Plugging the expressions of the parameters derived in Appendix D.1.3, we have $E_J \sim \frac{e^2}{\epsilon \ell_B} \frac{d_{\ell} L_y}{\ell_B^2} e^{-L_J/\xi}$. Numerical computations of the complete NLsM, including proper gate electrostatics, yield E_J of the same order of magnitude.

D.1.5 Charge gap of the exciton condensate and layer-polarized state and the resulting restrictions on ϕ_t

In this section, we use the HF Hamiltonian to estimate the charge gap of the exciton condensate ($m_z = 0$) and the layer-polarized state ($m_z \approx 1$), from which we determine the range of allowed ϕ_t in the single-split gate setup.

Assuming a uniform ground state, the Hatree-Fock Hamiltonian is

$$H_{\text{HF}} = \sum_{ab,k} (V_{ab}^H P_{bb} + U_a) c_{k,a}^\dagger c_{k,a} - \sum_{ab,k} V_{ab}^F P_{ba} c_{k,a}^\dagger c_{k,b}, \quad (D.44)$$

$$V_{ab}^H \equiv \frac{\tilde{V}_{ab}(0)}{2\pi\ell_B^2}, \quad V_{ab}^F \equiv \int \frac{d^2q}{(2\pi)^2} \tilde{V}_{ab}(\mathbf{q}) e^{-|\mathbf{q}|^2 \ell_B^2/2}$$

where $a = (l_a, \tau_a)$, $b = (l_b, \tau_b)$, $l_a = \pm$ denotes the up/down layer, τ denotes valley and spin flavor, U_a denotes the bare energy of each flavor, the screened Coulomb interaction $\tilde{V}_{ab}$ is independent of τ_a and τ_b . Note that it takes the same form for different Landau level orbitals k takes. Therefore, we only keep track of the flavor indices of fermion operators to simplify our notation.

For the exciton condensate phase $P_{ab} = \delta_{\tau_a, \tau_b} \delta_{\tau_a, K\uparrow}/2$, the HF Hamiltonian per orbital is

$$\sum_{l_a, l_b} \frac{V_{++}^H + V_{+-}^H - V_{++}^F}{2} c_{l_a K\uparrow}^\dagger c_{l_b K\uparrow} - \frac{V_{+-}^F}{2} c_{l_a K\uparrow}^\dagger \sigma_{l_a, l_b}^x c_{l_b K\uparrow} + \sum_{\tau_a \neq K\uparrow} \sum_{l_a} \frac{V_{++}^H + V_{+-}^H}{2} c_a^\dagger c_a \quad (D.45)$$

For this solution to be self-consistent, the gate voltage ϕ_0 must satisfy

$$\frac{V_{++}^H + V_{+-}^H - V_{++}^F - V_{+-}^F}{2} - e\phi_0 < 0$$

$$\frac{V_{++}^H + V_{+-}^H - V_{++}^F + V_{+-}^F}{2} - e\phi_0 > 0 \quad (D.46)$$

On the other hand, for the layer-polarized state $P_{ab} = \delta_{a,b} \delta_{a, +K\uparrow}$, we have

$$(V_{++}^H - V_{++}^F - U_\Delta) c_{+K\uparrow}^\dagger c_{+K\uparrow} + \sum_{\tau_a \neq K\uparrow} (V_{++}^H - U_\Delta) c_{+\tau_a}^\dagger c_{+\tau_a} + \sum_{\tau_a} (V_{+-}^H + U_\Delta) c_{-\tau_a}^\dagger c_{-\tau_a} \quad (D.47)$$

where $U_\Delta = \frac{d_\ell}{4d_g} e\phi_t$ is the layer polarization potential. For this solution to be self-consistent inside the junction, the average gate voltage of the top middle gate and the bottom gate must satisfy

$$V_{++}^H - V_{++}^F - e(\phi_0 + \frac{\phi_t}{2}) - U_\Delta < 0 \quad (D.48)$$

$$V_{++}^H - e(\phi_0 + \frac{\phi_t}{2}) - U_\Delta > 0 \quad (D.49)$$

$$V_{+-}^H - e(\phi_0 + \frac{\phi_t}{2}) + U_\Delta > 0, \quad (D.50)$$

Note that $V_{++}^H - V_{+-}^H \propto d_\ell$. Consider the case $d_\ell \ll \ell_B$ and $\Delta \propto \beta \sim d_\ell^2$, Eq. D.50 implies Eq. D.49. Thus, ϕ_t must satisfy

$$\frac{2(V_{++}^H - V_{++}^F - e\phi_0)}{1 + d_l/2d_g} < \phi_t < \frac{2(V_{+-}^H - e\phi_0)}{1 - d_l/2d_g} \quad (\text{D.51})$$

