The Mathematics and Physics of Moiré Superlattices

Mitchell Luskin (University of Minnesota),
Svetlana Jitomirskyaya (UC Berkeley),
Eunah Kim (Cornell University),
Lin Lin (University of California, Berkeley),
Allan MacDonald (University of Texas)

Sunday, October 22, 2023–Friday October 27, 2023

1 Overview of the Field

Moiré materials are formed by overlaying two dimensional crystals that have slightly different lattice constants, or that have a small relative rotation, thus creating larger moiré patterns like the beat effect. The advantage of moiré materials over real atomic materials is that their effective lattice constants are typically on the tens of nm length scale. At this length scale, the number of electrons per period of the pattern can be adjusted experimentally over a range of 1 to 10 simply by adjusting electrical gate voltages. The electron density is typically the most critical control parameter for any type of electronic phenomena. When the number of electrons per atom in a material changes by an amount of order 1, it changes its chemistry, i.e., it changes its quantum physics even at a high energy scale. Achieving an understanding of how smooth changes at the highest energy scales control transitions between quantum ground states with distinct properties, for example between superconductors and insulators, is the essential challenge of quantum materials physics. In moiré materials, quantum properties of interest are routinely studied experimentally over the full relevant range of electron density without introducing disorder from chemical dopants. The list of interesting known states of matter that have already been realized in moiré materials includes superconductors, Mott insulators, Chern insulators, charge-transfer insulators, ferromagnetic metals, and charge density-wave states. It is abundantly clear that many other states of matter are waiting in the wings.

Motivated by theoretical work that pointed to new opportunities, tremendous progress has been made over the past several years in using moiré superlattices formed from two-dimensional materials as a laboratory for the study of quantum materials. This development has opened up an exciting new scientific opening, one in which mathematics and theoretical physics have a very large role to play by identifying moiré systems that are likely to exhibit new or poorly understood electronic phenomena, by inventing mathematical methods that enable testable predictions of physical properties, and by unravelling the meaning of experimental observations.

This BIRS workshop combined expertise from mathematics and physics to push the frontiers of this field. The presentations and discussions identified new moiré superlattice systems of interest, derived and solved models that accurately describe their electronic properties, and invented new concepts to explain experimental surprises.

All steps above require active interactions between physicists and mathematicians. This field thus presents an excellent opportunity to foster cross-fertilization between different branches of mathematics as the building and simulation of the reduced models, as well as the analysis and physical interpretation of the results

require expertise from partial differential equations, operator theory, dynamical systems, geometry, topology, probability theory, optimization, and numerical linear algebra.

An exciting feature of the study of moiré theory is the recent and continuing development of experimental methods to probe the phenomena being investigated by theorists contemporaneously. This workshop included the active participation of several of the pioneering experimental moiré physicists.

2 Recent Developments and Open Problems

The nm length scale periodicity of moiré materials makes it possible for the first time to fabricate devices in which the number of magnetic flux quanta per period exceeds 1. This development opens new opportunities to study the math and physics embedded in Hofstadter-type electronic structure models that account for incommensurability between Aharonov-Bohm phase variations and matter periodicity. The emergence of moiré materials thus highlights new opportunities to make math progress by looking to nature, and to make physics progress by learning from math.

The natural incommensurability of twisted lattices has received little rigorous attention. At the same time, recently developed rigorous methods have unexplored potential to identify novel phenomena and inform our search for new phases of matter. Our workshop sought to motivate significant progress in both directions by bringing together leading mathematicians and physicists to collaborate on this search.

Closely related Hamiltonians can be generated simply by fabricating incommensurate moiré of moiré systems with two or more distinct twist angles or lattice constant differences, such as the twisted trilayer systems recently investigated by several workshop participants and the workshop organizer.

Moiré materials also present an exciting platform for designing topological phases with an unprecedented level of control. It has already been established that the alignment of magic-angle graphene with a boron nitride substrate creates a topological Chern insulator in which broken sublattice symmetry leads to a Dirac mass and therefore to non-zero Chern numbers in moiré bands. Several theoretical and experimental presentations described recent developments and opportunities for the development of mathematical foundations.

Moiré systems such as tBLG present significant and perhaps long-lasting challenges from a computational perspective. First, bilayer moiré systems at magic angles have a very large effective unit cell (called the moiré unit cell) consisting of approximately 10^4 atoms. The moiré lattice consists of many such unit cells, and therefore the physics of interest only occurs on a mesoscopic scale and the system size is well beyond 10^5 atoms. Bistritzer and MacDonald developed an emergent low-energy model in 2011 that is the basis for most current theoretical and computational investigations of twisted bilayer graphene.

