Topological Band Theory for Twisted Multilayer Graphene

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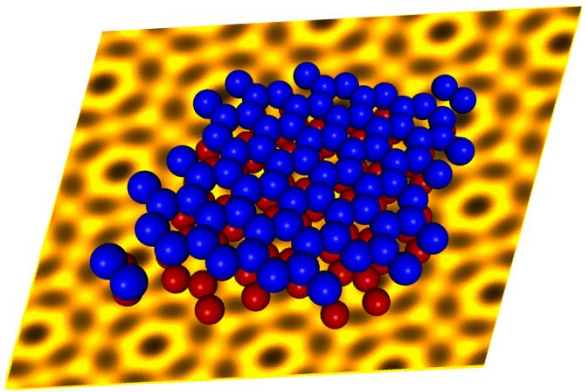
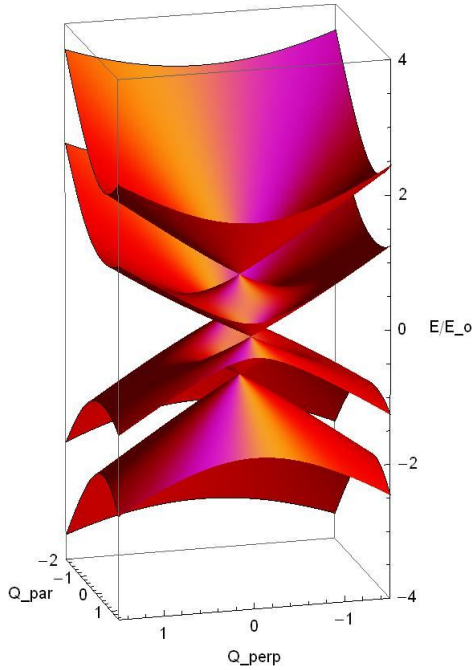




Topics for today:

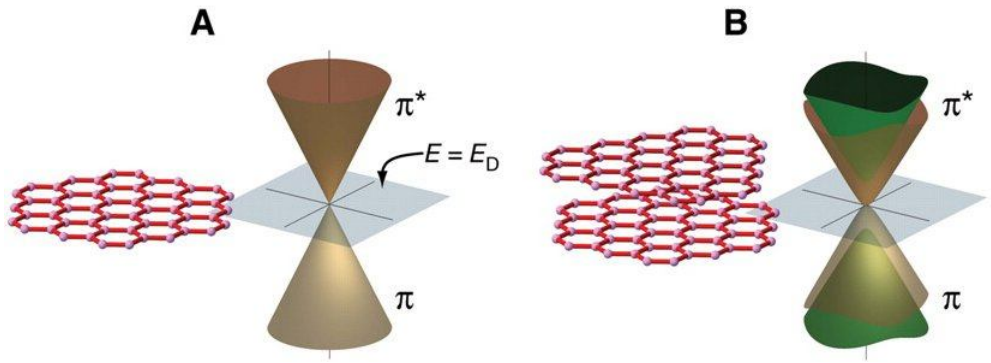
Introduction: Lattice structure of twisted FLG's

I. New approach to an old Hamiltonian

II. "Compensated" class near a topological transition.

III. "Uncompensated" new topological state in epitaxial FLG's

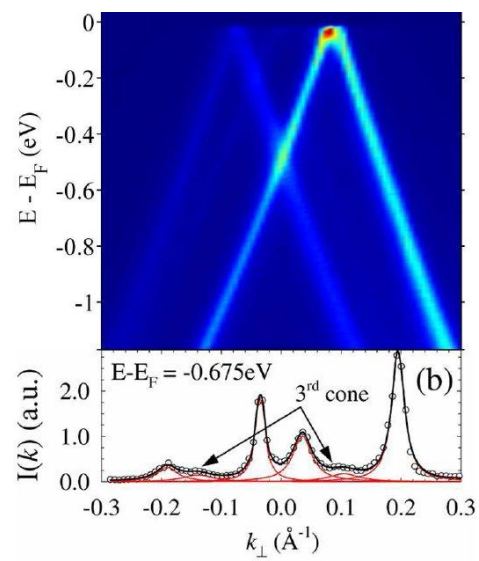
The interlayer coherence scale is large for a Bernal bilayer



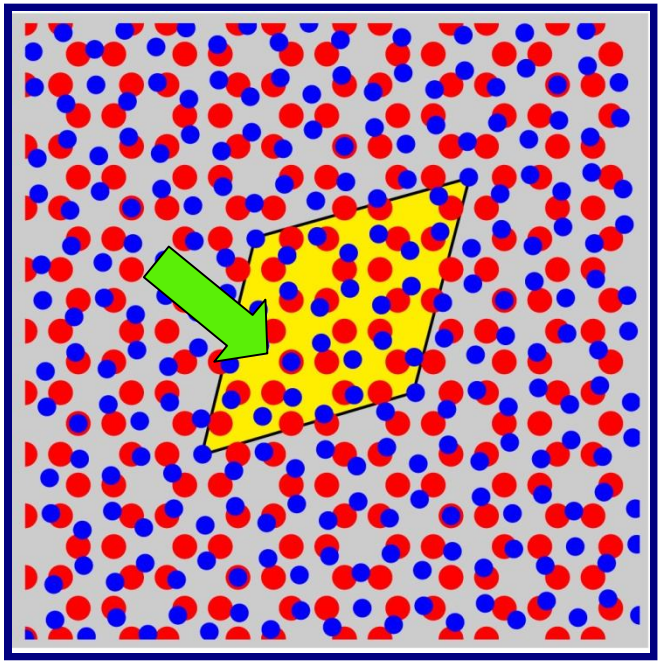
Single layer **Bernal Bilayer**

but is small in faulted multilayers

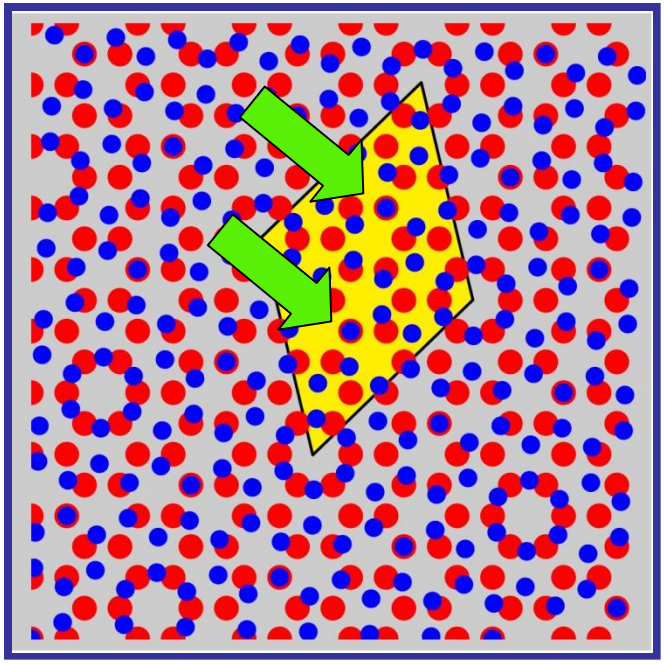
e.g. M. Sprinkle *et al.*
PRL 103, 226803 (2009) (ARPES)