Taking $e\phi_0 = \frac{V_{++}^H + V_{+-}^H - V_{++}^F - V_{+-}^F}{2}$, the lower bound given by Eq. D.46, we have

$$\frac{4\pi\beta}{1 + d_l/2d_g} < \phi_t < \frac{2(V_{+-}^F - 2\pi\beta)}{1 - d_l/2d_g}, \quad (\text{D.52})$$

where β is given by Eq. (D.29). The upper bound for ϕ_0 can only be smaller for other allowed values of ϕ_0 . In the limit $d_l \ll \ell_B, d_g$, the upper bound is approximately $2V_{+-}^F$.

In addition, according to the non-linear sigma model, the layer-polarized state is the true ground state only when $\Delta = \frac{d_\ell}{4d_g} \frac{e\phi_t}{2\pi} > \beta$. Thus, the allowed range of ϕ_t is

$$8\pi d_g \beta / d_l < e\phi_t < 2V_{+-}^F \quad (\text{D.53})$$

For the dual gate configuration, the parameters on the two sides of the inequalities are

$$\beta \approx \frac{d_\ell^2}{8\sqrt{2\pi}} \left(1 - \sqrt{\frac{2}{\pi}} d_g^{-1} \right), \quad V_{+-}^F = \sqrt{\pi/2} - d_\ell - (\ln 2) d_g^{-1}, \quad (\text{D.54})$$

therefore $\phi_{\min} = 8\pi d_g \beta / d_l \approx \sqrt{\pi/2} d_g d_\ell$, and $\phi_{\max} = 2V_{+-}^F \approx \sqrt{2\pi}$. As a result, ϕ_t has a smaller range of tunability at larger d_ℓ (smaller ℓ_B), and above a critical value $d_\ell d_g \approx 2\ell_B^2$ no ϕ_t can satisfy the constraints. The result can be verified with HF numerics, as shown in Fig. D.2.

Aside from point-like excitations, the exciton condensate state also admits charged excitations with extended pseudospin textures known as bimerons [256]. For the $m_z = 0$ state, each bimeron comprises of two merons with opposite vortices in the m_{xy} texture, with their core polarized in either one of the two layers. Each meron carries a charge $\pm e/2$, so the bimeron carries a charge ± 1 or 0. For $d_\ell/\ell_B \sim 0.2$, the charged and neutral bimeron energy is estimated to be $0.5V_{+-}^F$ and $0.25V_{+-}^F$ respectively [287], smaller than the charge gap from uniform HF analysis. Therefore we expect the realistic constraint on ϕ_t to be stronger but qualitatively close to our estimate.

D.2 Validity of lumped-element model

The actual device of the Josephson junction comprises three parts: the junction in the middle and two EC bulks on the two sides. The lumped-element model approximates each part as a locally defined component. For example, the expression of the Josephson energy $E_J \cos \varphi$ captures the phase difference φ across the junction by implicitly ignoring phase

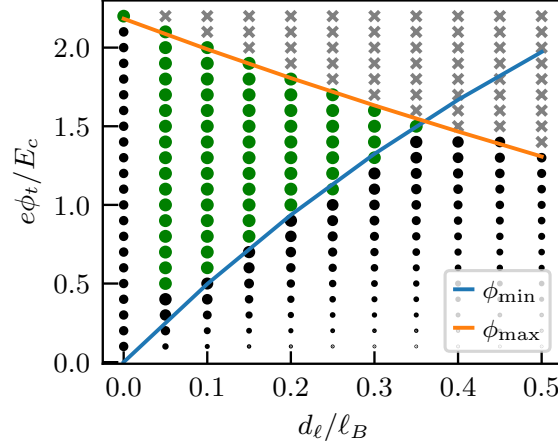


Figure D.2: HF result of m_z and filling ν at different d_ℓ and ϕ_t , with $d_g = 5\ell_B$, $L_x = 9L_y = 48\sqrt{2\pi}\ell_B$ and $L_J = L_x/2$. Crosses represent gapless states ($\nu > 1$), and circles represent gapped states ($\nu = 1$). The size of the circle is proportional to m_z^2 , with $m_z^2 > 0.99$ cases colored by green. The two curves correspond to $\phi_{\min} < \phi_t < \phi_{\max}$ in Eq. (D.53), which shows a decent agreement between the analytic results and the HF numerics.

variations within each EC bulk. The neglected contribution can be significant for certain device configurations, especially in the case of strongly-linked junctions. This section revisits the microscopic description of the Josephson junction and discusses when the lumped-element treatment is valid.

