Symmetry breaking and skyrmionic transport in twisted bilayer graphene

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N. Bultinck, SC and M. P. Zaletel, arXiv:1901.08110
Twisted bilayer graphene

- Bilayer graphene with a relative twist angle $\theta$
- Nearly flat bands close to the *magic angle* $\theta \sim 1.09^\circ$

Bistritzer, MacDonald, PNAS 2011

Animation: quantamagazine.org
Twisted bilayer graphene

- Bilayer graphene with a relative twist angle $\theta$
- Nearly flat bands close to the magic angle $\theta \sim 1.09^\circ$

Bistritzer, MacDonald, PNAS 2011

Figure: Koshino et al, PRX 2018
Twisted bilayer graphene

- 8 active low-energy bands (2 layer, 2 valley, 2 spin)
- Inversion $C_{2z}$ and time-reversal $T$ protects Dirac cones 
  \[ \text{Po et al, PRX 2018} \]
- Dirac cones within the same valley have identical chirality
  \[ \text{Related work: Yuan et al, Koshino et al, Isobe et al, Zou et al, Kang et al, lots of others...} \]

Figure: Koshino et al, PRX 2018
Twisted bilayer graphene

- Correlated insulators at integer fillings of Moire unit cells
- Superconductivity on doping away from these insulators

Cao et al. Nature\textsuperscript{2}, 2018

Yankowitz \textit{et al.}, Science 2018
Twisted bilayer graphene

- Correlated insulators at integer fillings of Moiré unit cells
- Superconductivity on doping away from these insulators

Lu et al, arXiv:1903.06513
Transport in TBG aligned with h-BN

- Insulator at charge neutrality ($\nu = 0$) – Dirac cones gapped out!
- Resistance peaks at $\nu = 2$ and $\nu = 3$ (insulating?)

Sharpe et al, Science 2019
Transport in TBG aligned with h-BN

- Insulator at charge neutrality ($v = 0$) – Dirac cones gapped out!

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- Resistance peaks at $\nu = 2$ and $\nu = 3$ (insulating?)

Sharpe et al, Science 2019
Transport in TBG aligned with h-BN

- What is the nature of the insulators at $\nu = 0, 2$ and $3$?
- Do we need to invoke interactions, or does a band picture suffice?

Sharpe et al., Science 2019
Transport in TBG aligned with h-BN

- Large anomalous Hall effect at $\nu = 3$ (out of 4 conduction bands), not quite quantized with $\sigma_{xy} \sim 0.5 \ e^2/h$

- Hysteresis loop in presence of a coercive magnetic field

- Signatures of chiral edges from non-local resistance (?)

Sharpe et al, Science 2019
**Transport in TBG aligned with h-BN**

- **Key feature of the device**: One graphene layer is very closely aligned with hexagonal Boron Nitride (h-BN) substrate

- **Effects of h-BN**
  1. Broken inversion ($C_{2z}$) symmetry (Dirac cones get gapped)
  2. Additional Moire potential (weaker than the original one)

- **Hypothesis**: Gapped bands can have Chern numbers $+C$ for valley K and $-C$ for valley $K'$

- **Interaction-driven valley polarization** $\rightarrow$ anomalous Hall effect

- **Full valley + spin polarization** can cause quantized anomalous Hall conductance

  \[
  \text{At } \nu = 3 : (K, \uparrow), (K, \downarrow), (K', \uparrow) \]
Chern bands and Valley Zeeman effect

- Band structure calculations using monolayer free-electron bands coupled via interlayer tunneling
  
  \[ \Delta_t = 0 \text{ meV}, \Delta_b = 0 \text{ meV} \]

- Added sublattice potential + phenomenological lattice relaxation

- Gaps at the Dirac cones \( \rightarrow \) Insulator at \( \nu = 0 \)

Bands in a single valley (others by time-reversal and spin-rotation symmetries)

- \( C = 1 \)
- \( C = -1 \)

Bistritzer, MacDonald, PNAS 2011
Chern bands and Valley Zeeman effect

- Band structure calculations using monolayer free-electron bands coupled via interlayer tunneling
  Bistritzer, MacDonald, PNAS 2011
- Added sublattice potential + phenomenological lattice relaxation
- Gaps at the Dirac cones → Insulator at $\nu = 0$

Bands in a single valley (others by time-reversal and spin-rotation symmetries)
Chern bands and Valley Zeeman effect

- Generically, topologically non-trivial bands in large parts of the phase diagram
- $C = \pm 1$ for valleys related by time-reversal symmetry
- Large valley Zeeman effect due to orbital magnetic moment, $g_v = -2$ to -6
- Chern bands + spontaneous polarization + valley Zeeman lead to anomalous Hall effect and hysteresis in $R_{xy}$

