Title: Excited state spectrum of strongly interacting magic-angle twisted bilayer graphene at three- quarters filling

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Abstract: The interplay between strong electronic interaction and non-trivial topology in magic-angle twisted bilayer graphene (tBLG) yields many intriguing phenomena that range from superconductivity to a spontaneous quantum anomalous Hall state with Chern number ±1. WIth the equilibrium phase diagram under much scrutiny, a better theoretical understanding of the excitation spectrum of tBLG is crucial to reveal experimental signatures of competing phases and discern possible pathways of controlling their behavior out of equilibrium. To this end, we study an effective Wannier-orbital model from Kang and Vafek (2019) in the strong coupling limit, which captures the Chern state at three quarters filling as well as its competition with proximal stripe charge order. We compute the density and chiral excitation spectra as well as the charge gap as a function of the overlap of neighboring Wannier orbitals. Our results provide an experimental signature to detect the transition from the stripe phase to the Chern phase and offer insight into steering of the quantum anomalous Hall state via low-frequency driving.

# Excited state spectrum of strongly interacting magic-angle twisted bilayer graphene at three-quarters filling

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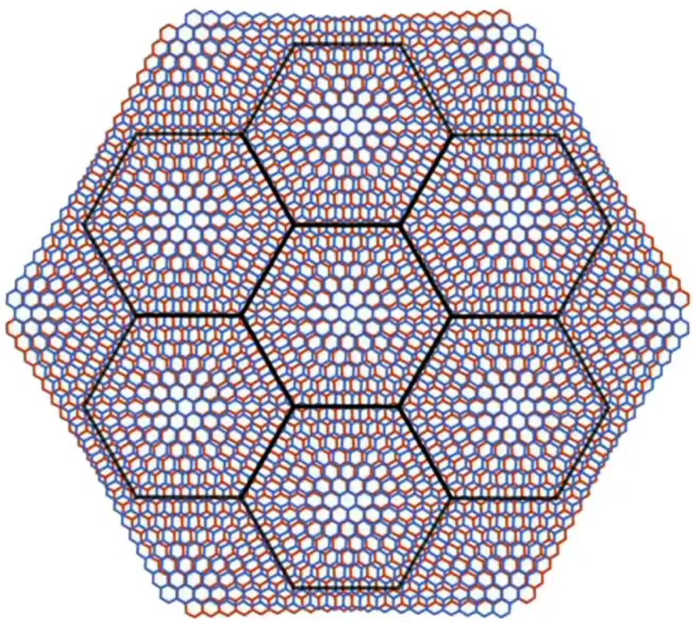
Prof. Martin Claassen

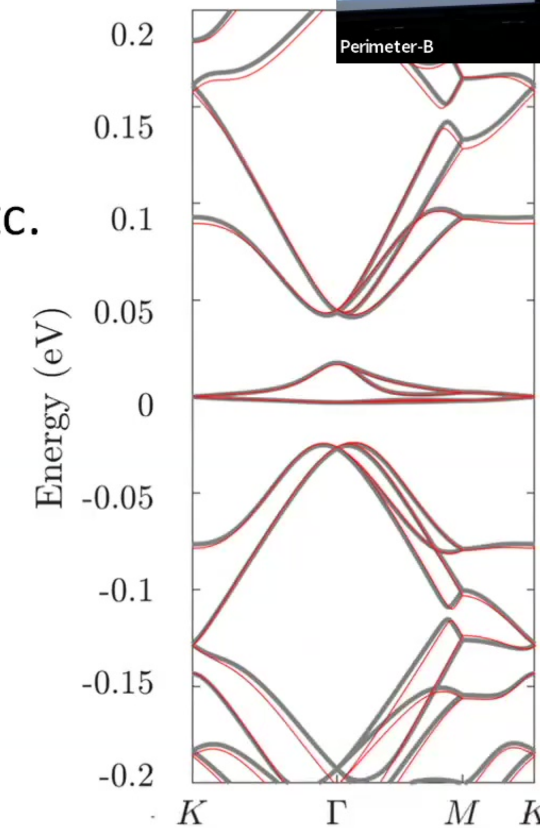

# Introduction

On twisted bilayer graphene (tBLG)

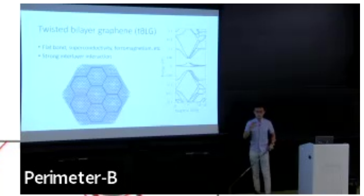
# Twisted bilayer graphene (tBLG)