Even more challenging is direct simulation at the mean-field (Hartree-Fock or DFT) level due to the cubic scaling with respect to the number of atoms. Because the physics of interest is an energy scale that is on the order of meVs around the flat energy bands, compared to the atomic energy scale that is at least 10^3 times larger, direct numerical simulation must be very accurate, or the behavior at the scale of the moiré unit cell may not exceed numerical inaccuracy tolerances. Hence, reduced order modeling (ROM) is essential for studying moiré physics. Reduced order modeling is also important in order to study correlated electronic structures beyond the mean-field level, where current processes for constructing effective many-body models from first principles are highly empirical, and standard correlated solvers can often only treat systems with up to 100 orbitals. Such a reduction often involves identifying relevant localized orbitals in the moiré unit cell. However, recent works indicate that the localization step is not simple either, due to topology obstructions. This gives rise to the challenge of finding a mathematically principled way to faithfully and systematically derive the reduced model for interacting electrons of moiré systems. Even when the model is identified, the accurate solution of the reduced model at the interacting level is also very expensive. Therefore, it is challenging to solve the interacting model at the proper level of quantum many-body physics that balances the efficiency and accuracy.

These examples demonstrate that accurate modeling and simulation of moiré systems is a very challenging and interdisciplinary field. The standard methods of electronic structure theory fail. All steps above require active interactions between mathematicians and physicists. This field is also an excellent opportunity to foster cross-fertilization between different branches of mathematics as the building and simulation of the reduced models, as well as the analysis and physical interpretation of the results require expertise from partial differential equations, operator theory, dynamical systems, geometry, topology, probability theory,

optimization, and numerical linear algebra.

3 Presentation Highlights

3.1 Allan MacDonald: Some math and physics moiré material challenges

In this talk I will highlight three interesting and important challenges facing moiré materials researchers: i) How can we build a better models of moiré materials ? ii) Can we open new ground in the math and physics of quasi-periodic Hamiltonians? iii) Can we develop a predictive understanding of fractional Chern insulator states in moiré materials? For i) twisted bilayer graphene seems to be the most challenging case. Current models do not fully account for the non-local nature of the interactions between flat band electrons and the negative energy sea, and this may be necessary if we are ever to achieve a quantitative understanding of the competition between superconducting, Fermi liquid, and magnetic states. For ii), the moiré material platform allows creation of flexibly tunable quasiperiodic two-dimensional Hamiltonians. The physical properties of these systems will be influenced by interactions as well as by single-particle physics. There is an opportunity, I believe, to pose new mathematical questions. One important goal is to learn how to calculate and how to measure the quantum numbers that characterize spectral gaps. For iii), we are in early days. The discovery of fractional Chern insulator states in moiré materials is a breakthrough event in condensed matter physics. Can we use the tunability of moiré materials to stabilize fractionalized states that support non-Abelian quasiparticles?

3.2 Kin Fai Mak: Magnetism in doped moiré Mott insulators

Moiré materials provide a highly controllable platform to explore the strong electronic correlation phenomena. Specifically, Mott insulators with a lattice of local magnetic moments have been observed in semiconductor moiré bilayers in the flat band limit. In this talk, I will discuss experiments studying magnetism in doped moiré Mott insulators. One observation involves the spin polarons—bound states of a doped hole and a spin flip—in a hole-doped triangular lattice Mott insulator. The second involves the emergence of ferromagnetism at the onset of a Kondo breakdown transition in a moiré Kondo lattice (a lattice of local moments exchange-coupled to conduction electrons).

3.3 Lin Lin: Exact ground state of interacting electrons in magic angle graphene

One of the most surprising theoretical discoveries of magic angle twisted bilayer graphene is that in the chiral limit, certain single Slater determinants can be the ground state of the flat-band interacting Hamiltonian. This provides an explanation of the correlated insulating phase at integer filling. We investigate the symmetry attributes of the interacting Hamiltonian and the resulting ground states. This allows us to study systems beyond TBG, including TBG-like systems with 4 flat bands per valley, and equal twist-angle trilayer graphene systems (joint work with Simon Becker and Kevin Stubbs).

