Topological Band Theory for Twisted Multilayer Graphene

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Topics for today:

Introduction: Lattice structure of twisted FLG’s

I. New approach to an old Hamiltonian

II. “Compensated” class near a topological transition.

III. “Uncompensated” new topological state in epitaxial FLG’s
The interlayer coherence scale is large for a Bernal bilayer. But is small in faulted multilayers. 

Faults are indexed by a 2D graphene translation vector \((m,n)\) and occur in complementary partners with the same commensuration area but opposite sublattice exchange symmetry.
Two types of low energy physics

- SE odd
- SE even

Bernal

- no pseudospin rotation in AA stacking
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**Canonical long wavelength theory:** Layer decoupling from the momentum mismatch across a rotational fault

\[ H_{\text{eff}} u(\mathbf{r}) = -i\hbar v_F \left( \mathbf{\sigma} \cdot \nabla \right) u(\mathbf{r}) \]

J.M.B. Lopes dos Santos, N.M.R. Peres and A.H. Castro Neto

Dilemma

Family behavior missing from the small angle theory

Truncated interlayer amplitudes*:

Real-space (position dependent) pseudospin coupling matrices

*Interpretation of small angle approximation for a/L << 1
Small angle partners

$\theta = 3.89^\circ$

$\theta = 56.11^\circ$
with their coupled Dirac cones

$\theta = 3.89^\circ$

$\theta = 56.11^\circ$
Spatially modulated coupling

\[
\hat{T}(\vec{r}) = \hat{t}_0 + \sum_{n=1}^{6} \hat{t}_n e^{i\vec{G}_n \cdot \vec{r}}
\]
with expansion coefficients

\[ \hat{t}_n = t_G \begin{pmatrix} e^{-i\vec{G}_n \cdot \vec{r}_\gamma} & e^{-i\vec{G}_n \cdot \vec{r}_\alpha} \\ e^{-i\vec{G}_n \cdot \vec{r}_\beta} & e^{-i\vec{G}_n \cdot \vec{r}_\gamma} \end{pmatrix} \]

\[ t_G \begin{pmatrix} z & 1 \\ \overline{z} & z \end{pmatrix} \quad \text{(even n)} \quad \& \quad t_G \begin{pmatrix} \overline{z} & 1 \\ z & \overline{z} \end{pmatrix} \quad \text{(odd n)} \]

\[ t_0 = \begin{pmatrix} c_{aa} & c_{ab} \\ c_{ba} & c_{bb} \end{pmatrix}; \quad c_{aa} = c_{bb}, \quad c_{ab} = c_{ba} \]
Slonczewski-Weiss-McClure model

isotropic two center tight binding model

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Parameterization</th>
<th>I</th>
<th>II</th>
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<tbody>
<tr>
<td>$t_\sigma$</td>
<td>$(\gamma_1 - \gamma_3)/9$</td>
<td>43.3</td>
<td>8.3</td>
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TABLE I: Fourier coefficients (meV units) for the interlayer hopping operator Eqn. 2, fitted to the Slonczewski Weiss McClure parameterization for Bernal stacked layers. Model I: $\gamma_1 = 390$ meV, $\gamma_3 = \gamma_4 = 0$. Model II: $\gamma_1 = 390$ meV, $\gamma_3 = 315$ meV and $\gamma_4 = 44$ meV.
Model I: q=0 term in K-point basis

\[ T_{ij} \rightarrow T_{ij} e^{i\tilde{G} \cdot \bar{\tau}_i - i\tilde{G} \cdot \bar{\tau}_j} \]

\[ T_1 = w \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \]

\[ T_2 = w \begin{pmatrix} z & 1 \\ \bar{z} & z \end{pmatrix} \]

\[ T_3 = w \begin{pmatrix} \bar{z} & 1 \\ z & \bar{z} \end{pmatrix} \]

\[ w = \frac{\gamma_1}{3} = 130 \text{ meV} \quad (\text{TB est. } \sim 110 \text{ meV}) \]
Scaling Relations

\[
\Delta K = \frac{8\pi}{3a} \sin\left(\frac{\theta}{2}\right) \quad Q = \frac{q}{\Delta K}
\]

\[
E_\theta = \hbar v_F \Delta K = \frac{8\pi \hbar v_F}{3a} \sin\left(\frac{\theta}{2}\right) \quad \varepsilon = \frac{E}{E_\theta}
\]

\[
\tilde{c} = \frac{3ac}{8\pi \hbar v_F \sin\left(\frac{\theta}{2}\right)}
\]

only \(\theta\)-dependent parameter:
strong coupling at small angles
Canonical picture

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- **Decoupled**
- **Isotropic q=0 coupling**

- Van Hove sing.

