Anomalous Hall Crystals or Moiré Chern Insulators? Spontaneous versus explicit translational symmetry breaking in graphene pentalayers

1. **Theory of fractional quantum anomalous Hall phases in pentalayer rhombohedral graphene moiré structures**
   Authors: Zhihuan Dong, Adarsh S. Patri, and T. Senthil
   arXiv:2311.03445

2. **Fractional quantum anomalous Hall effects in rhombohedral multilayer graphene in the moiréless limit and in Coulomb imprinted superlattice**
   Authors: Boran Zhou, Hui Yang, and Ya-Hui Zhang
   arXiv:2311.04217

3. **Anomalous Hall Crystals in Rhombohedral Multilayer Graphene I: Interaction-Driven Chern Bands and Fractional Quantum Hall States at Zero Magnetic Field**
   Authors: Junkai Dong, Taige Wang, Tianle Wang, Tomohiro Soejima, Michael P. Zaletel, Ashvin Vishwanath, and Daniel E. Parker
   arXiv:2311.05568

4. **Theory of fractional Chern insulator states in pentalayer graphene moiré superlattice**
   Authors: Zhongqing Guo, Xin Lu, Bo Xie, Jianpeng Liu
   arXiv:2311.14368

5. **Moiré Fractional Chern Insulators III: Hartree-Fock Phase Diagram, Magic Angle Regime for Chern Insulator States, the Role of the Moiré Potential and Goldstone Gaps in Rhombohedral Graphene Superlattices**
   Authors: Yves H. Kwan, Jiabin Yu, Jonah Herzog-Arbeitman, Dmitri K. Efetov, Nicolas Regnault, and B. Andrei Bernevig
   arXiv:2312.11617

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The advent of highly-tunable moiré heterostructures of atomically thin materials has revitalized the exploration of complex orders in two-dimensional materials. While the study of two-dimensional electron gases (2DEGs) is a venerable one, for instance leading to the discovery of the integer and fractional quantum Hall effects, the introduction of the moiré superlattice due to the mismatch of lattice spacing or twist angle between the layers adds a new layer of complexity. This is because purely electrostatic gating can be used to tune electron densities that are comparable to those required to fully fill a Bloch band formed by the superlattice, whose wavelength typically is in the tens of nanometers. (In contrast, gating is less able to access features of the microscopic band structure due to the lattice-scale periodicity of a few angstrom.) Apart from allowing experimentalists to access wide doping ranges in a single sample, in this regime the traditional 2DEG approximation of treating the electron dispersion as parabolic within the effective mass approximation is often no longer appropriate and one needs to consider band structure in its full richness, including the plethora of phenomena linked to band topology. A second feature of these systems is the fact that the moiré-reconstructed bands are often 'narrow', in that interaction effects equal or exceed the bandwidth. Consequently, moiré heterostructures have become an important platform for exploring the interplay of interactions and topology in two dimensions, both in theory and experiment, as discussed in this Journal Club on several previous occasions.

This commentary is devoted to a relatively new entrant to the moiré roster: rhombohedral pentalayer graphene (R5G) aligned with a hexagonal boron (hBN) nitride substrate. First, let me briefly summarize the experimental setting before turning to the main focus of this commentary: their theoretical analysis. (A more detailed discussion of experiments is in a recent commentary by Ashvin Vishwanath (JCCM, December 2023).) n-layer rhombohedral graphene consists of graphene layers crystallographically stacked in a staircase-like pattern. The interlayer tunnelling Hamiltonian that captures physics along the stacking direction is reminiscent of the Su-Schrieffer-Heefer model, in that the low-energy electron states are 'zero modes' confined near the top and bottom of the stack. The dispersions of each of these 'zero modes' exhibits an n-fold band touching and a valley degeneracy inherited from a single graphene layer*. If one side of the multilayer is (nearly) aligned with hBN the slight lattice mismatch between graphene and hBN strongly modifies the band structure, leading to nearly flat bands that are very sensitive to the application of a perpendicular displacement field D. (Many different works have studied the single-particle physics of the pentalayer; a detailed recent treatment is in Ref. [2].) The experiments on R5G-hBN [1] are performed at large values of D, where a single-particle calculation nominally gives conduction bands with Chern number $C = \pm 5$ (the valleys acquire equal and opposite Chern numbers in a manner that preserves time reversal symmetry) but which are poorly isolated from other bands (the gaps are very small). This makes two of the experimental results very striking:

- they report a state with IQAH response $\sigma_{xy} = \pm\frac{e^2}{h}$ at a filling $\nu = 1$ corresponding to a single filled moiré band, consistent with a $|C| = 1$ Chern insulator;
- they further report FQAH response with $\sigma_{xy} = \left\{\frac{2}{3}, \frac{3}{5}, \frac{4}{7}, \frac{4}{9}, \frac{3}{7}, \frac{2}{5}\right\}\frac{e^2}{h}$ at filling factors $\nu = \frac{2}{3}, \frac{3}{5}, \frac{4}{7}, \frac{4}{9}, \frac{3}{7}, \frac{2}{5}$ of the moiré superlattice, consistent with the formation of fractional

*Owing to the negligible spin-orbit coupling in graphene, there is an additional near-exact SU(2) spin symmetry present throughout, that we will not comment on explicitly.