Rotationally Faulted Bilayers



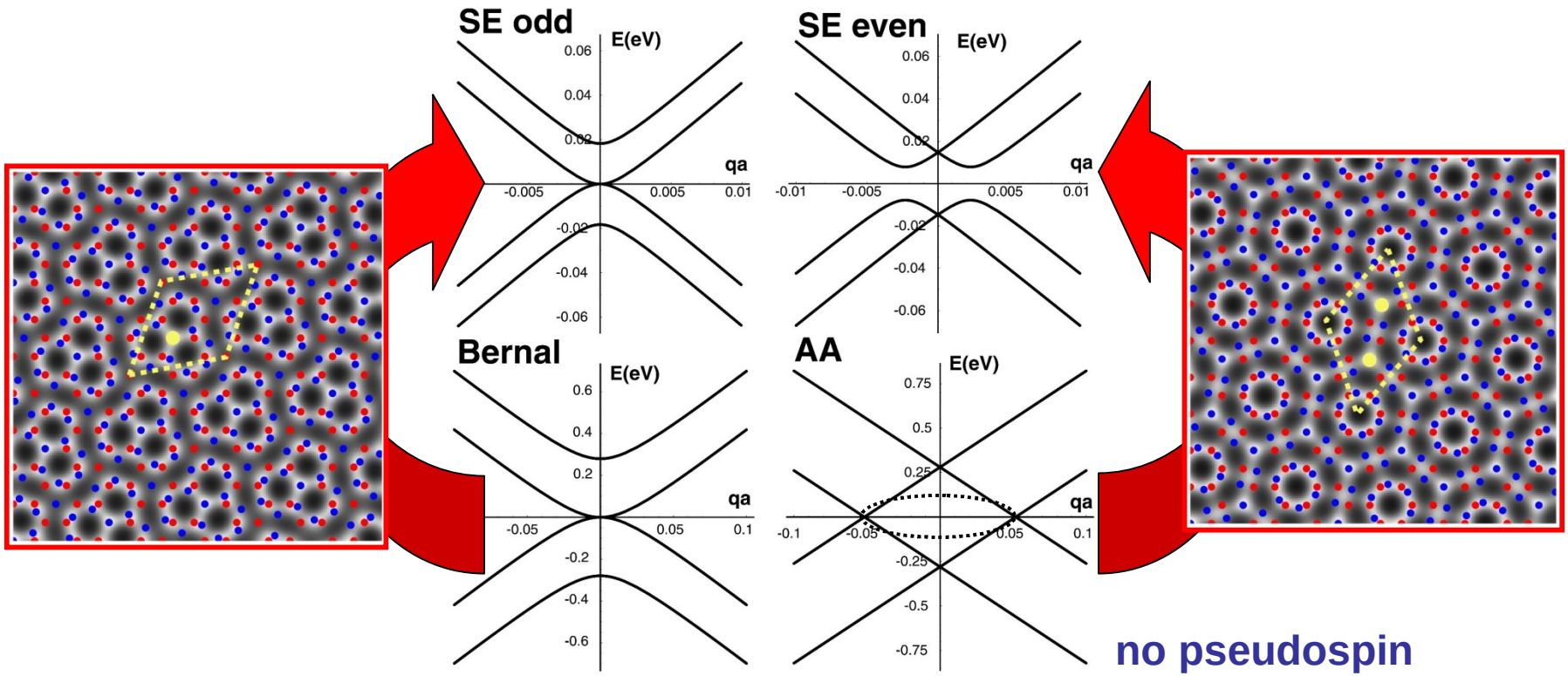
32.204°



27.796°

Faults are indexed by a 2D graphene translation vector ***(m,n)*** *and occur in complementary partners with the* ***<u>same</u>*** *commensuration area but* ***<u>opposite</u>*** *sublattice exchange symmetry*

Two types of low energy physics



no pseudospin rotation in AA stacking

Introduction: Lattice structure of twisted FLG's

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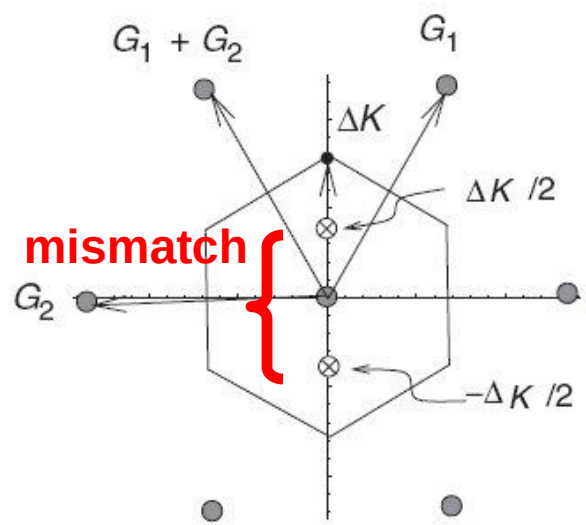
Canonical long wavelength theory: *Layer decoupling from the momentum mismatch across a rotational fault*

$$H_{eff}\,u(\vec{r}) = -i\hbar v_F\left(\vec{\sigma}\bullet\nabla\right)u(\vec{r})$$

pseudo-spinor wf



J.M.B. Lopes dos Santos, N.M.R. Peres and A.H. Castro Neto
Physical Review Letters 99, 256802 (2007))

R. Bistritzer and A. H. MacDonald, *PNAS* 108, 12233 (2011)

Dilemma

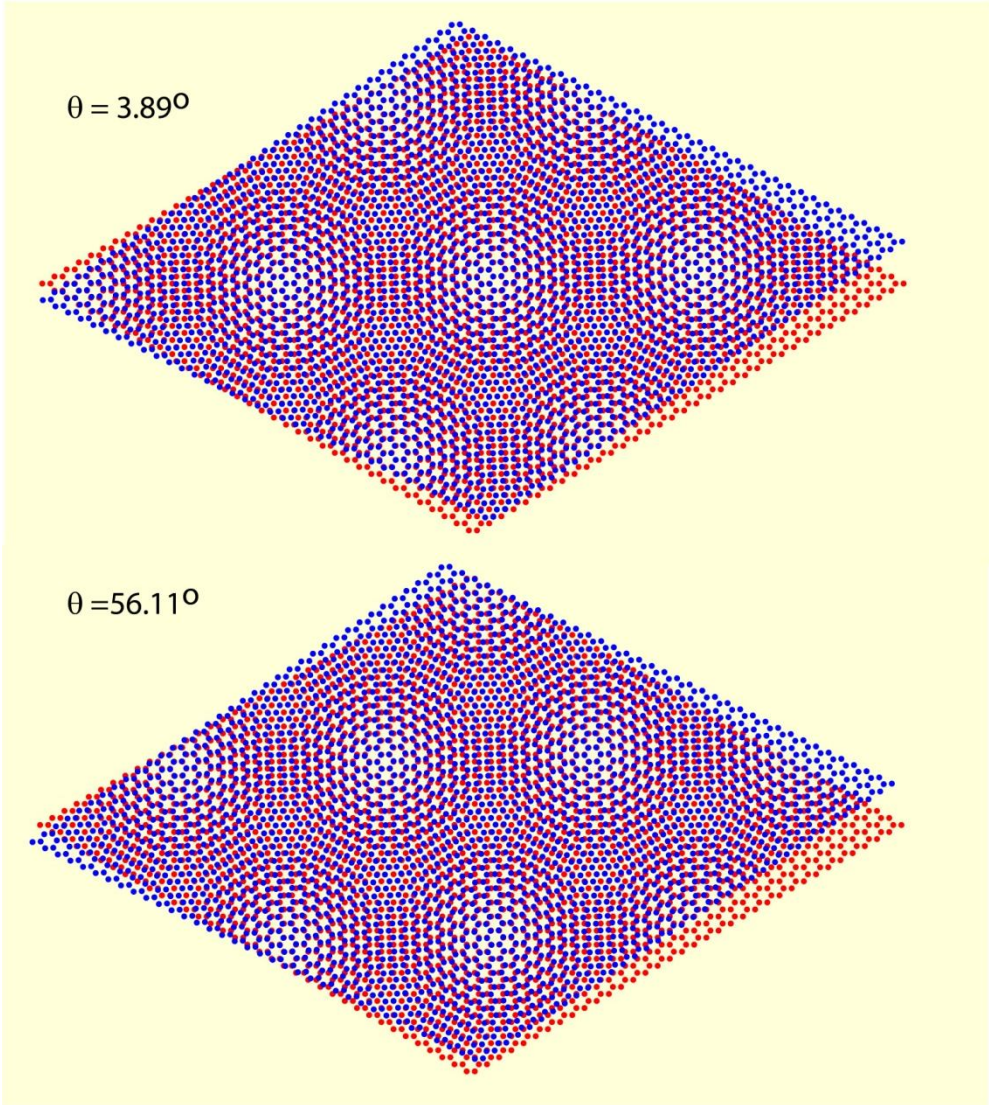
Family behavior missing from the small angle theory

Truncated interlayer amplitudes*:

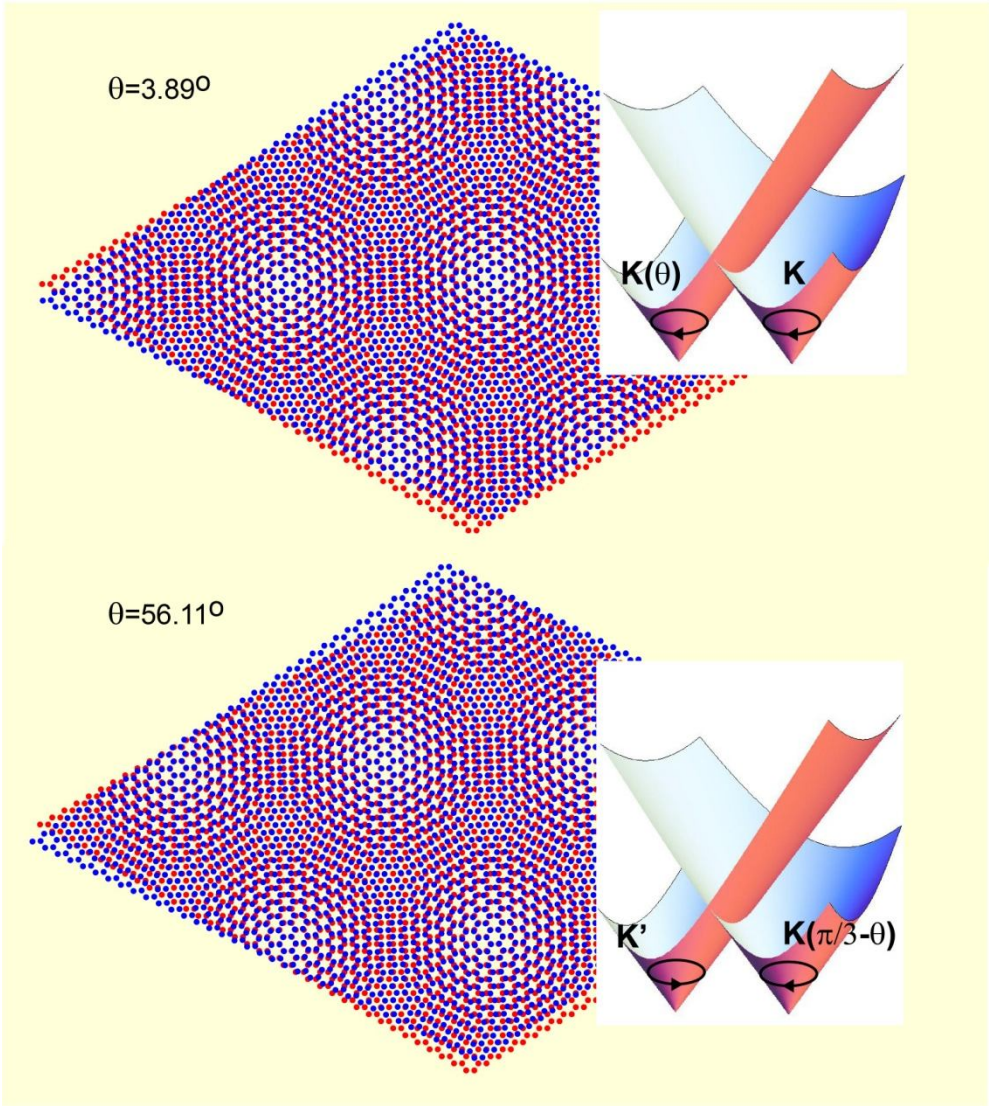
Real-space (position dependent) pseudospin coupling matrices

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

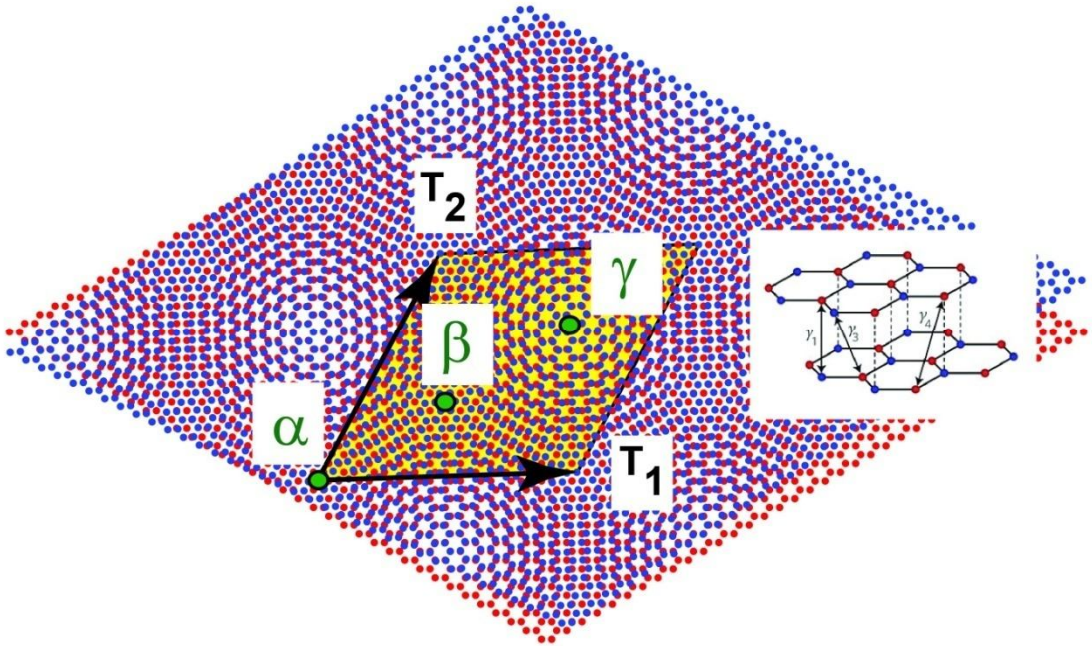
Small angle partners



with their coupled Dirac cones



Spatially modulated coupling



$$\hat{T}(\vec{r}) = \hat{t}_0 + \sum_{n=1}^{6} \hat{t}_n \, e^{i\vec{G}_n \bullet \vec{r}}$$

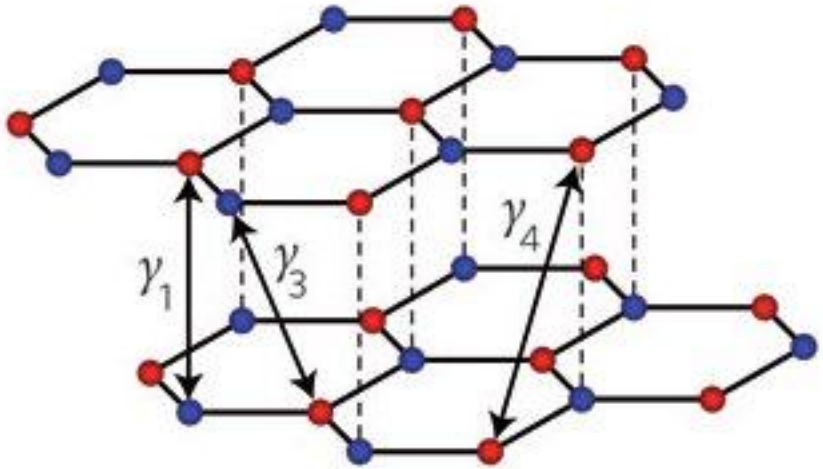
with expansion coefficients

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

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

$$t_0 = \begin{pmatrix} c_{aa} & c_{ab} \\ c_{ba} & c_{bb} \end{pmatrix}; \quad c_{aa} = c_{bb}, c_{ab} = c_{ba}$$

Slonczewski-Weiss-McClure model



isotropic two center tight binding model

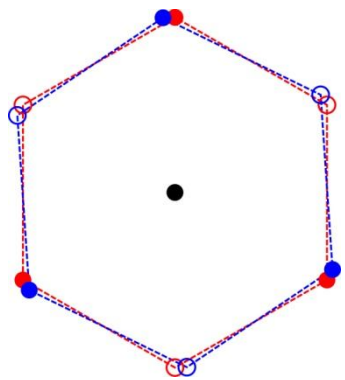
Coefficient	Parameterization	I	II
$t_{\mathcal{G}}$	$(\gamma_1 - \gamma_3)/9$	43.3	8.3
c_{aa}	$\gamma_4 + (\gamma_1 - \gamma_3)/3$	130.0	69.0
c_{ab}	$(\gamma_1 + 2\gamma_3)/3$	130.0	340.0