Sharpe et al, Science 2019
Chern bands and Valley Zeeman effect

• Toy model: Two bands with opposite Chern numbers ±1 described by dispersive lowest Landau levels, with screened isotropic Coulomb interaction $u_0$

• Metal $\rightarrow$ Valley polarized metal $\rightarrow$ Valley polarized insulator transition at half-filling when $W/u_0$ is tuned

• Anomalous Hall effect if valley-polarization is non-zero, quantized if fully valley + spin polarized
Recently, perfectly quantized anomalous Hall effect has been observed at the $\nu = 3$ in twisted bilayer graphene.

Serlin et al, arXiv:1907.00261
Fate of inter-valley coherence

- In quantum Hall bilayers, such a ferromagnetic state is unstable to inter-layer coherence in presence of small interaction anisotropy.

- What makes our state stable to intervalley coherence (IVC)?
Fate of inter-valley coherence

- In quantum Hall bilayers, such a ferromagnetic state is unstable to inter-layer coherence in presence of small interaction anisotropy?

- What makes our state stable to intervalley coherence (IVC)?

- Twist: Valleys have opposite Chern numbers

\[ \Phi(k) = \langle c_k^\dagger, + c_k, - \rangle \]

- The phases of the electron creation operators in ± valleys wind around the BZ by ±2\(\pi\)

- Phase of \(\Phi(k)\) must wind by 4\(\pi\) around the BZ → Nodes in \(\Phi(k)\) lower correlation energy gain
Lack of IVC at low interaction anisotropy; excitonic vortex lattice phase is possible when anisotropy is cranked up.

(A) Valley-polarized insulator (B) Exciton vortex lattice (C) Partially polarized metal (D) Unpolarized metal
• Lack of IVC at low interaction anisotropy; excitonic vortex lattice phase is possible when anisotropy is cranked up.

(A) Valley-polarized insulator  (B) Exciton vortex lattice  (C) Partially polarized metal  (D) Unpolarized metal
Transport in TBG aligned with h-BN

- In a perpendicular magnetic field $B_\perp$, $\rho_{xx}$ increases till $B_\perp = 6T$ and then decreases at filling $\nu = 2$

Sharpe et al, Science 2019
Symmetry breaking at $\nu = 2$

- Arrange the insulators according to the symmetries they break, and systematically check against the transport data

- $U(2)^+ \times U(2)^-$ from charge conservation, valley conservation and independent $SU(2)$ spin rotations in $\pm$ valleys in the decoupled limit

<table>
<thead>
<tr>
<th>Fully Valley-polarized spin-singlet (VP)</th>
<th>Inter-valley coherent state (IVC)</th>
<th>Spin-polarized valley symmetric (FM or SVL)</th>
</tr>
</thead>
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<tr>
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Symmetry breaking at $\nu = 2$

- Arrange the insulators according to the symmetries they break, and systematically check against the transport data

- $U(2)_+ \times U(2)_-$ from charge conservation, valley conservation and independent SU(2) spin rotations in $\pm$ valleys in the decoupled limit

- No anomalous Hall effect at $\nu = 2$
Symmetry breaking at $\nu = 2$

Inter-valley coherent state (IVC): $\langle \tau^x \rangle \neq 0$ or $\langle \tau^x s \rangle \neq 0$

$$H_M = \sum_k c_k^\dagger \left[ \Phi(k) \tau^x - g_V(k) \mu_B B_\perp \tau^z + (\varepsilon_{+,k} - \varepsilon_{-,k}) \tau^z \right] c_k$$

- If $\Phi(k) = \Phi_0$, then the charge gap $\Delta_c$ increases with $B_\perp$

$$\Delta_c(B_\perp) = 2 \sqrt{(\varepsilon_{+,k} - \varepsilon_{-,k} - g_V(K) \mu_B B_\perp)^2 + \Phi^2}$$

- But, the IVC order parameter $\Phi(k)$ from opposite Chern bands is momentum dependent; it must have nodes in the BZ.