3.4 Fabian Faulstich: Interacting models for twisted bilayer graphene: Towards a quantum chemistry approach

We present a numerical study of an interacting Bistritzer-MacDonald (IBM) model of TBG using a suite of methods in quantum chemistry, including Hartree-Fock, coupled cluster singles, doubles (CCSD), and perturbative triples (CCSD(T)), as well as a quantum chemistry formulation of the density matrix renormalization group method (DMRG). At integer filling, all numerical methods agree in terms of energy and $C_{2z}T$ symmetry breaking. Additionally, as part of our benchmarking, we explore the impact of different schemes for removing "double-counting" in the IBM model. Our results at integer filling suggest that cross-validation of different IBM models may be needed for future studies of the TBG system. After benchmarking our approach at integer filling, we perform a systematic study of the IBM model near integer filling. In this regime, we find that the ground state can be in a metallic and $C_{2z}T$ symmetry breaking phase. The ground state appears

to have low entropy, and therefore can be relatively well approximated by a single Slater determinant. Furthermore, we observe many low entropy states with energies very close to the ground state energy in the near integer filling regime.

3.5 Shiwei Zhang: Treating electron interactions in moiré systems

The interplay between strong interactions and the unique environment created by moiré superlattices is believed to be a key for many of the most exciting phenomena seen in these two-dimensional materials. It is then important to treat both one- and two-body effects in a balanced and accurate way. This presents outstanding theoretical, algorithmic, and computational challenges. I will describe our preliminary work on developing and applying quantum Monte Carlo methods to treat moiré systems. This includes a study of the interacting Bistritzer-MacDonald model beyond specialized fillings which are sign-problem-free, calculations in a continuum model of two-dimensional electron gas in moiré potentials, and the parametrization of an exchange-correlation functional for density-functional theory calculations in two-dimensional materials.

3.6 Leni Bascones: Heavy quasiparticles and cascades without symmetry breaking in twisted bilayer graphene

Twisted bilayer graphene (TBG) exhibits a plethora of electronic phases. Among the variety of correlated states, the cascades in the spectroscopic properties and in the compressibility happen in a much larger energy [1,2,3], twist angle and temperature range than other effects, pointing to a hierarchy of phenomena. In this work [4], we show that the spectral weight reorganization associated to the formation of local moments and heavy quasiparticles, and not a symmetry breaking process, is responsible for the cascade phenomena. Among the phenomena reproduced in this framework are the cascade flow of spectral weight, the oscillations of the remote band energies and the asymmetric jumps of the inverse compressibility. Due to the fragile topology of TBG, we predict a strong momentum differentiation in the incoherent spectral weight. In the talk, I will also address other possible measurements which may help distinguishing the phenomenology of the cascades discussed here from proposals involving symmetry breaking.

[1] Wong et al, Nature 582, 198 (2020) [2] Zondiner et al, Nature 582, 203 (2020) [3] Polski et al, arXiv:2205.05225 [4] A. Datta, M.J. Calderón, A. Camjayi, E. Bascones, Nature Comms. 14, 5036 (2023)

3.7 Eslam Khalaf: Spin polarons in topological ferromagnets: application to graphene moire heterostructures

Understanding the phase diagram of twisted bilayer graphene and related moiré systems is a central theoretical challenge. While the ground states at integer fillings have been shown in many cases to be simple flavor ferromagnets, the charge excitations above such states can be non-trivial due to band topology. Conventional approaches to understand such excitations as real space topological textures fail to account for the distinct momentum space features of Chern bands and obscures their comparison to single particle excitations. Here, we present a general fully momentum space formulation for the problem of charge excitations in Chern bands. In the limit of (normal-ordered) contact interactions in an ideal flat band, we construct exact analytical wavefunctions for the lowest energy excitation with charge ±e and spin n+1/2 , a spin polaron. Away from this ideal limit, we show that these analytical wavefunctions are excellent variational states describing a bound state of an electron/hole with n spin flips. We show that the ansatz can be cast in the form of an antisymmetrized electron-hole geminal power and develop a diagrammatic approach to evaluate the expectation values of operators in such states, allowing us to study relatively large number of spin flips and large system sizes. We apply our formalism to study charge excitations in twisted bilayer graphene and find that (i) in the chiral limit, multispin flip polarons are the lowest energy charge excitations at charge neutrality and at non-zero integer fillings when doping towards neutrality. In the realistic limit, we find that the multispin flip states are the lowest charged excitations at $\nu = \pm(1-\epsilon)$ for any strong coupling state and at $\nu = \pm(2-\epsilon)$ for the time-reversal intervalley coherent state (TIVC) but not the Krammers intervalley coherent state (KIVC). We discuss the experimental implications of these results for low strain devices.