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

$$T_{ij} \rightarrow T_{ij}\ e^{i\vec{G}'\bullet\vec{\tau}_i' - i\vec{G}\bullet\vec{\tau}_j}$$

$$T_1 = w\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$



$$T_2 = w\begin{pmatrix} z & 1 \\ \bar{z} & z \end{pmatrix} \qquad T_3 = w\begin{pmatrix} \bar{z} & 1 \\ z & \bar{z} \end{pmatrix}$$

$$w = \frac{\gamma_1}{3} = 130 \text{ meV (TB est. } \sim 110 \text{ meV)}$$

Scaling Relations

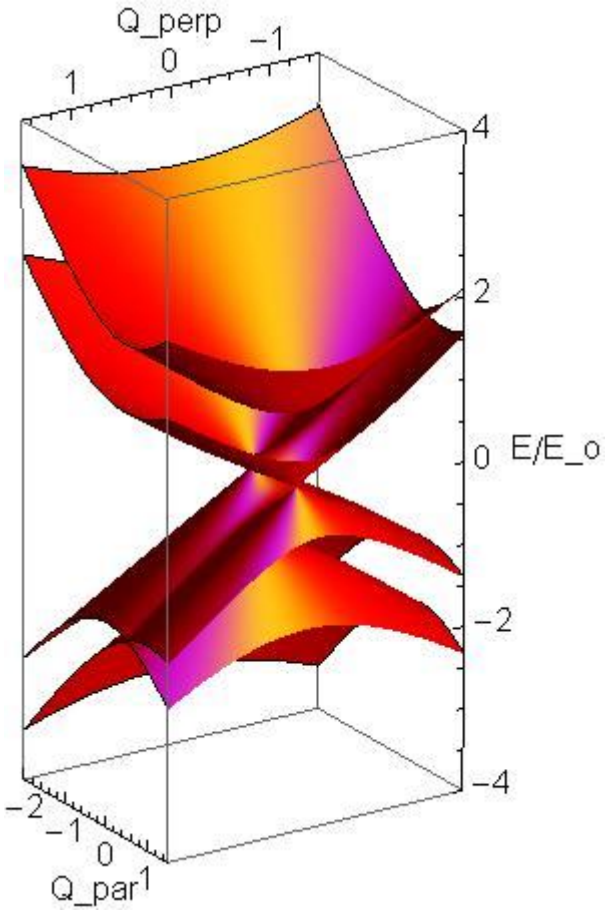
$$\Delta K = \frac{8\pi}{3a}\sin\left(\frac{\theta}{2}\right) \qquad Q = \frac{q}{\Delta K}$$

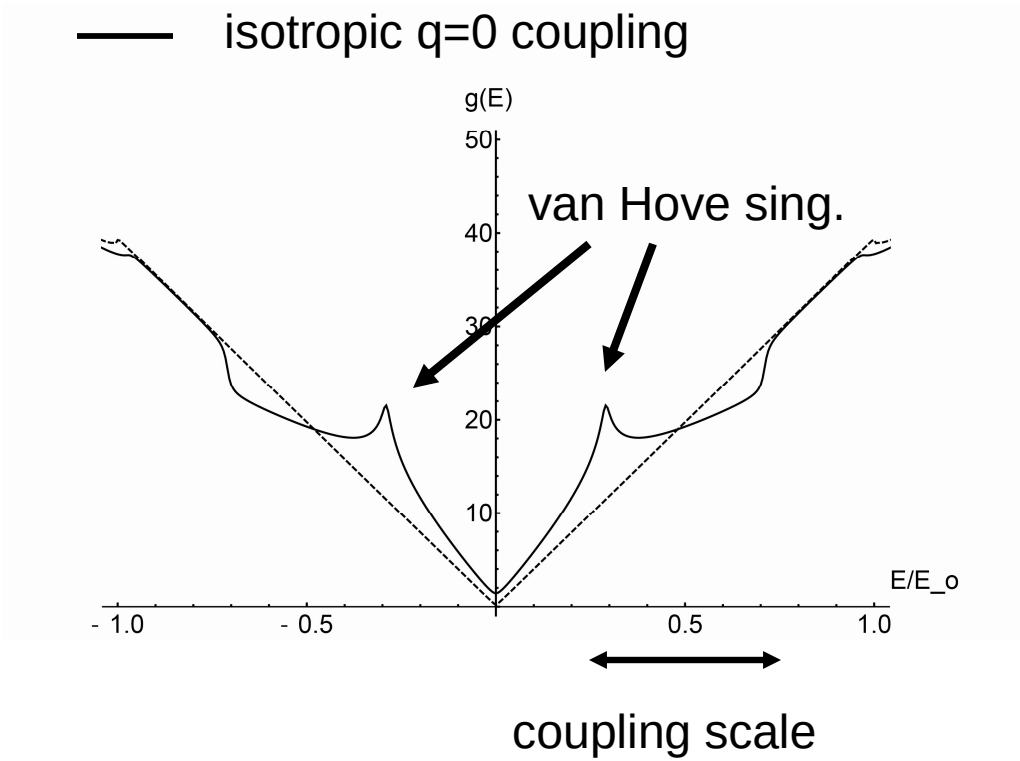
$$E_\theta = \hbar v_F \Delta K = \frac{8\pi\hbar v_F}{3a}\sin\left(\frac{\theta}{2}\right) \qquad \varepsilon = \frac{E}{E_\theta}$$

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

only θ-dependent parameter:
strong coupling at small angles

Canonical picture





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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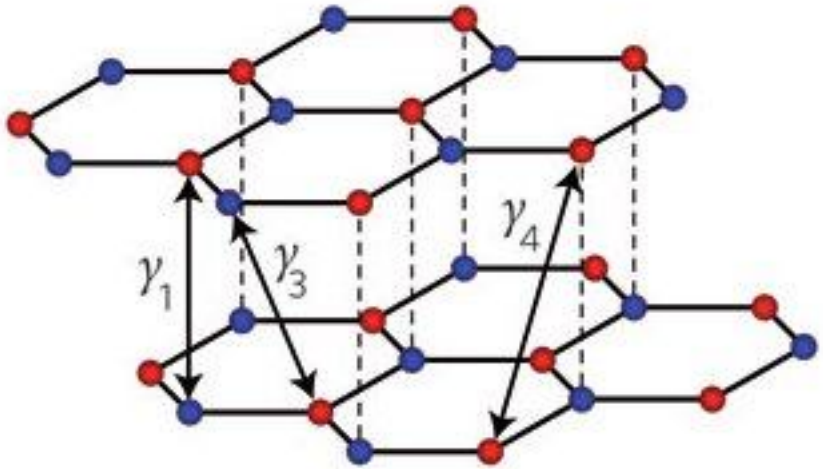
II. "Compensated" class near a topological transition.