- Flat band, superconductivity, ferromagnetism, etc.
- Strong interlayer interaction

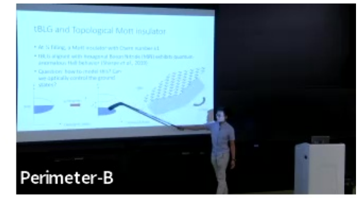




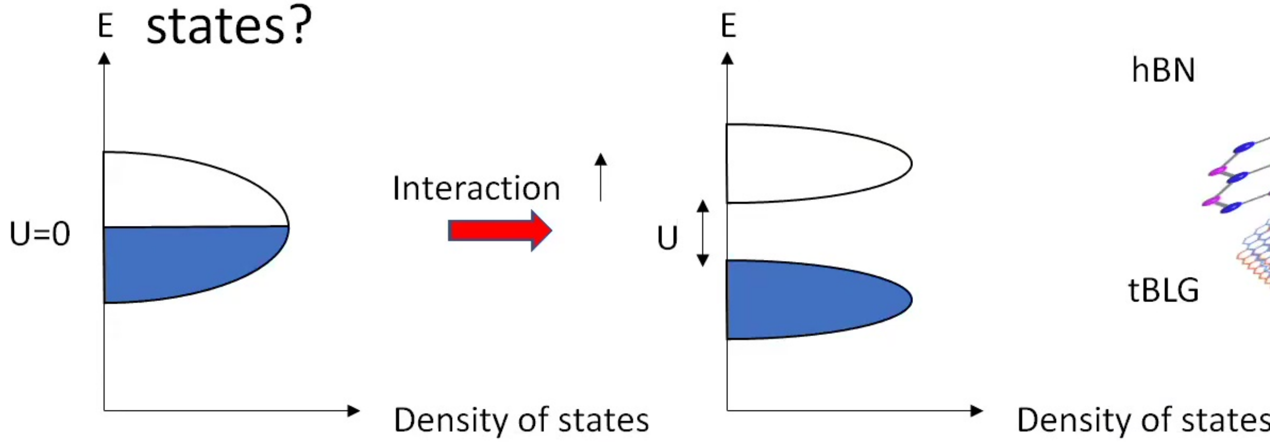
Fang *et al.* (2019)

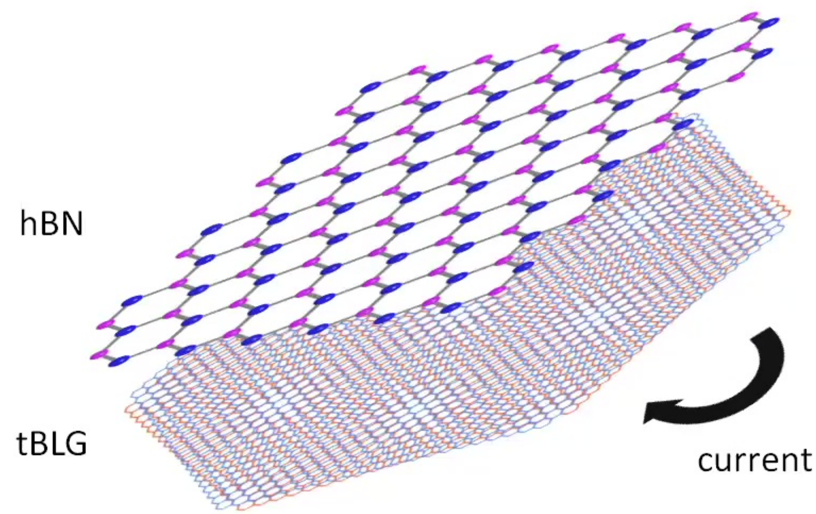


# tBLG and Topological Mott insulator



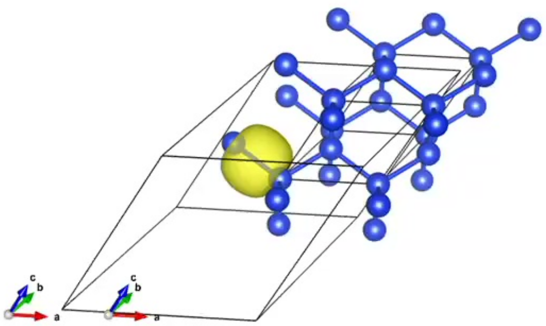

- At ¾ filling, a Mott insulator with Chern number ±1
- tBLG aligned with hexagonal Boron Nitride (hBN) exhibits quantum anomalous Hall behavior (Sharpe *et al.*, 2019)
- Question: how to model this? Can we optically control the ground states?