3.8 Eunah Kim: Fractionalization in 1/3 filled twisted bilayer graphene

The best-established example of fractionalization starts from the partially filling flat kinetic energy dispersion, namely the fractional quantum Hall effect. We will show that twisted bilayer graphene systems present new platforms for arriving at fractionalization: fractional correlated insulating state. Various 1/3 filled twisted bilayer graphene are expected to form Chern number=0 incompressible states driven by the extended fidget spinner-shaped Wannier orbitals. The geometric frustration due to the orbital shapes leads to charge 1/3 excitations with restricted mobility. The restricted mobility limited to the sub-dimension gives fracton-like character to the charge 1/3 excitations. I will discuss theoretical predictions on how to detect such fractional correlated insulators and preliminary experimental results.

3.9 Simon Becker: The mathematics of the chiral limit – What we know and what we don't know!

I will report on 3-4 years of mathematical analysis on the chiral limit of the BMH model and report on our understanding for bilayer and multilayer systems, and what open questions remain. My understanding of the subject has been shaped by collaborations with Mark Embree, Tristan Humbert, Ryan Kim, Izak Oltman, Martin Vogel, Jens Wittsten, Mengxuan Yang, Xiaowen Zhu, and Maciej Zworski.

3.10 Patrick Ledwith: Vortexable Chern bands and fractional Chern insulators in moiré graphene and transition metal dichalcogenides

Fractional Chern insulators realize the remarkable physics of the fractional quantum Hall effect (FQHE) in crystalline systems with Chern bands. The lowest Landau level (LLL) is known to host the FQHE, but not all Chern bands are suitable for realizing fractional Chern insulators (FCI). Previous approaches to stabilizing FCIs focused on mimicking the LLL through momentum space criteria. Here instead we take a real-space perspective by introducing the notion of vortexability. Vortexable Chern bands admit a fixed operator that introduces vortices into any band wavefunction while keeping the state entirely within the same band. Vortexable bands admit trial wavefunctions for FCI states, akin to Laughlin states. In the absence of dispersion and for sufficiently short-ranged interactions, these FCI states are the ground state – independent of the distribution of Berry curvature. Vortexable Chern bands emerge naturally in chiral twisted graphene, and fractional Chern insulators were subsequently observed experimentally. Recently, zero-field fractional Chern insulators, and potentially a zero-field composite Fermi liquid, were also observed in the nearly-vortexable twisted $MoTe_2$. New and exciting nearly-vortexable platforms are also appearing, including periodically strained graphene and helically twisted graphene.

3.11 Senthil Todadri: Quantum anomalous Hall physics in moiré bilayers: proximate phases and phase transitions

Quantum Hall phases are the most exotic experimentally established quantum phases of matter. Recently they have been discovered at zero external magnetic field in two dimensional moiré materials. I will describe recent work on their proximate phases and associated phase transitions that is motivated by the high tunability of these moire systems. These phase transitions (and some of the proximate phases) are exotic as well, and realize novel 'beyond Landau' criticality that have been explored theoretically for many years. I will show that these moiré platforms provide a great experimental opportunity to study these unconventional phase transitions and related unconventional phases, thereby opening a new direction for research in quantum matter.

3.12 Raquel Queiroz: Stability of chiral Landau levels and its implications for twisted heterostructures

Perfectly flat bands in moiré materials have intimate connections to Landau levels of Dirac fermions. In this talk, we will investigate how the robustness of zeroth Landau level to chiral disorder relates to the stability

of moiré flat bands against certain types of disorder. In light of moiré TMDs, we will also discuss the implications for massive Dirac fermions where the chiral symmetry is explicitly broken.

3.13 Jie Shan: Fractional Chern insulators and electric-field-induced topological phase transitions in moiré $MoTe_2$

The recent discovery of fractional Chern insulators (FCIs), which can exhibit the fractional quantum anomalous Hall effects, has attracted much scientific interest. I will discuss thermodynamic studies on the FCIs and the non-topological states in twisted bilayer $MoTe_2$. I will particularly focus on the nature of the electric-field-induced transitions between the FCIs and the non-topological states. I will also compare our thermodynamic studies with recent transport studies and discuss its implications.

3.14 Francisco Guinea: Superconductivity in graphene stacks

Superconductivity has been observed in a number of twisted and untwisted graphene multilayers. The dependence of the superconducting properties on the geometry of the graphene stack will be discussed. The possibility of novel phenomena due to non trivial order parameters will also be highlighted.