III. "Uncompensated" topological state in epitaxial FLG's

Slonczewski-Weiss-McClure model



SWMcC model contains a (strong) threefold lattice anisotropy

Coefficient	Parameterization	I	II
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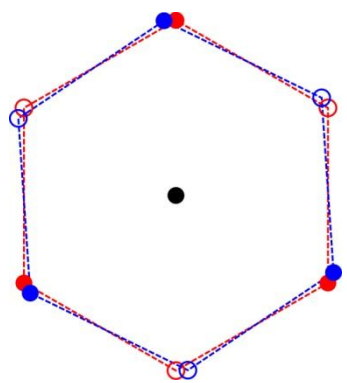
Model II q=0 term in K-point basis

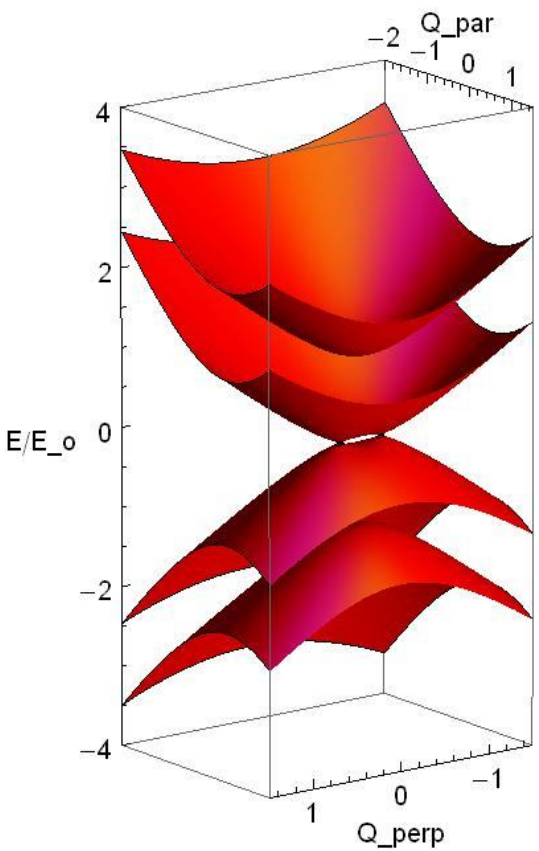
$$T_1 = w\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \rightarrow c_{ab}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = c_{ab}\sigma_x\tau_x$$

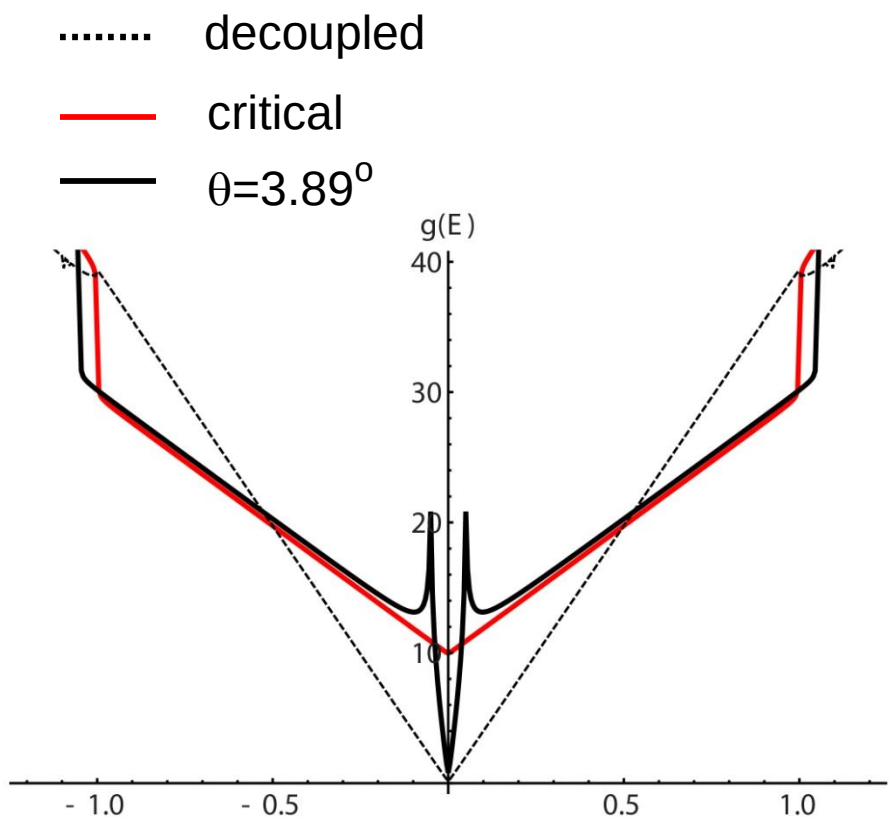


$$T_2 = c_{ab}\begin{pmatrix} 0 & 1 \\ \bar{z} & 0 \end{pmatrix}$$

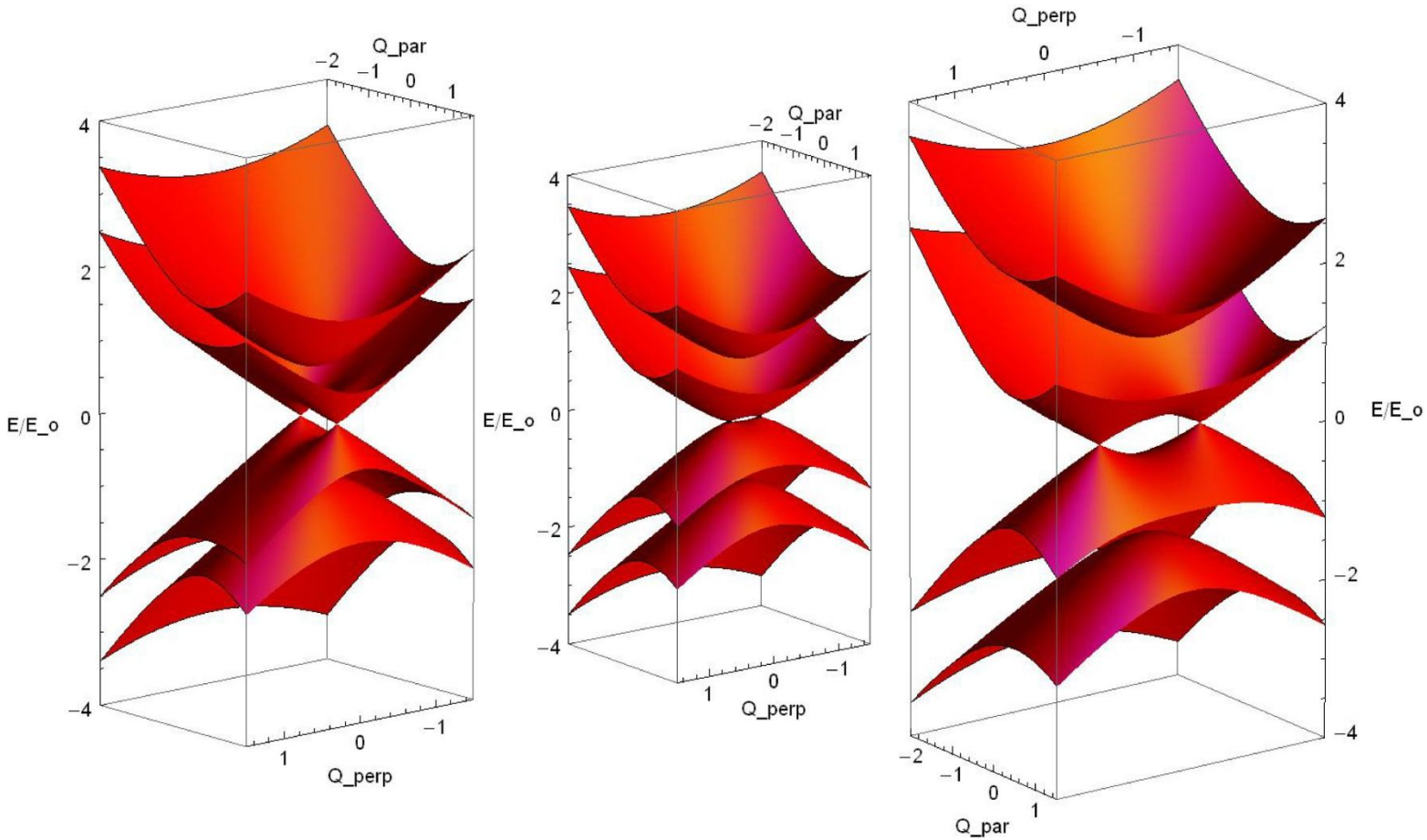
$$T_3 = c_{ab}\begin{pmatrix} 0 & 1 \\ z & 0 \end{pmatrix}$$