Chern insulators (FCIs) on doping a $|C| = 1$ band, rather than a band with $|C| > 1$.

In addition, these responses are attributed to the electrons *further away* from the hBN where the moiré potential is quite weak. Furthermore, as mentioned above, single-particle computations are inconsistent with an isolated band with $|C| = 1$. This naturally raises the question of precisely what role is played by the moiré potential, which, together with the formation of Chern insulator (CI) and fractional Chern insulator (FCI) states without a progenitor in the single-particle band structure, constitute the main mysteries of R5G-hBN.

Addressing these puzzles has been the focus of the five recommended papers, that are the vanguard of what promises to be much future work attacking this problem. All five of these recommended papers identify an interaction-driven mechanism for forming a $|C| = 1$ first conduction band that is separated from other bands, by means of self-consistent Hartree-Fock (SCHF) mean field calculations. In a well-known recent example of interaction-induced QAH [4] the Chern band topology is present already at the single-particle level. The role of interactions is restricted to driving flavour symmetry breaking so as to lift the degeneracy between $C = +1$ and $C = -1$ bands and spontaneously break time reversal symmetry. In contrast, interactions play a bigger role in R5G-hBN: beyond just breaking the fourfold spin-and-valley degeneracy, they drive a reconstruction of the bands leading to the formation of an isolated $|C| = 1$ band. While theoretically it has been shown [5] that FCIs can in principle arise even in bands with vanishing Berry curvature (an even more stringent constraint than simply requiring the Chern number to vanish), experimental examples of such 'intrinsically interacting' CIs are rare [6]. As such, it is a vivid example of how the closely competing energy scales of the bare dispersion and the interactions in moiré materials mean that it is often difficult to attribute phenomena exclusively to band theory and the effect of strong correlations: the substantial Berry curvature of the single-particle bands acts in concert with interactions to give rise to the emergent $|C| = 1$ band.

The first four papers also construct effective single-band problems for modelling the FCI physics, typically by doping holes into the the SCHF bands (with their $|C| = 1$ structure) and using numerical exact diagonalization (ED) of the resulting many-body problem; the third paper also performed density-matrix renormalization group (DMRG) simulations. Here, there are occasional discrepancies between these numerical results and experiments. For example, the first paper reports FCIs also at $\nu = \frac{1}{3}$, at odds with experiments; while the fourth paper also finds such a state, it is significantly weaker than that at $\nu = 2/3$. The other two papers focus on specific fillings or subsets of fillings without exploring all the fractions seen in experiment. While there is less consensus than in the case of the SCHF results, these studies do prove the principle that doping into the interaction-induced Chern band can lead to FCIs. My sense is that more extensive and exhaustive numerical studies, in particular those that go beyond single-band-projection, will be needed to better assess the competition between the FCIs and competing states. Other issues that appear worth considering include asking how the stability of the underlying $|C| = 1$ band — which after all is itself a consequence of interactions — evolves as it is doped towards lower electron density. Hopefully, such future studies will resolve some of the theory-experiment discrepancies and flesh out the proximate phases to the FCIs.

A more subtle — and to my mind more conceptually interesting — puzzle is linked to the precise role played by the moiré potential from the hBN. As noted above, for the sign

of displacement field in the experiments, the mobile electrons are localized on the other side of the pentalayer from the hBN, and consequently *prima facie* feel a rather weak moiré potential. One might ask: is the moiré potential essential? The second and third papers explored the effect of dialling the coupling between hBN and the R5G to zero, and observed that the interaction-induced $|C| = 1$ band survived despite the absence of the moiré potential that results from the hBN-R5G coupling. This led the authors of those papers to conjecture that the actual role of the moiré potential is merely as a weak pinning field for a state of matter that spontaneously breaks continuous translational symmetry (akin to a Wigner crystal) and simultaneously exhibits a QAHE (like a Chern insulator). Such a QAH-Wigner crystal hybrid [7] — dubbed an "anomalous Hall crystal" (AHC) by the third recommended paper — would be conceptually distinct from a CI. For instance, it would show signatures of spontaneous translational symmetry breaking, such as the presence of a "pseudo-Goldstone mode", i.e. a very soft phonon whose gap is set by the scale of the weak "extrinsic" moiré pinning, and as such would be much weaker than the interaction scale.