Our discussion is based on the NLsM of the Josephson junction Eq. (7), quoted below for the reader's convenience

$$\frac{E[\mathbf{m}]}{L_y} = \int dx \frac{\rho_{xy}}{2} [(\partial_x m_x)^2 + (\partial_x m_y)^2] + \frac{\rho_z}{2} (\partial_x m_z)^2 + \frac{\beta}{2} m_z^2 - \Delta(x) m_z. \quad (\text{D.55})$$

We place the junction at $0 < x < L_J$ and two EC bulks at $-L_x < x < 0$ and $L_J < x < L_J + L'_x$ respectively. In principle, both the left and right EC islands contribute to the capacitance and inductance in the lump-element description. Below we focus on the left EC bulk and fix $\varphi(L_J) = 0$ to get rid of the right EC island to simplify our discussion. Including the right EC bulk only complicates the calculation but will not quantitatively change the conclusion.

Based on the discussion in the main text, we can approximate the junction energy by $-E_J \cos \varphi(0)$, and assume $m_z \approx 0$ and slow-varying in the left EC islands. We have

$$\frac{E[\mathbf{m}]}{L_y} \approx \int_{-L_x}^0 dx \left(\frac{\rho}{2} (\partial_x \varphi)^2 + \frac{\beta}{2} m_z^2 - \frac{eV(x)}{4\pi} m_z \right) - \varepsilon_J \cos \varphi(0). \quad (\text{D.56})$$

where $\varepsilon_J = E_J/L_y$ is the lumped-element Josephson energy per unit width. The energy reduces to that for a single capacitance $C_J^{-1} \propto \beta$ if we take $\partial_x \varphi = 0$. Below we estimate

corrections to the lumped-element approximation due to spatial fluctuations in φ . We set $\ell_B = 1$ for simplicity.

Specifically, we examine the system's response to an applied driving voltage and analyze how the spatial variation of φ modifies the resonant frequency. To capture such dynamics, a fully quantum mechanical treatment of the problem is required. We choose the pair of canonical variables to be the phase φ and the electron density $\Pi_\varphi = \hbar n = \hbar m_z / 4\pi$, which is consistent with the choice of the main text (for example Eq. (4)). The Hamiltonian reads

$$H = \int_{-L_x}^0 dx \left(\frac{\rho}{2} (\partial_x \varphi)^2 + \frac{8\pi^2 \beta}{\hbar^2} \Pi_\varphi^2 - \frac{eV(x, t)}{\hbar} \Pi_\varphi \right) - \varepsilon_J \cos \varphi(0). \quad (\text{D.57})$$

In the bulk, the equations of motion of (φ, Π_φ) are

$$\begin{cases} \partial_t \varphi(x) = \frac{\partial H}{\partial \Pi_\varphi(x)} = \frac{16\pi^2 \beta}{\hbar^2} \Pi_\varphi(x) - \frac{e}{\hbar} V(x) \\ \partial_t \Pi_\varphi(x) = -\frac{\partial H}{\partial \varphi(x)} = \rho \partial_x^2 \varphi(x). \end{cases} \quad (\text{D.58})$$

which leads to

$$(\partial_t^2 - v^2 \partial_x^2) \varphi = \frac{e}{\hbar} \frac{\partial V(x, t)}{\partial t}, \quad v = \frac{4\pi}{\hbar} \sqrt{\rho \beta}. \quad (\text{D.59})$$

On the two boundaries $x = 0$ and $x = -L_x$, the current conservation law provides the proper boundary conditions

$$\varepsilon_J \sin \varphi(0) + \rho \partial_x \varphi(0) = 0, \quad \rho \partial_x \varphi(-L_x) = 0. \quad (\text{D.60})$$

Now, we turn on an AC driving voltage $V(x, t) = V_0 \cos \omega t$ and consider the following trial solution

$$\varphi(x, t) = \Re[(\varphi_0 + A_k \cos(k(x + L_x)))e^{i\omega t}], \quad \omega^2 = v^2 k^2. \quad (\text{D.61})$$

The boundary condition at $x = -L_J$ is automatically satisfied. The bulk equation of motion determines φ_0 :

$$-\omega^2 \Re[\varphi_0 e^{i\omega t}] = \frac{e}{\hbar} \Re V_0 i \omega e^{i\omega t} \implies \varphi_0 = \frac{e V_0}{i \hbar \omega}. \quad (\text{D.62})$$

At the boundary $x = 0$, we assume $|\varphi(0, t)| \ll 1$ and have a linearized equation

$$\varepsilon_J \varphi_0 + A_k (\varepsilon_J \cos k L_x - \rho k \sin k L_x) = 0, \quad (\text{D.63})$$

The resonance, when $A_k \rightarrow \infty$, occurs at wave vectors that satisfy the following condition

$$k L_x \tan k L_x = \varepsilon_J L_x / \rho, \quad (\text{D.64})$$

The resonance condition has infinitely many solutions, but only the lowest resonant solution k_J is relevant at low probe frequency.