Model I: coupled layer spectra





Decrease rotation angle



increasing c

Topological Transition

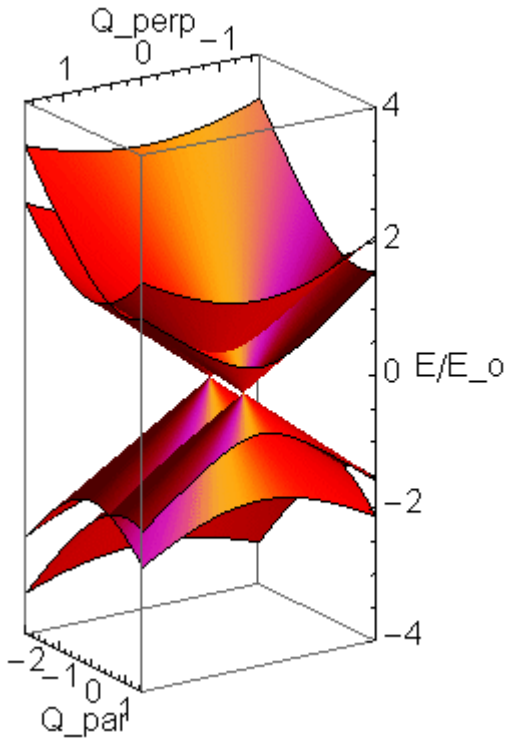
$$H = \begin{pmatrix} \sigma \bullet (-i\nabla) & \tilde{c}\sigma_x \\ \tilde{c}\sigma_x & \sigma \bullet (-i\nabla - (1)\hat{e}_{\Delta K}) \end{pmatrix}$$

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

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

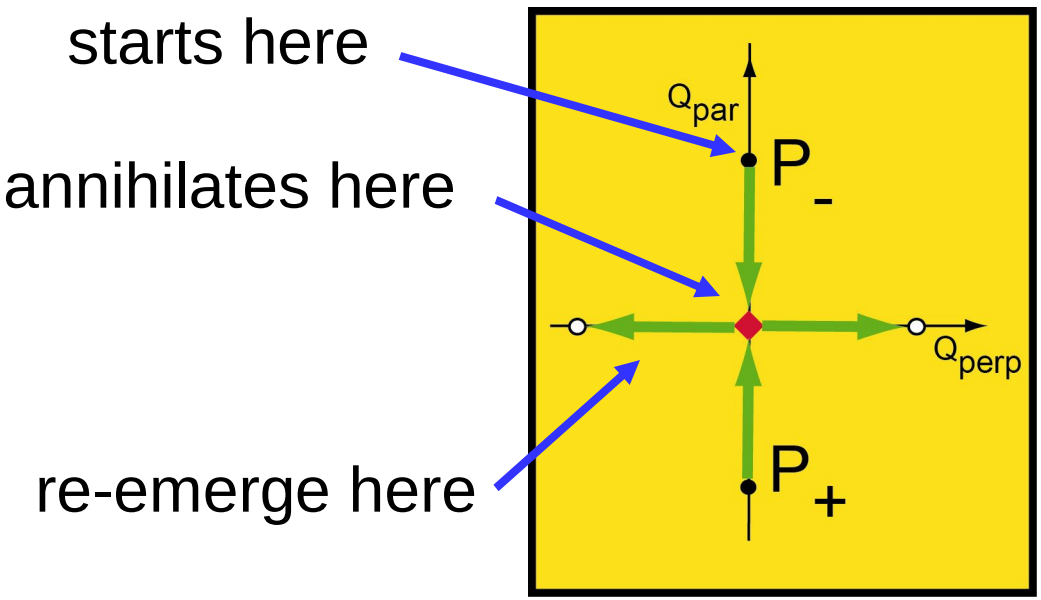
"Compensated" (opposite helicities)

Topological Transition

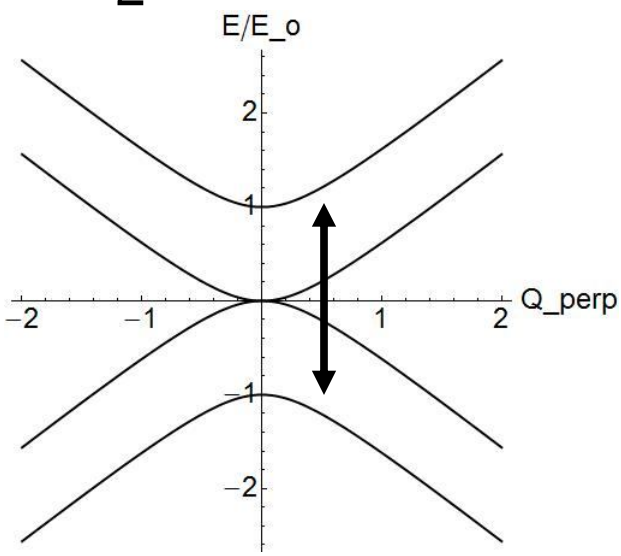


Decrease angle: increase coupling strength

Spectral reconstruction



$$\tilde{c} = \frac{1}{2}$$



Pair annihilation for compensated DP's

Converge/collapse/diverge with increasing c

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

$$w\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

$$c_{ab}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$ anisotropic (-)

$$c_{aa}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$ anisotropic (+)

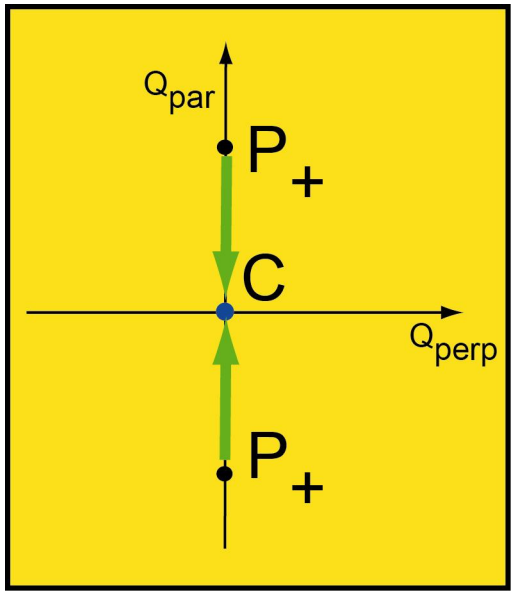
Topological Transition

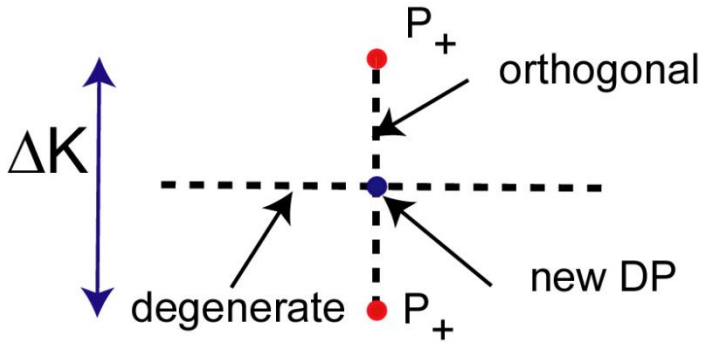
$$H = \begin{pmatrix} \sigma \bullet (-i\nabla) & \tilde{c}\, I \\ \tilde{c}\, I & \sigma \bullet (-i\nabla + \hat{e}_x) \end{pmatrix}$$

$$H = \begin{pmatrix} H_K(\vec{q}) & \tilde{c}\, I \\ \tilde{c}\, I & H_K(\vec{q} - \Delta\vec{K}) \end{pmatrix}$$

"Uncompensated" (same helicity)