- Coupling scale
Part I Conclusion:

Canonical long wavelength model projects the \( q=0 \) (i.e. averaged) interlayer amplitudes onto the K-point (pseudospin) basis.
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Slonczewski-Weiss-McClure model

SWMcc model contains a (strong) threefold lattice anisotropy

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Model II q=0 term in K-point basis

\[ T_1 = w \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \rightarrow c_{ab} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = c_{ab} \sigma_x \tau_x \]

\[ T_2 = c_{ab} \begin{pmatrix} 0 & 1 \\ \frac{1}{z} & 0 \end{pmatrix} \]

\[ T_3 = c_{ab} \begin{pmatrix} 0 & 1 \\ z & 0 \end{pmatrix} \]
Model I: coupled layer spectra

\[ \theta = 3.89^\circ \]
Decrease rotation angle
Topological Transition

\[ H = \begin{pmatrix} \sigma \cdot (-i \nabla) & \tilde{c}\sigma_x \\ \tilde{c}\sigma_x & \sigma \cdot (-i \nabla - (1) \hat{e}_{\Delta K}) \end{pmatrix} \]

\[ \tilde{H} = \begin{pmatrix} I & 0 \\ 0 & \sigma_x \end{pmatrix} H \begin{pmatrix} I & 0 \\ 0 & \sigma_x \end{pmatrix} \]

\[ \tilde{H} = \begin{pmatrix} H_K(\bar{q}) & \tilde{c} I \\ \tilde{c} I & \sigma_x H_K(\bar{q} - \Delta \bar{K})\sigma_x \end{pmatrix} \]

“Compensated” (opposite helicities)
Topological Transition

Decrease angle: increase coupling strength
Spectral reconstruction

Pair annihilation for compensated DP’s
Converge/collapse/diverge with increasing $c$

$\tilde{c} = \frac{1}{2}$
Part II Conclusion:

The SWMcC model contains a (large) threefold lattice anisotropy

Topological transition in small angle regime:

Relativistic (linear) bands → Massive (curved) bands
Dirac point annihilation and regeneration
BUT
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Reverse sign of anisotropy

-isotropic

\[ w \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \]

\[ c_{ab} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \]  
\text{anisotropic (-)}

\[ c_{aa} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \]  
\text{anisotropic (+)}
Topological Transition

\[ H = \begin{pmatrix} \sigma \cdot (-i\nabla) & \tilde{c} \ I \\ \tilde{c} \ I & \sigma \cdot (-i\nabla + \hat{e}_x) \end{pmatrix} \]

\[ H = \begin{pmatrix} H_K(\tilde{q}) & \tilde{c} \ I \\ \tilde{c} \ I & H_K(\tilde{q} - \Delta \tilde{K}) \end{pmatrix} \]

“Uncompensated” (same helicity)
Symmetry-protected crossing

Bilayer version of absence of backscattering
Second generation Dirac points

uncompensated

new DP

compensated
Helicity eigenstates

compensated hybridized cones

uncompensated symmetry-protected
Symmetry-protected intersection
Velocity renormalization (C)

\[ \hat{v}_+ = \frac{\partial \hat{H}}{\partial q_-} = v_F \hat{\sigma}_+ \rightarrow v_F (1 - \tilde{c}^2) \hat{\sigma}_+ \]

\[ \hat{v}_- = \frac{\partial \hat{H}}{\partial q_+} = v_F \hat{\sigma}_- \rightarrow v_F (1 - \tilde{c}^2) \hat{\sigma}_- \]

\[ v_F^* = v_F (1 - 9\tilde{c}^2) \]

perturbative, isotropic reduction
Velocity renormalization (U)

\[ \hat{v}_+ = \frac{\partial \hat{H}}{\partial q_-} = v_F \hat{\sigma}_+ \rightarrow v_F (\hat{\sigma}_+ - \tilde{c}^2 \hat{\sigma}_-) \]

\[ \hat{v}_- = \frac{\partial \hat{H}}{\partial q_+} = v_F \hat{\sigma}_- \rightarrow v_F (\hat{\sigma}_- - \tilde{c}^2 \hat{\sigma}_+) \]

\[ v_F^* = v_F (1 - \tilde{c}^4 \cos(2\phi)) \]

perturbative with twofold anisotropy
(vanishes after sum over $\Delta K$ triad)
Special features of the uncompensated state

- SYMMETRY-PROTECTED BAND CROSSING
- SECOND GENERATION DIRAC POINTS: DEGENERATE AT DISCRETE POINTS (NOT LINES)\(^1\).
- NO PERTURBATIVE VELOCITY RENORMALIZATION
- EXTENDED (STRONGER) VAN HOVE SINGULARITY

These are properties of the SiC (000 bar 1) epitaxial graphenes!

\(^1\) ARPES: Is there a linear band splitting along Q\(_{\text{perp}}\)?
Part III Conclusion:

Sign reversal of anisotropy identifies a second topological class ("uncompensated")

Interlayer hybridization prevented by pseudospin orthogonality at discrete symmetry-protected second generation Dirac singularities.

The Fermi velocity is unrenormalized in weak coupling
Small angle partners

\[ \theta = 3.89^\circ \]

\[ \theta = 56.11^\circ \]
Topological class from lattice anisotropy

compensated

\[ \gamma_3 > \gamma_4 \]

uncompensated

\[ \gamma_4 > \gamma_3 \]
More questions:

- **Coupling shifts** $\Delta K$'s
  *(commensuration at *small* magic angles?)*

- **Topological analysis of multilayers**
  *(topological semimetals)*

- **New physics in flat band land**
Theory Collaborators:

Charlie Kane
Markus Kindermann
Andy Rappe
Two-center TB is isotropic coupling, misses lattice anisotropy in T

Density functional calculations on short-period structures are not in the continuum limit.

Conventional SWMcC has $\gamma_3 > \gamma_4$ (compensated class).
Note this is a fit to Bernal stacked structure.

$\gamma_4 > \gamma_3$ is required for strong coupling in AA zones.