While an appealing theoretical idea, the fifth recommended paper injects some skepticism into the discussion. Via a careful analysis of the collective mode spectrum, they demonstrate that for at least a certain subset of reasonable models of R5G-hBN, the interaction-renormalized effect of the moiré potential is *not* small. In identifying "reasonable models" they highlight one of the key challenges in moiré modelling: the sensitivity of numerical studies to the "background" charge density about which one normal-orders the interactions. This is not an innocuous choice: it has the physical meaning, roughly, of deciding which aspects of the interactions have already been incorporated into the structure of an individual layer, and which constitute the leftover pieces necessary to retain in the many-body moiré problem. While similar challenges arise in principle in conventional crystals, they are elevated in the moiré setting owing to the comparable scales of kinetic and potential energy and the extent of interaction renormalization of bands even at the mean-field level. Previous experience suggests that different subtraction schemes lead to somewhat distinct phase boundaries, but that typically the effects are more significant for excitations or order-parameter textures rather than for ground-state phase structure [8]. In contrast, in R5G-hBN, the authors of the fifth paper show that the choice of subtraction scheme is crucial even at a gross qualitative level, in addressing the relative importance of the moiré potential. In the so-called "charge neutral" scheme where one normal-orders interactions with respect to the non-interacting bands at charge neutrality, they find that the occupied valence bands (which correspond to the electrons near the hBN layer that feel the moiré potential most strongly) do not significantly influence the distant conduction bands; in this limit, they find the HF phase diagram to be nearly independent of the hBN potential, consistent with the conjectured behaviour of an AHC. In stark contrast, for a different "average" subtraction scheme the moiré potential generated by the occupied valence bands is sufficiently strong that it introduces a considerable gap into the pseudo-Goldstone mode, such that in the Chern insulator phase this is even undercut by another collective mode linked to valley pseudospin. Consequently this suggests that the moiré potential strongly breaks translational symmetry, rather than serving merely as a weak pinning potential for an underlying 'pristine' spontaneously-symmetry-broken state. At minimum, one cannot neglect it in comparison to interaction effects that set the scale of the valley fluctuations. The paper also studies the effect of different "stackings" distinguished by the alignment of the B and N atoms relative to the inequivalent C atoms,

again finding a dichotomy between the schemes, with the charge neutrality scheme showing little dependence and the average scheme showing contrasting phase diagrams for the two stackings. The analysis of collective modes is complementary to the other works, and given the laudably painstaking attention paid to the subtraction scheme and similar subtleties, one should take these results as a serious challenge to the AHC scenario, indicating that a moiré FCI with strong explicit translational symmetry breaking could better describe the observed physics. However, since there is as yet no consensus on the 'correct' subtraction scheme, this is likely not the last word on the problem.

Ultimately, more experiments will be needed to distinguish between the two competing scenarios. In this vein, it may prove fruitful to draw on the large body of work around dynamical signatures of charge-density wave order [9], possibly with an eye on how Chern band topology might modify these results. Finally, while much of the existing work is (quite sensibly) focused on precise numerical studies to establish theoretical models that are quantitatively consistent with experiment, it would be very appealing to develop a more wholistic theoretical picture of the emergence of interaction-induced topology in multilayer graphene and other moiré systems, as well as analytically tractable toy models that can shed qualitative light on the mechanisms behind the formation of AHCs. In any event, given the pace of experimental and theoretical progress on the topic, it seems likely that we will hear quite a lot more about this and related problems in the very near future.

References

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[2] Jonah Herzog-Arbeitman *et al*, arXiv:2311.12920 (2023).

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[6] Though there are other moiré problems where the single-particle and interacting band structure differ in their topology: for instance 'ABC' trilayer graphene on hBN [G. Chen *et al*, arXiv:1905.06535] where the interacting bands have $|C| = 2$ rather than the $|C| = 3$ predicted by single-particle calculations.

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[8] For a (highly subjective) list of examples from this correspondent's own experience, see Y.H. Kwan *et al* Phys. Rev. B **104**, 115404 (2021); Phys. Rev. X **11**, 041063 (2021); *ibid* **12**, 031020 (2022), and G. Wagner *et al*, Phys. Rev. Lett. **128**, 156401 (2022), where the role of various subtraction schemes have been considered in some detail.

[9] G. Grüner Rev. Mod. Phys. **60**, 1129 (1988).