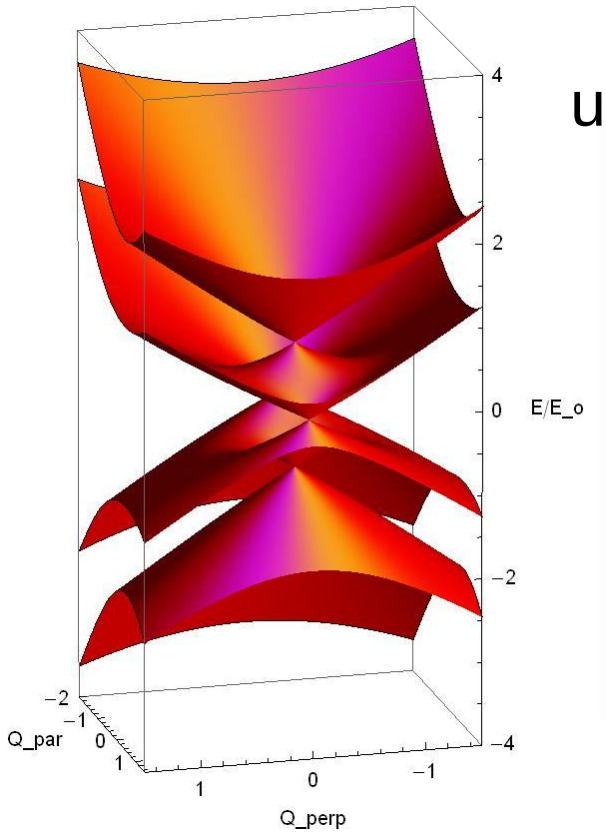
Symmetry-protected crossing

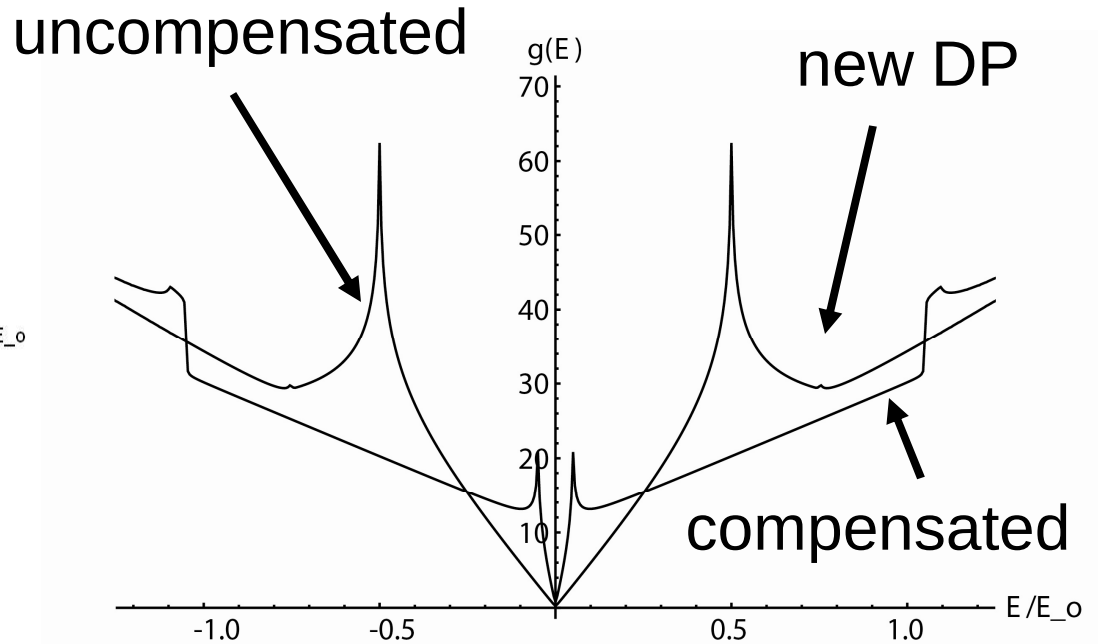




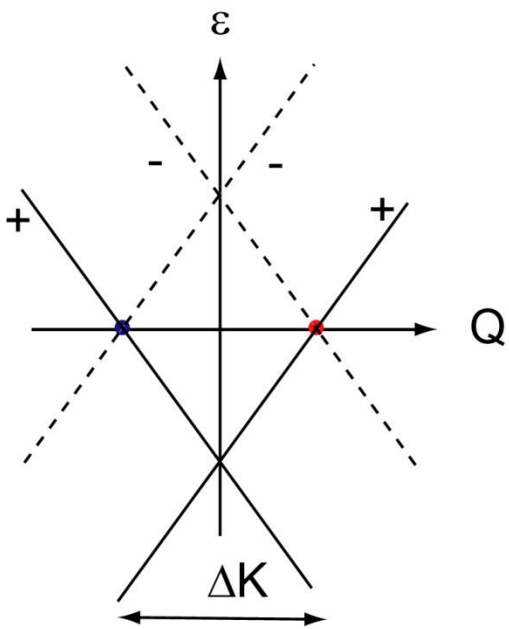
Bilayer version of absence of backscattering

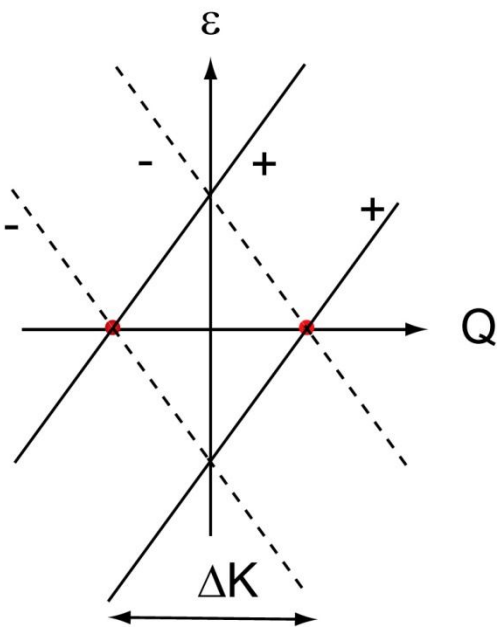
Second generation Dirac points





Helicity eigenstates

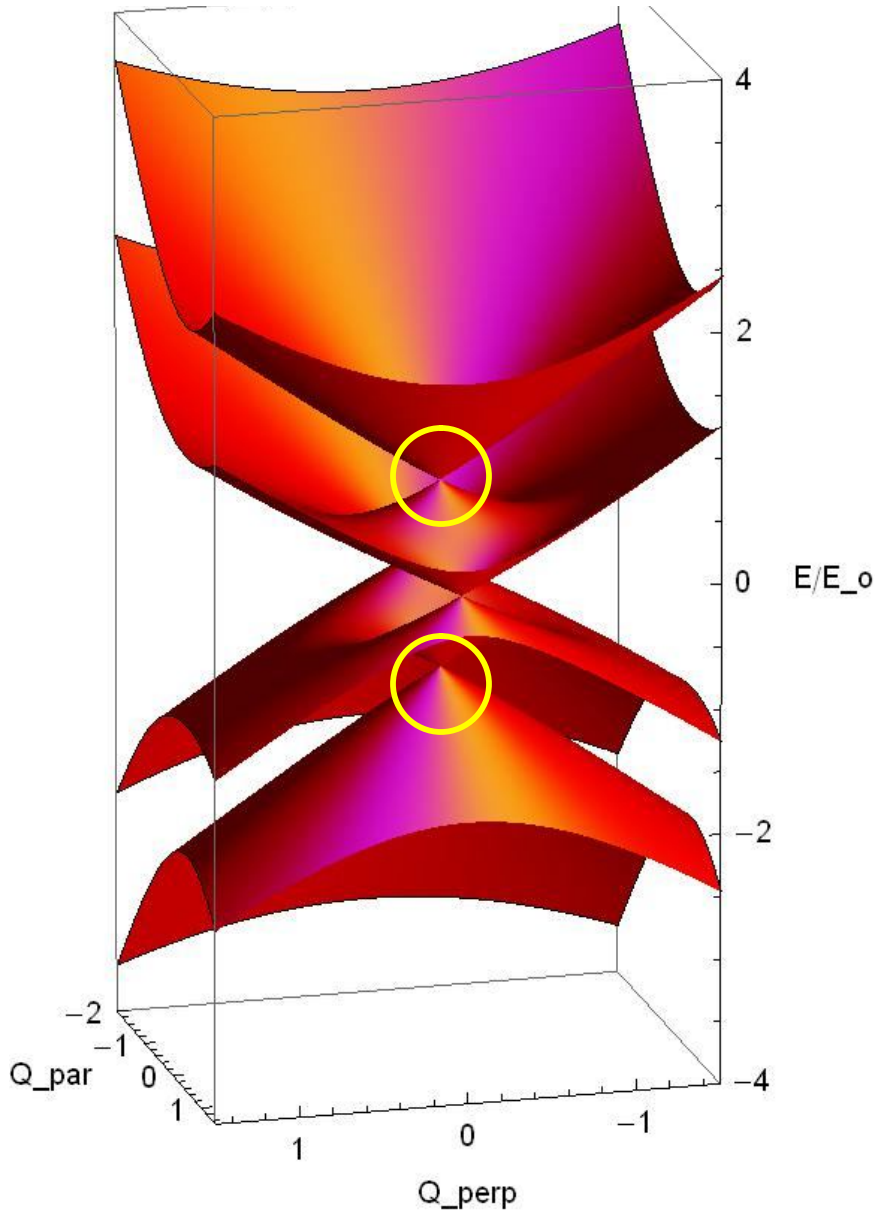




<u>compensated</u>
hybridized cones

<u>uncompensated</u>
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 ΔK 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_perp?