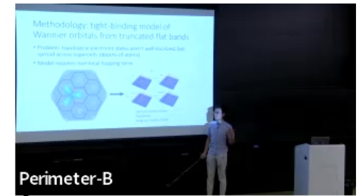



# Methodology: tight-binding model of Wannier orbitals from truncated flat bands


- Magic-angle tBLG has prohibitively large unit cell (~1000 atoms)
- Simplification: consider tight-binding models from the two flat bands
- Assumption: significant energy gap with excited states
- To construct model, use Wannier orbitals: maximally localized states from Fourier transforms of Bloch wavefunctions

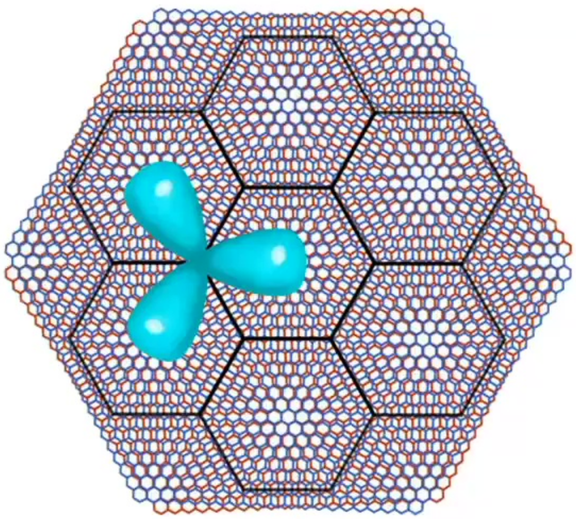


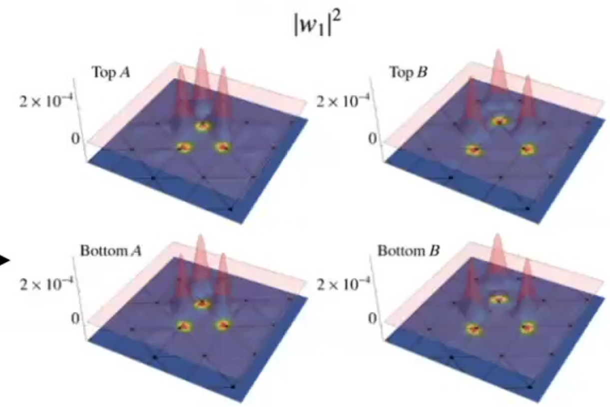
From ABINIT's tutorial



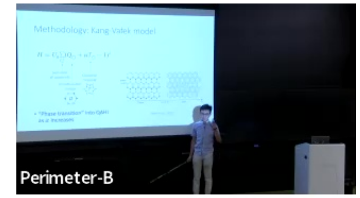

# Methodology: tight-binding model of Wannier orbitals from truncated flat bands

- Problem: topological electronic states aren't well-localized, but spread across supercells (dozens of atoms)
- Model requires non-local hopping term






Wannierization of two flat bands
Kang and Vafek, (2018)



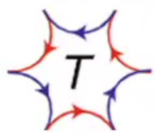

# Methodology: Kang-Vafek model

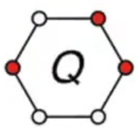
$$H = U_0 \sum_{\hexagon} (Q_{\hexagon} + \alpha T_{\hexagon} - 1)^2$$