3.15 Mikito Koshino: Topological moiré trilayers

In addition to the extensive study of twisted moiré bilayers in the past decade, the scope of investigation has extended to encompass multilayer systems including three or more layers. Particular attention has recently been directed toward twisted trilayer systems which consists of three layers arranged in a specific rotational configuration. A twisted trilayer is characterized by two twist angles between adjacent layers, offering a vast parameter space that remains largely unexplored. In the first part of my talk, we will present systematic theoretical studies on the lattice relaxation and the electronic structures in general twisted trilayer graphenes [1]. We show that the relaxed lattice structure forms a patchwork of moiré-of-moiré domains, where a moiré pattern given by layer 1 and 2 and another pattern given by layer 2 and 3 become locally commensurate. The electronic band calculation reveals a wide energy window featuring sparsely distributed highly one-dimensional electron bands. These one-dimensional states exhibit a sharp localization at the boundaries between supermoiré domains, and they are identified as a topological boundary state between distinct Chern insulators. In the latter part of our discussion, we will explore the electronic structure of hBN/graphene/hBN trilayer system with arbitrary twist angles. We find that the electronic spectrum displays fractal minigaps akin to the Hofstadter butterfly. We demonstrate that each of minigaps is uniquely labeled by six topological numbers associated with the quasicrystalline Brillouin zones, and these numbers can be expressed as second Chern numbers through a formal connection with the quantum Hall effect in four-dimensional space [2,3].

[1] N. Nakatsuji, T. Kawakami, and M. Koshino, arXiv:2305.13155; Phys. Rev. X, in press. [2] M. Koshino, H. Oka, Phys. Rev. Research 4, 013028 (2022) [3] H. Oka and M. Koshino, Phys. Rev. B 104, 035306 (2021)

3.16 Jennifer Cano: Topological flat bands in bilayer graphene with a superlattice potential

We propose an externally imposed superlattice potential as a platform for engineering topological phases, which has both advantages and disadvantages compared to a moiré superlattice. We show that a superlattice potential applied to Bernal-stacked bilayer graphene can generate flat Chern bands, similar to those in twisted bilayer graphene, whose bandwidth can be as small as a few meV. Further, the flat band has a favorable band geometry for realizing a fractional Chern insulator at partial filling. The superlattice potential offers flexibility in both lattice size and geometry, making it a promising alternative to achieve designer flat bands without a moiré heterostructure.

3.17 Oskar Vafek: Interacting narrow bands of twisted bilayer graphene in magnetic field

In the first part of the talk I will discuss magneto-transport experiments on twisted bilayer graphene at 1.32 degree twist angle, i.e., away from the magic value. Despite the absence of correlated states at B=0, the theoretical explanation of these experiments provides insight into the origin of the Landau level degeneracy near the charge neutrality point and the role of heterostrain [1]. Equipped with this understanding, I will present a comprehensive Hatree-Fock study of interacting electrons in finite magnetic field while varying the electron density, twist angle and heterostrain. Within a panoply of correlated Chern phases emerging at a range of twist angles, I will present a unified description for the ubiquitous sequence of states with the Chern number t for $(s,t) = \pm(0,4), \pm(1,3), \pm(2,2)$ and $\pm(3,1)$. Correlated Chern insulators at unconventional sequences with $s+t \neq \pm 4$ are also found, as well as with fractional s. I will discuss their nature [2].

[1] Xiaoyu Wang et al. PNAS2023 Vol. 120 No. 34 e2307151120 [2] Xiaoyu Wang and O.Vafek arXiv.2310.xxxx

3.18 Dumitru Calugaru: Heavy-fermion physics in twisted bilayer graphene

Twisted bilayer graphene (TBG) displays two seemingly contradictory characteristics: (1) quantum-dot-like behavior in STM suggesting electron localization; (2) transport experiments indicating an itinerant nature. Both aspects can be naturally captured by a topological heavy-fermion model where topological conduction electron bands interact with local moments. We study the local-moment physics and the Kondo effect within this model. We reveal that at integer fillings ($\nu = -2, -1, 0, 1, 2$), the RKKY interactions favor ferromagnetic states satisfying a U(4) Hund's rule. Conversely, at non-integer fillings, the Kondo effect becomes significant, resulting in a Kondo resonance in the spectral function. Through our heavy-fermion model, we also explore the transport properties of TBG. We identify two primary types of carriers: incoherent f electrons and coherent c electrons. The coherent c electrons dominate the transport properties and give rise to a fully negative Seebeck coefficient at positive fillings. We also show that our model can also reproduce various aspects of the physics of TBG, including a natural explanation of the IKS state and its wavevector, as well as the reason for the existence of stronger correlated states for positive integer fillings, despite the bare band structure being more dispersive on that side.