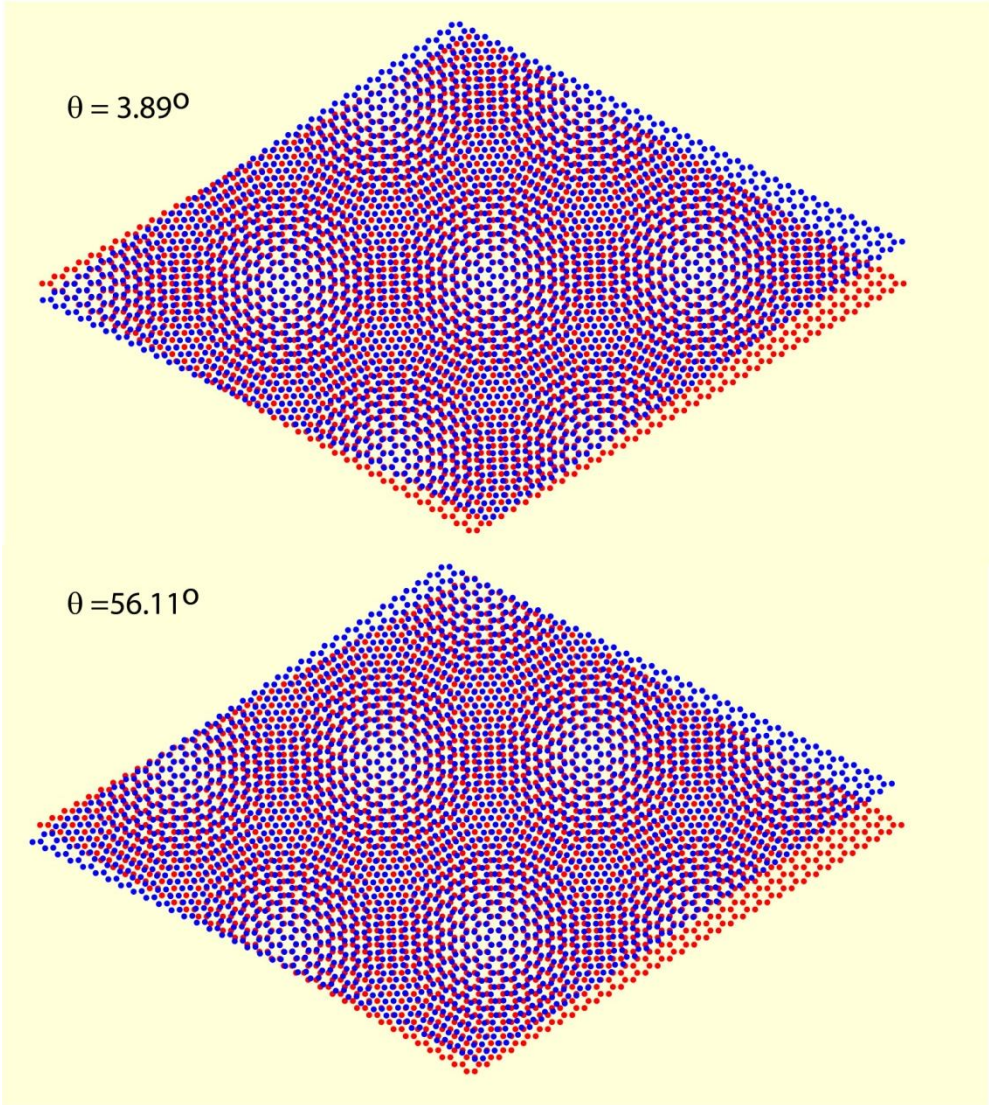
Part III Conclusion:

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

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

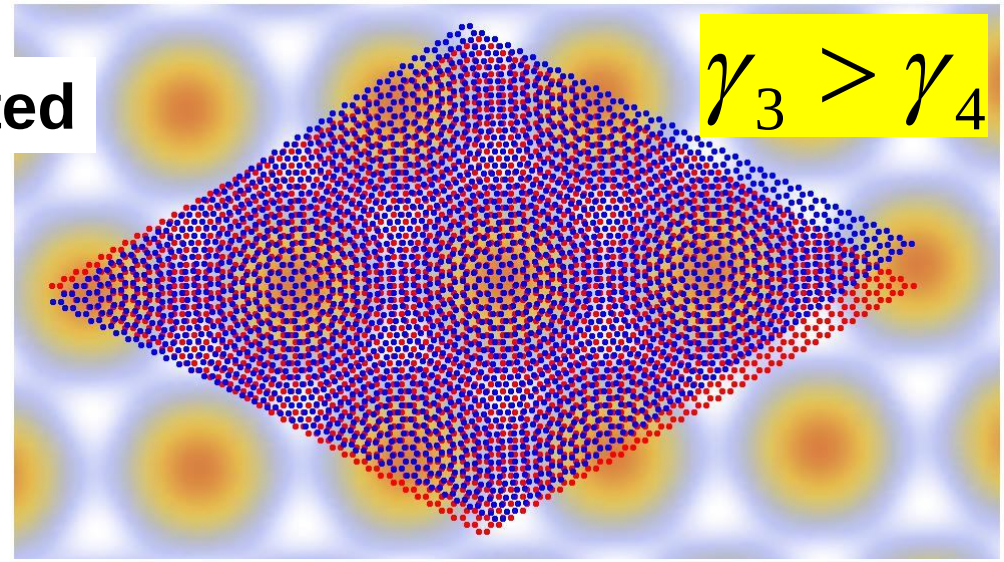
The Fermi velocity is unrenormalized in weak coupling

Small angle partners

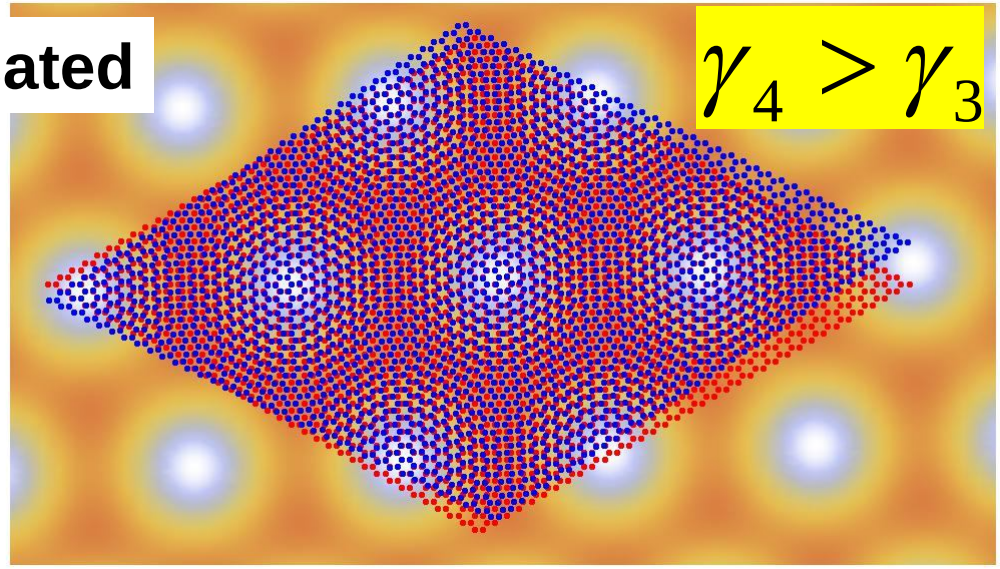


Topological class from lattice anisotropy

compensated



uncompensated



More questions:

- ***Coupling shifts ΔK's***
  (commensuration at small magic angles?)
- ***Topological analysis of multilayers***
  (topological semimetals)
- ***New physics in flat band land***

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UNIVERSITY of PENNSYLVANIA

Theory Collaborators:

Charlie Kane
Markus Kindermann
Andy Rappe

Comments

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.