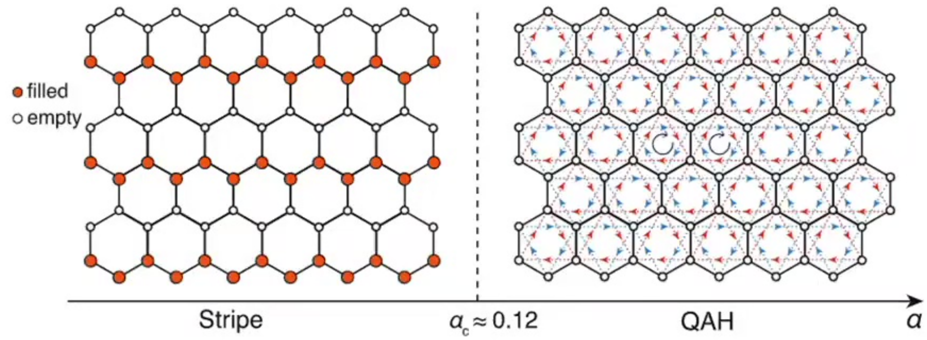
Sum over all supercells

On-site cluster charge

Coulomb hopping



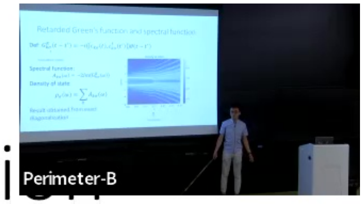




- "Phase transition" into QAHI as $\alpha$ increases

Chen *et al.*, 2021

# Retarded Green's function and spectral function




**Def:** $G^R_{k\sigma}(t-t') = -i\langle\{c_{k\sigma}(t), c^\dagger_{k\sigma}(t')\}\rangle\theta(t-t')$

Sublattice index

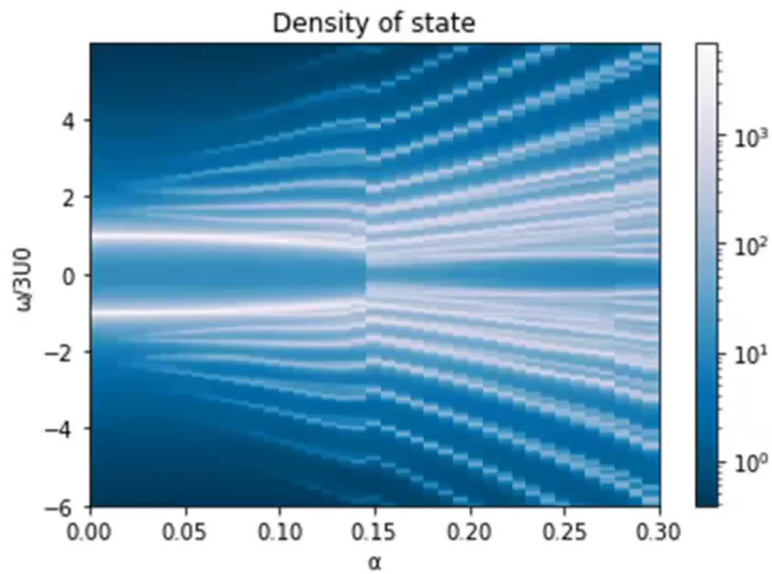
**Spectral function:**

$$A_{k\sigma}(\omega) = -2Im(\mathrm{G}^R_{k\sigma}(\omega))$$

**Density of state:**

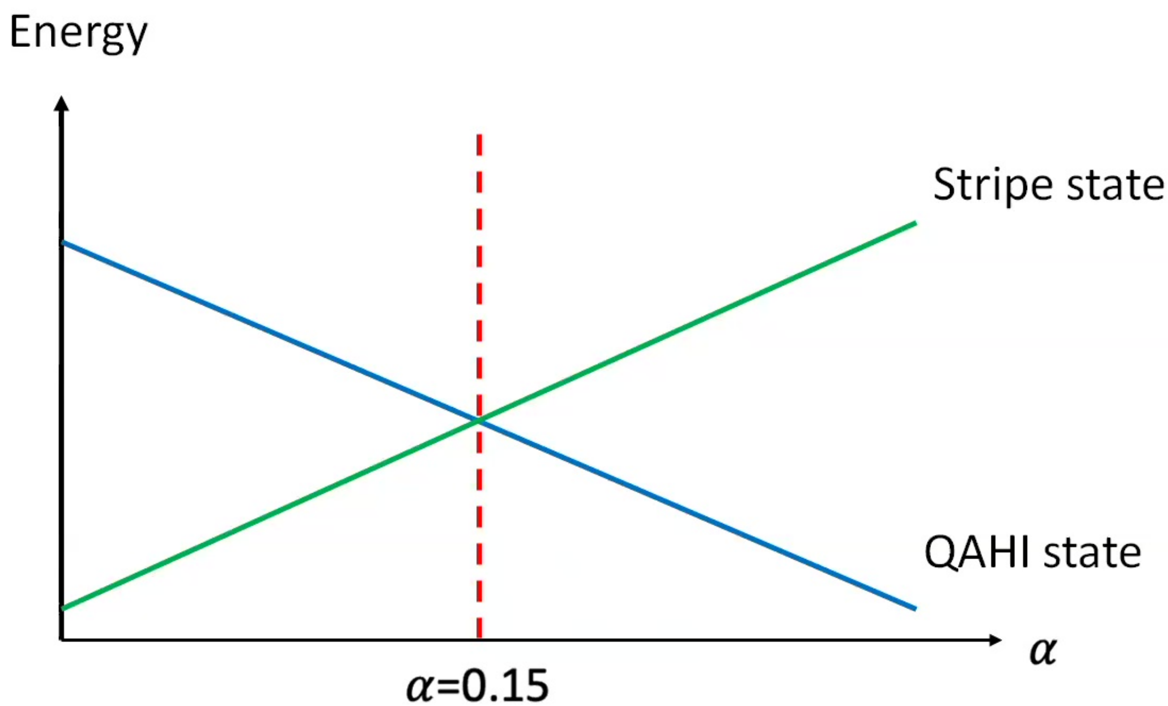
$$\rho_\sigma(\omega) = \sum_k A_{k\sigma}(\omega)$$