If we assume $k_J L_x \ll 1$, we can approximate $\tan(k_J L_x) \approx k_J L_x$. Then we have $k_J = \sqrt{\varepsilon_J / \rho L_x}$ and

$$\omega_J^2 = v^2 k_J^2 = \left(\frac{4\pi}{\hbar}\right)^2 \frac{\beta}{L_x} \frac{1}{\varepsilon_J^{-1}}. \quad (\text{D.65})$$

Recalling that $E_J = \varepsilon_J L_y$ and $C_J^{-1} = 16\pi^2 \beta / L_x L_y$, this recovers the lumped-element result $\omega_J = e\sqrt{E_J / C_J} / \hbar$ in Eq. (3). Meanwhile, a more accurate solution of k_J is given by the series expansion of $\varepsilon_J L_x / \rho$:

$$k_J = \sqrt{\frac{\varepsilon_J}{\rho L_x}} \left(1 - \frac{\varepsilon_J L_x}{6\rho} + \frac{11}{360} \left(\frac{\varepsilon_J L_x}{\rho}\right)^2 + \dots\right). \quad (\text{D.66})$$

Physically, $\varepsilon_J L_x / \rho$ can be interpreted as the ratio of the edge inductance from Josephson energy $L_{\text{edge}} \sim \varepsilon_J^{-1}$ and bulk kinetic inductance $L_{\text{bulk}} \sim L_x / \rho$. To see its contribution more clearly, we express the corresponding resonance frequency as in Eq. (D.65)

$$\omega_J^2 = \left(\frac{4\pi}{\hbar}\right)^2 \frac{\beta}{L_x} \frac{1}{\varepsilon_J^{-1} + \frac{L_x}{3\rho} + \dots}, \quad (\text{D.67})$$

in which the edge inductance (ε_J^{-1}) is substituted with the sum of edge and bulk inductance in series ($\varepsilon_J^{-1} + \frac{L_x}{3\rho}$). We also note that including contribution from the right EC island will merely add quantitative modifications to the capacitance β / L_x on the numerator and the inductance on the denominator. Therefore, the accurate ω_J should account for the inductance of both the edge and the bulk, and the lumped-element model is valid only when the bulk inductance is negligible, or quantitatively,

$$k_J L_x = \omega_J L_x / v \ll 1 \Leftrightarrow \varepsilon_J L_x / \rho \ll 1 \quad (\text{D.68})$$

The two equivalent conditions cover different perspectives: the second from the strength of Josephson coupling, and the first from the resulting resonant frequency. The same conclusion can be applied to the right EC bulk, leading to similar conditions: $\omega_J L'_x / v \ll 1 \Leftrightarrow \varepsilon_J L'_x / \rho \ll 1$.

Finally, we estimate when the lumped-element treatment is justified in realistic devices. From previous sections we have $v \sim \sqrt{\rho\beta} / \hbar \sim E_c d_\ell / \hbar \sim \alpha_{\text{BN}} d_\ell c$ (with $\alpha_{\text{BN}} = \frac{1}{4.4} \frac{1}{137}$ the fine-structure in hBN and c the velocity of light) and $\varepsilon_J \sim \sqrt{\rho\beta} \exp(-L_J \sqrt{\beta/\rho}) \sim E_c d_\ell \exp(-\sqrt{2} L_J d_\ell)$ (for weakly-linked junction). If we take $L_x = 5 \mu\text{m}$ and $d_\ell = 0.2 \ell_B = 2 \text{ nm}$ ($B = 6.5 \text{ T}$), the conditions leads to

$$\nu_J \ll 20 \text{ GHz} \Leftrightarrow L_J > 240 \text{ nm (with } \varepsilon_J L_x / \rho = 0.1) \quad (\text{D.69})$$

Note that resonance can still be observed in experiments even when deviating from the above conditions, but needs to be corrected accordingly to match the theoretical description.