- At the nodes, we expect the gap to decrease
Symmetry breaking at $\nu = 2$

Inter-valley coherent state (IVC): $\langle \tau^x \rangle \neq 0$ or $\langle \tau^x s \rangle \neq 0$

$$H_M = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger [\Phi(\mathbf{k}) \tau^x - g_V(\mathbf{k}) \mu_B B_\perp \tau^z + (\varepsilon_{+}\mathbf{k} - \varepsilon_{-}\mathbf{k}) \tau^z] c_{\mathbf{k}}$$

- For Chern $\pm 1$ bands, there can be two $2\pi$ nodes or a single $4\pi$ node.
- Consider two $2\pi$ nodes at the $K_+$ and $K_-$ points (assuming $C_6$)
- By time-reversal $\varepsilon_+ - \varepsilon_-$ has opposite sign at the two points, so the gap decreases at one point and increases at the other

$$\Delta_c(B_\perp) = 2|\varepsilon_{+}\mathbf{K} - \varepsilon_{-}\mathbf{K} - g_V(\mathbf{K}) \mu_B B_\perp|$$
Symmetry breaking at $\nu = 2$

Inter-valley coherent state (IVC): $\langle \tau^x \rangle \neq 0$ or $\langle \tau^x s \rangle \neq 0$

$$H_M = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger \left[ \Phi(\mathbf{k}) \tau^x - g_V(\mathbf{k}) \mu_B B_\perp \tau^z + (\varepsilon_{+,\mathbf{k}} - \varepsilon_{-,\mathbf{k}}) \tau^z \right] c_{\mathbf{k}}$$

- Nearly degenerate flat bands
  - $\Phi(\mathbf{k}) = \text{const in the MBZ}$
- $\Phi(\mathbf{k})$ has nodes in the MBZ

- For $\varepsilon_{+,\mathbf{K}} - \varepsilon_{-,\mathbf{K}} = 1.5$ meV, $g_V(\mathbf{K}) = 15$, the gap closes at $B_\perp = 3-4$ T
Symmetry breaking at $\nu = 2$

Inter-valley coherent state (IVC): $\langle \tau^x \rangle \neq 0$ or $\langle \tau^x s \rangle \neq 0$

$$H_M = \sum_k c_k^\dagger [\Phi(k)\tau^x - g_V(k)\mu_B B_\perp \tau^z + (\varepsilon_+, k - \varepsilon_-, k)\tau^z] c_k$$

- A $4\pi$ node in $\Phi(k)$ must occur at the $\Gamma$ point (with time-reversal)
- $g_V$ at the $\Gamma$ point is smaller; spin Zeeman becomes important

Metallic, $\rho_{xx}(B_\perp)$ drops

Insulating, $\rho_{xx}(B_\perp)$ rises
Symmetry breaking at $\nu = 2$

Inter-valley coherent state (IVC): $\langle \tau^x \rangle \neq 0$ or $\langle \tau^x s \rangle \neq 0$

$$H_M = \sum_k c_k^\dagger [\Phi(k)\tau^x - g_V(k)\mu_B B_\perp \tau^z + (\varepsilon_+,k - \varepsilon_-,k)\tau^z] c_k$$

- Both scenarios for $\rho_{xx}(B_\perp)$ are possible for a $4\pi$ node in $\Phi(k)$
- However, a nodal $\Phi(k)$ does not gap out the electrons completely and results in less correlation energy gain
- In a coarse-grained description, a double vortex in $\Phi(k)$ costs twice the energy of two single vortices
- Therefore, IVC order can be consistent with transport, but it is unlikely
Symmetry breaking at $\nu = 2$

- Arrange the insulators according to the symmetries they break, and systematically check against the transport data.

- $U(2)_+ \times U(2)_-$ from charge conservation, valley conservation and independent SU(2) spin rotations in $\pm$ valleys in the decoupled limit.

- Fully Valley-polarized spin-singlet (VP) $\langle \tau^z \rangle \neq 0$

- Inter-valley coherent state (IVC) $\langle \tau^x \rangle \neq 0$
  or $\langle \tau^x s \rangle \neq 0$

- Spin-polarized valley symmetric (FM or SVL) $\langle s \rangle \neq 0$
  or $\langle \tau^z s \rangle \neq 0$

Unlikely
Symmetry breaking at $\nu = 2$

Spin-polarized valley symmetric FM or SVL: $\langle s \rangle \neq 0$ or $\langle \tau^z s \rangle \neq 0$

$$H_M = \sum_k c_k^\dagger [M_S s^z - g_V(k)\mu_B B_\perp \tau^z + (\varepsilon_{+,k} - \varepsilon_{-,k})\tau^z] c_k$$

- The remaining possibilities for an insulator are a valley-unpolarized ferromagnet (+,↑;-↑) or spin-valley locked state (+,↑;-↓)
- To distinguish these two: Evaluate inter-valley coupling due to projected Coulomb and phonons
- Numerically, we find $J_{\text{Coulomb}}^{IV} \approx -0.2$ meV, $J_{\text{phonons}}^{IV} \approx 0.08$ meV
- Ferromagnetic state seems more favorable, but the scales are very close!
Symmetry breaking at $\nu = 2$