3.19 Eric Cances: Semiclassical analysis of moiré Hamiltonians

The method introduced in [1] allows one to construct an approximate Kohn-Sham Hamiltonian for (incommensurate) twisted bilayer graphene. In the first part of the talk, I will show how an effective moiré-scale continuum model, similar though not identical to the Bistritzer-MacDonald model, can be derived from this Hamiltonian by simple variational approximation [2]. In the second part of the talk, I will show that methods from semiclassical analysis can be used to study the density-of-states of this Hamiltonian in the limit of small twist angles [3].

[1] G. Tritsaris, S. Shirodkar, E. Kaxiras, P. Cazeaux, M. Luskin, P. Plechac, and E. Cancès, Perturbation theory for weakly coupled two–dimensional layers, J. Mater. Res. 31 (2016) 959–966 [2] E. Cancès, L. Garrigue and D. Gontier, Simple derivation of moiré-scale continuous models for twisted bilayer graphene, Phys. Rev. B 107 (2023) 155403. [3] E. Cancès and L. Meng, Semiclassical analysis of two-scale electronic Hamiltonians for twisted bilayer graphene, in preparation.

3.20 Guillaume Bal: Robust asymmetric interface transport in topological insulators

The surprising robustness to perturbation of the asymmetric transport observed along interfaces separating distinct insulating bulks has a topological origin. This talk reviews recent classifications of partial differential operators modeling such systems. A classification by means of domain walls provides a topological invariant whose calculation as an explicit integral is straightforward. A general bulk-interface correspondence then proves that the invariant also describes the quantized aforementioned asymmetric transport. The theory is illustrated on several examples of applications and in particular gated twisted bilayer graphene models.

3.21 Dionisios Margetis: Chirality and edge plasmons in the twisted bilayer graphene

In this talk, I will discuss recent progress in understanding implications of the electrical conductivity tensor, coming from the Kubo formalism, for the twisted bilayer graphene (TBG) and similar heterostructures. The use of a spatially homogeneous and isotropic tensor conductivity has led us to the analytical derivation of a dispersion relation for non-retarded edge plasmons. This relation explicitly depends on the chiral response of the system. I will describe a correspondence of the chiral optical plasmon in the TBG to the magnetoplasmon in the single-layer graphene, by introducing an effective magnetic field. If time permits, I will also discuss related extensions of the theory to the twisted trilayer and quadrilayer graphene systems. In the analysis, the long-range electrostatic interaction is retained via application of the Wiener-Hopf method of factorization to systems of integral equations for scalar fields.

3.22 Daniel Massatt: Observables of an incommensurate bilayer linear Schrödinger equation

We formulate a plane-wave basis representation of an incommensurate bilayer linear Schrödinger equation. We use the representation to find algorithms for a number of fundamental electronic observables such as the local density of states of spatial configurations, total density of states, and the local density of states in momentum space, which is a parallel object to electronic band structure in the absence of periodicity. We further prove the equivalence of the density of states in the plane-wave formulation to that of the density of states of the real space Schrödinger equation through a properly averaged thermodynamic limit. The methodology relies on tracking the plane-wave scattering between incommensurate potentials and using these 'hopping' parameters to construct a matrix describing the coupling of all interacting plane-waves, which we find to be indexed by a four-dimensional lattice. The algorithm relies on truncation of the matrix via an energy truncation and hopping distance truncation with rigorous convergence rates.

3.23 Alexander Watson: Moiré materials from atomic to moiré scales

I will review progress towards realistic yet manageable models of the electronic properties of twisted bilayer graphene and other moiré materials. First, I will present a general approach to modeling atomic relaxation in moire materials using interatomic potentials. Then, I will discuss a general framework for deriving corrections to effective continuum models such as the Bistritzer-MacDonald model.

3.24 Wencai Liu: Algebraic geometry, complex analysis and combinatorics in spectral theory of periodic graph operators

In this talk, we will discuss the significant role that the algebraic properties of Bloch and Fermi varieties play in the study of periodic graph operators. I will begin by highlighting recent discoveries about these properties, especially the irreducibility. Then, I will show how we can use these findings, together with techniques from complex analysis and combinatorics, to study spectral and inverse spectral problems arising from periodic graph operators.

3.25 Xiaowen Zhu: Cantor spectrum of a 1D moiré model

It is known that the magnetic Schrödinger operator on a 2D lattice with irrational flux has Cantor spectrum, which illustrates the well-known picture of "Hofstadter butterfly". In this talk, I will introduce the proof of Cantor spectrum for another model - a 1D moiré model. In particular, the moiré pattern plays a key role in the exhibition of Cantor spectrum in a relatively robust way that is intrinsically different from magnetic fields. This implies further potential of understanding other moiré-pattern models. The talk is based on a joint work with Simon Baker and Svetlana Jitomirskaya.