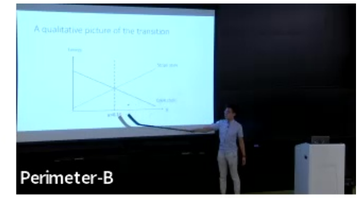
Result obtained from exact diagonalization



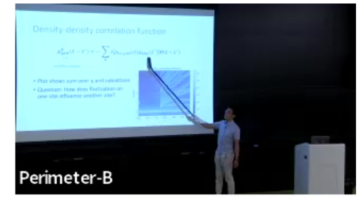

Transition

# A qualitative picture of the transition



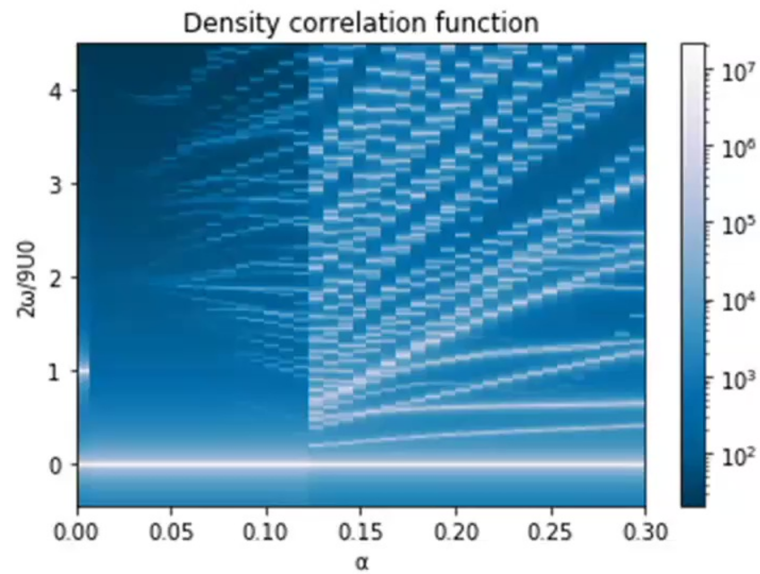
# Density-density correlation function



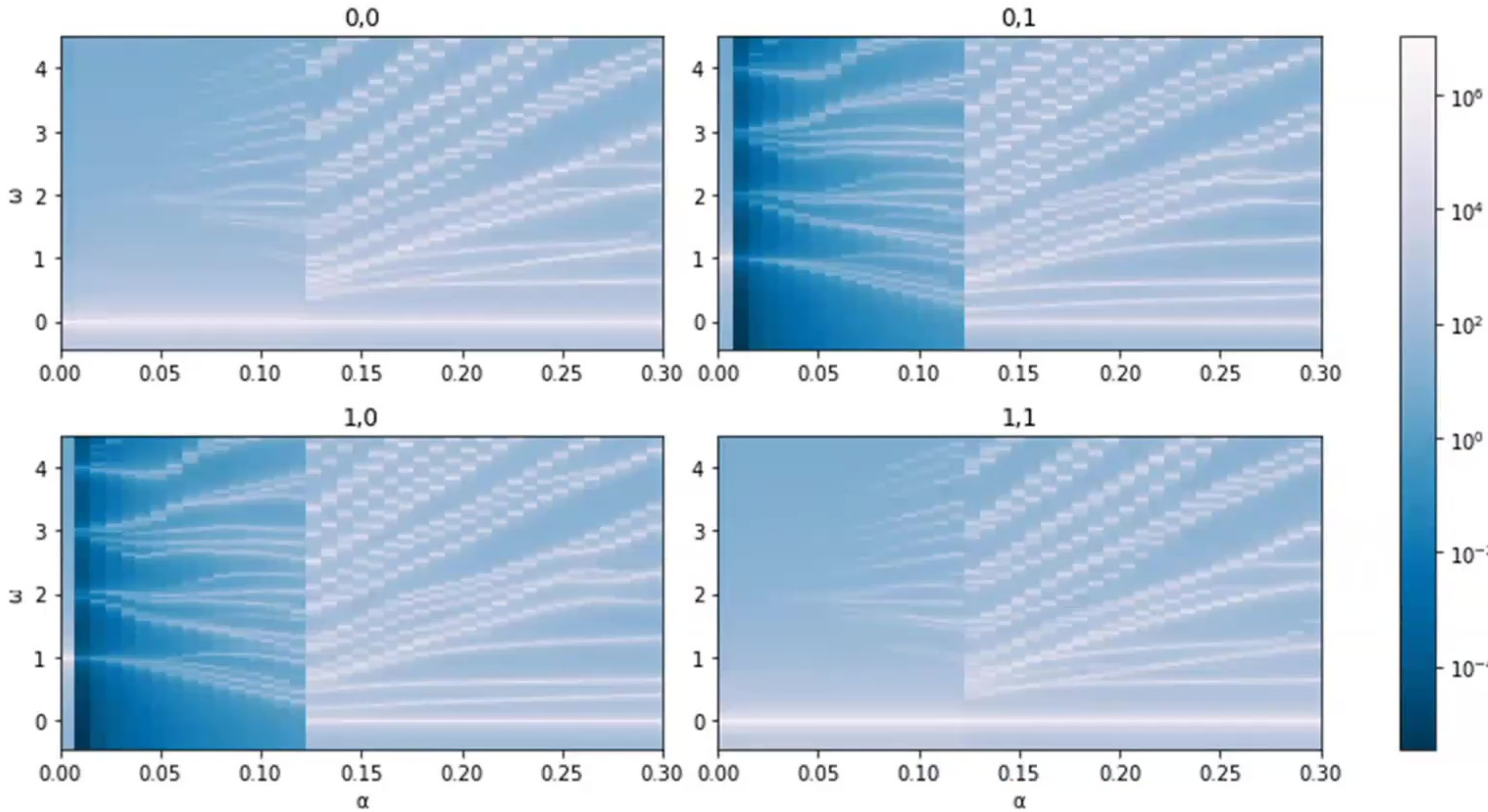

$$\rho^{R}_{q\sigma\theta}(t-t') = -\sum_{k} i\langle \rho_{k+q\sigma\theta}(t)\rho_{k\theta\sigma}(t')\rangle\theta(t-t')$$

Sublattice indices

- Plot shows sum over q and sublattices
- Question: How does fluctuation on one site influence another site?

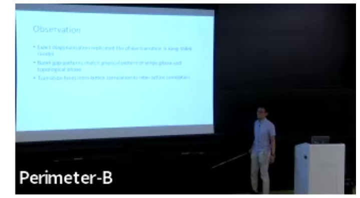


# Density correlation function across sublattices




A clear transition from same-sublattice phase to inter-sublattice correlated phase

# Observation




- Exact diagonalization replicated the phase transition in Kang-Vafek model
- Band gap patterns match physical pattern of stripe phase and topological phase
- Transition from intra-lattice correlation to inter-lattice correlation

# Future work: Floquet optical manipulation


- Light changes properties
- E.g. Floquet-driven QAHI in monolayer graphene (McIver *et al.*, 2020), superconductor modes based on symmetry (Claassen *et al.*, 2019)
- Question: can you optically drive the two degenerate chiral ground states from one to another?