Spin-polarized valley symmetric FM or SVL: $\langle s \rangle \neq 0$ or $\langle \tau^z s \rangle \neq 0$

$$H_M = \sum_{\mathbf{k}} c_{\mathbf{k}}^\dagger [M_S s^z - g_V(\mathbf{k})\mu_B B_\perp \tau^z + (\varepsilon_{+,\mathbf{k}} - \varepsilon_{-,\mathbf{k}})\tau^z] c_{\mathbf{k}}$$

- Let us consider the valley-unpolarized ferromagnet ($\uparrow, \uparrow$; $\downarrow, \downarrow$)
- Even for this state, the particle-hole gap goes down with $B_\perp$
- Therefore, one would expect that $\rho_{xx}(B_\perp)$ decreases as $B_\perp$ goes up
Symmetry breaking at $\nu = 2$

Spin-polarized valley symmetric FM or SVL: $\langle s \rangle \neq 0$ or $\langle \tau^z s \rangle \neq 0$

$$H_M = \sum_k c_k^\dagger [ M_S s^z - g_V(k)\mu_B B_\perp \tau^z + (\varepsilon_{+,k} - \varepsilon_{-,k})\tau^z ] c_k$$

- Let us consider the valley-unpolarized ferromagnet ($+,\uparrow;-\uparrow$)
- Even for this state, the particle-hole gap goes down with $B_\perp$
- Therefore, one would expect that $\rho_{xx}(B_\perp)$ decreases as $B_\perp$ goes up
- However, Chern bands host additional charged excitations associated with spin textures: skyrmions!

Sondhi et al, PRL 1993  Y. Zhang et al, PRB 2019  Figure: Wikipedia
Symmetry breaking at $\nu = 2$

Spin-polarized valley symmetric FM or SVL: $\langle s \rangle \neq 0$ or $\langle \tau^z s \rangle \neq 0$

$$H_M = \sum_k c_k^{\dagger} [M_S s^z - g_V(k) \mu_B B_\perp \tau^z + (\varepsilon_+,k - \varepsilon_-,k) \tau^z] c_k$$

- Net charge gap $\Delta_c$ is set by the energy $2E_{sk}$ required to create a skyrmion pair, as long as $2E_{sk}$ is smaller than the particle-hole energy $E_{p-h}$.
- $E_{p-h}$ decreases linearly with $B_\perp$ due to the Zeeman terms.
- $E_{sk}$ is determined by the competition between screened Coulomb and Zeeman energies. It increases sub-linearly with $B_\perp$ (at small $B_\perp$) and then saturates when the skyrmion size becomes small.
Symmetry breaking at $\nu = 2$

Spin-polarized valley symmetric FM or SVL: $\langle s \rangle \neq 0$ or $\langle \tau^z s \rangle \neq 0$

$$H_M = \sum_k c_k^\dagger \left[ M_S s^z - g_V(k) \mu_B B_\perp \tau^z + (\varepsilon_{+,k} - \varepsilon_{-,k}) \tau^z \right] c_k$$

\[ \Delta_c = 2E_{sk} \sim B_\perp^{1/2} \text{ for small } B_\perp \]
Symmetry breaking at $\nu = 2$

Spin-polarized valley symmetric FM or SVL: $\langle s \rangle \neq 0$ or $\langle \tau^z s \rangle \neq 0$

\[ H_M = \sum_k c_k^\dagger [M_S s^z - g_V(k)\mu_B B_\perp \tau^z + (\varepsilon_{+}(k) - \varepsilon_{-}(k))\tau^z] c_k \]

- We generalize the expression for spin-stiffness to take into account inhomogeneities of Berry curvature.

\[ \rho_s = \frac{1}{8A} \left( \frac{1}{N} \sum_{k'} F(k')^2 \right) \left( \frac{1}{N} \sum_k V(k)f^2(k)|k|^2 \right) \]

- Numerically, we find that $E_{p-h} \approx 48$ meV, and $2E_{sk} \approx 21$ meV for a sublattice splitting $\Delta_t = 15$ meV

Figure: Wikipedia
Symmetry breaking at \( \nu = 2 \)

Spin-polarized valley symmetric FM or SVL: \( \langle s \rangle \neq 0 \) or \( \langle \tau_z s \rangle \neq 0 \)

\[
H_M = \sum_k c_k^\dagger \left[ M_S s^z - g_V(k) \mu_B B_\perp \tau^z + (\varepsilon_{+,k} - \varepsilon_{-,k}) \tau^z \right] c_k
\]