3.26 Daniele Guerci: Interplay of moiré patterns: TBG on aligned hBN and helical trilayer graphene

In my presentation, I will explore two illustrative examples where the interplay of two moiré patterns to the formation of large moiré domains where commensuration is restored: TBG on aligned hBN and helical trilayer graphene. The latter gives rise to a topological Chern mosaic dominated by regions of ABA/BAB stacking forming a periodic triangular pattern on the moiré of moiré scale. I will provide a detailed exploration of the origins of the electronic bands in the chiral limit. Exact results will reveal the existence of a Chern 2 band with unique properties that cannot be reduced to a single lowest Landau level [1-3]. Notably, our predictions are consistent with recent experimental findings [4], underscoring the significance of these moiré patterns in uncovering novel topological phenomena.

[1] D. Guerci, Y. Mao, C. Mora, arXiv:2305.03702 (2023) [2] D. Guerci, Y. Mao, C. Mora, arXiv:2308.02638 (2023) [3] Y. Mao, D. Guerci, C. Mora, PRB 107, 125423 (2023) [Editors' Suggestion] [4] L. Xia, P. Jarillo-Herrero et al., arXiv:2310.12204 (2023)

3.27 Daniel Bennett: Twisted bilayer graphene revisited: where is the "magic"?

The moiré pattern observed experimentally in twisted bilayer graphene (tBLG) clearly shows the formation of different types of domains. These domains can be explained by the atomic relaxation, both in-plane and out-of-plane, using continuum elasticity theory and the Generalized Stacking Fault Energy (GSFE) concept. Moreover, the atomic relaxation significantly affects the electronic states, leading to a pair of flat bands at the charge neutrality point which are separated by band gaps from the rest. These features appear for a small range of twist angles, that we call the "magic range", around the twist angle of 1 degree. We discuss how all these aspects of the system are crucial for understanding the origin of correlated states and superconductivity in tBLG. We also present a minimal model that can capture these features with 2 flat and 2 auxiliary bands and explore the implications of the model for correlated electron behavior in the context of the Hubbard model.

4 Scientific Progress Made

Active discussions occurred during the presentations, breaks, meals, and along hiking trails on Wednesday afternoon. Informal sessions were also held the hour before dinner, For example, an informal session was held on Wednesday on interacting Bistritzer-MacDonald models and on Thursday on configuration-based relaxation models for twisted trilayer graphene and other multi-layer heterostructures.

5 Outcome of the Meeting

The moiré mathematics community has recently begun to investigate interacting models for twisted bilayer graphene and other 2D heterostructures. The opportunity for the mathematical community to have detailed discussion with the theoretical physicists who developed these interacting models will enable further collaboration between mathematicians and physicists on the investigation of correlated phases in moiré systems and the development of rigorous mathematical foundations.

References

[1] Eva Y Andrei and Allan H MacDonald. Graphene bilayers with a twist. *Nature Materials*, 19(12):1265–1275, 2020.

[2] Artur Avila and Svetlana Jitomirskaya. The ten martini problem. *Annals of Math.*, 70:303–342, 2009.

[3] S. Becker, S. Jitomirskaya, and R. Han. Cantor spectrum of graphene in magnetic fields. *Invent. math*, 218:979–1041, 2019.

[4] Simon Becker, Mark Embree, Jens Wittsten, and Maciej Zworski. Spectral characterization of magic angles in twisted bilayer graphene. *Phys. Rev. B*, 103:165113, Apr 2021.

[5] Simon Becker and Maciej Zworski. From the chiral model of tbg to the bistritzer–macdonald model, 2023.

[6] Rafi Bistritzer and Allan H MacDonald. Moiré bands in twisted double-layer graphene. *Proceedings of the National Academy of Sciences*, 108(30):12233–12237, 2011.

[7] Eric Cancès, Paul Cazeaux, and Mitchell Luskin. Generalized Kubo formulas for the transport properties of incommensurate 2D atomic heterostructures. *J. Math. Phys.*, 58:063502 (23pp), 2017.

[8] Éric Cancès, Louis Garrigue, and David Gontier. Simple derivation of moiré-scale continuous models for twisted bilayer graphene. *Phys. Rev. B*, 107:155403, Apr 2023.

[9] Yuan Cao, Valla Fatemi, Ahmet Demir, Shiang Fang, Spencer L Tomarken, . . . , Efthimios Kaxiras, and Pablo Jarillo-Herrero. Correlated insulator behaviour at half-filling in magic-angle graphene superlattices. *Nature*, 556(7699):80–84, 2018.

[10] Yuan Cao, Valla Fatemi, Shiang Fang, Kenji Watanabe, Takashi Taniguchi, Efthimios Kaxiras, and Pablo Jarillo-Herrero. Unconventional superconductivity in magic-angle graphene superlattices. *Nature*, 556(7699):43–50, 2018.

[11] S. Carr, D. Massatt, S. B. Torrisi, P. Cazeaux, M. Luskin, and E. Kaxiras. Relaxation and Domain Formation in Incommensurate 2D Heterostructures. *Phys. Rev. B*, page 224102 (7 pp), 2018.

[12] Stephen Carr, Daniel Massatt, Shiang Fang, Paul Cazeaux, Mitchell Luskin, and Efthimios Kaxiras. Twistronics: manipulating the electronic properties of two-dimensional layered structures through the twist angle. *Phys. Rev. B*, 95:075420, 2017.

[13] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim. The electronic properties of graphene. *Rev. Mod. Phys.*, 81:109–162, Jan 2009.

[14] Paul Cazeaux, Drake Clark, Rebecca Engelke, Philip Kim, and Mitchell Luskin. Relaxation and domain wall structure of bilayer moiré systems. *Journal of Elasticity*, 2023.

[15] Paul Cazeauz, Mitchell Luskin, and Daniel Massatt. Energy minimization of 2D incommensurate heterostructures. *Arch. Rat. Mech. Anal.*, 235:1289–1325, 2019.

[16] Junkai Dong, Patrick J. Ledwith, Eslam Khalaf, Jong Yeon Lee, and Ashvin Vishwanath. Many-body ground states from decomposition of ideal higher chern bands: Applications to chirally twisted graphene multilayers. *Phys. Rev. Res.*, 5:023166, Jun 2023.

[17] Fabian M. Faulstich, Kevin D. Stubbs, Qinyi Zhu, Tomohiro Soejima, Rohit Dilip, Huanchen Zhai, Raehyun Kim, Michael P. Zaletel, Garnet Kin-Lic Chan, and Lin Lin. Interacting models for twisted bilayer graphene: A quantum chemistry approach. *Phys. Rev. B*, 107:235123, Jun 2023.

[18] Daniel Massatt, Stephen Carr, and Mitchell Luskin. Electronic observables for relaxed bilayer 2D heterostructures in momentum space. *Multiscale Model. Simul.*, to appear.

[19] Hoi Chun Po, Liujun Zou, Ashvin Vishwanath, and T. Senthil. Origin of mott insulating behavior and superconductivity in twisted bilayer graphene. *Phys. Rev. X*, 8:031089, Sep 2018.

[20] Zhi-Da Song and B. Andrei Bernevig. Magic-angle twisted bilayer graphene as a topological heavy fermion problem. *Phys. Rev. Lett.*, 129:047601, Jul 2022.

[21] Grigory Tarnopolsky, Alex Jura Kruchkov, and Ashvin Vishwanath. Origin of magic angles in twisted bilayer graphene. *Phys. Rev. Lett.*, 122:106405, Mar 2019.

[22] Alexander Watson and Mitchell Luskin. Existence of the first magic angle for the chiral model of bilayer graphene. *J. Math. Phys.*, 62:091502 (32pp), 2021.

[23] Alexander B. Watson, Tianyu Kong, Allan H. MacDonald, and Mitchell Luskin. Bistritzer-MacDonald dynamics in twisted bilayer graphene. *J. Math. Phys. (Editor's Choice)*, 64:031502 (38pp), 2023.

[24] Fengcheng Wu, Timothy Lovorn, Emanuel Tutuc, and Allan H MacDonald. Hubbard model physics in transition metal dichalcogenide moiré bands. *Physical review letters*, 121(2):026402, 2018.

[25] Ziyan Zhu, Stephen Carr, Daniel Massatt, Mitchell Luskin, and Efthimios Kaxiras. Twisted trilayer graphene: A precisely tunable platform for correlated electrons. *Phys. Rev. Lett.*, 125:11604 (6 pp), 2020.

[26] Ziyan Zhu, Paul Cazeaux, Mitchell Luskin, and Efthimios Kaxiras. Modeling mechanical relaxation in incommensurate trilayer van der Waals heterostructures. *Phys. Rev. B*, page 224107 (14 pp), 2020.

[27] Maciej Zworski, Mengxuan Yang, and Zhongkai Tao. Mathematical results on the chiral model of twisted bilayer graphene (with an appendix by mengxuan yang and zhongkai tao), 2023.