- Additional corrections due to Coulomb and Zeeman terms can be accounted for by an effective two-component non-linear sigma model

\[
\mathcal{L} = \sum_\alpha (A[n_\alpha] \cdot \partial_t n_\alpha(r) + \frac{\rho_s}{2} (\nabla n_\alpha(r))^2 + g_s \mu_B n_\alpha(r) \cdot B) - \frac{\rho_s}{2} [(n_+(r) - n_-(r))^2 - \frac{1}{2} \int dr' V(r - r') \rho(r) \rho(r')
\]

\[
E_{sk} = 4\pi \rho_s + \alpha E_C \left[ \left( \frac{\Delta}{E_C} \right) \ln \left( 1 + \frac{E_C}{\Delta} \right) \right]^{\nu}
\]

\[
\rho(r) = -\frac{C_e}{4\pi} n \cdot (\partial_x n \times \partial_y n)
\]

\[
E_C \sim \rho_s, \Delta = g_s \mu_B B_{\text{eff}}
\]

- The skyrmion still remains the lowest energy charged excitation

Figure: Wikipedia
Symmetry breaking at $\nu = 2$

Spin-polarized valley symmetric FM or SVL: $\langle s \rangle \neq 0$ or $\langle \tau^z s \rangle \neq 0$

- Skyrmions as charge carriers can explain the resistivity curve, both for the valley-unpolarized ferromagnet and the spin-valley locked state!

Figure: Wikipedia

- $\rho_{xx}$ decreases
- $\rho_{xx}$ peaks
- $\rho_{xx}$ increases

$\Delta_c$

$\Delta_{p-h}$

$2E_{sk,FM}$

$2E_{sk,SVL}$

$\frac{\tilde{\rho}_s}{g_s \mu_B}$

$B_{FM}$

$B_{SVL}$

$8\pi \rho_s$
Symmetry breaking at $\nu = 2$

- Arrange the insulators according to the symmetries they break, and systematically check against the transport data

- $U(2)_+ \times U(2)_-$ from charge conservation, valley conservation and independent SU(2) spin rotations in $\pm$ valleys in the decoupled limit

**Consistent, exciting possibility**

- Fully Valley-polarized spin-singlet (VP) $\langle \tau^z \rangle \neq 0$

- Inter-valley coherent state (IVC) $\langle \tau^x \rangle \neq 0$ or $\langle \tau^x s \rangle \neq 0$

- Spin-polarized valley symmetric (FM or SVL) $\langle s \rangle \neq 0$ or $\langle \tau^z s \rangle \neq 0$
Fun with skyrmions: Pairing

- Two skyrmions from the same valley naturally attract; hence skyrmion pairing can lead to superconductivity in doped samples. Y. Zhang et al, PRB 2019

- Skyrmions from opposite valleys can pair in the valley-unpolarized SVL. This phase transition proceeds by a deconfined quantum critical point.

- Charge 2e skyrmion pairs are defects of the magnetic order parameter, while superconducting vortices carry spin!


Experimental probes

- The ferromagnet breaks time-reversal, can be probed via µSR

- The spin-valley locked state is harder to detect; it breaks spin-rotation but not time-reversal as spins from opposite valleys anti-align

- May probe magnon dispersion at non-zero $B_\perp$ (gapped in FM, gapless in canted SVL) via thermodynamic probes, or spin currents

- If one can trap a skyrmion in impurities, local magnetometers like scanning nanosquids or NV centers

- Careful study of the charge activation gap with $B_\perp$ can also tell FM and SVL apart

SC, S. Sachdev, PRB 2015
Lachman et al, Science 2015,
Dovzhenko et al, Nat. Comms 2018
Conclusions and Outlook

• Chern bands can appear in TBG on aligning with h-BN substrate

• A spin and valley polarized insulator/metal can lead to anomalous Hall effect at odd fillings ($\nu = 3$)
  Y. Zhang, D. Mao, T. Senthil, arXiv:1901.08209,
  M. Xie, A. Macdonald, arXiv:1812.04213,
  Y. Lin, R. Nandkishore, arXiv:1901.00500

• A ferromagnetic insulator with skyrmionic excitations is consistent with the peculiar non-monotonic magnetoresistance at $\nu = 2$

• Why is there no insulator at $\nu = 1$?

• Chern bands seem ubiquitous in Moire devices (like tri-layer graphene on h-BN). Do skyrmions play a role in transport?
  G. Chen et al, Nature 2019, Y. Zhang et al, PRB 2019

• How important is the substrate alignment? Is $C_{2z}$ broken spontaneously?
  S. Liu et al, arXiv:1905.07409
Thank you for your attention!