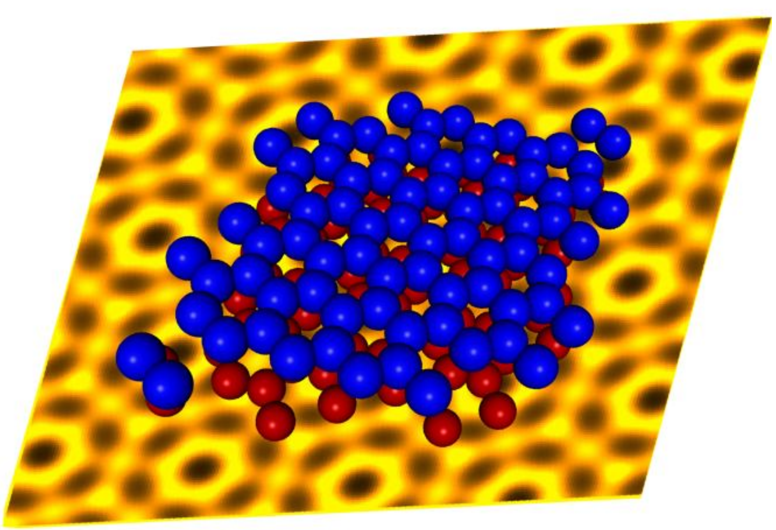
An unexpected turn for twisted graphenes

Gene Mele
University of Pennsylvania



Twisted Graphenes:

I. Introduction: what, where, why

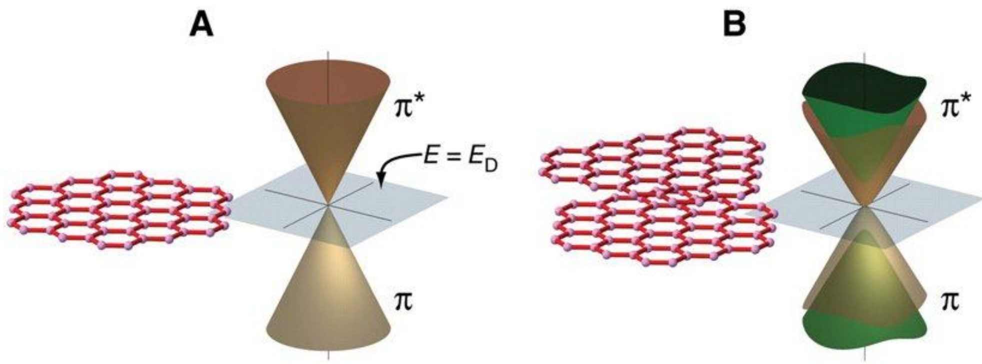
II. Family behavior of low energy physics

III. New approach to an old Hamiltonian

IV. "Compensated" class near a
topological transition

V. "Uncompensated" new topological state
in twisted FLG's

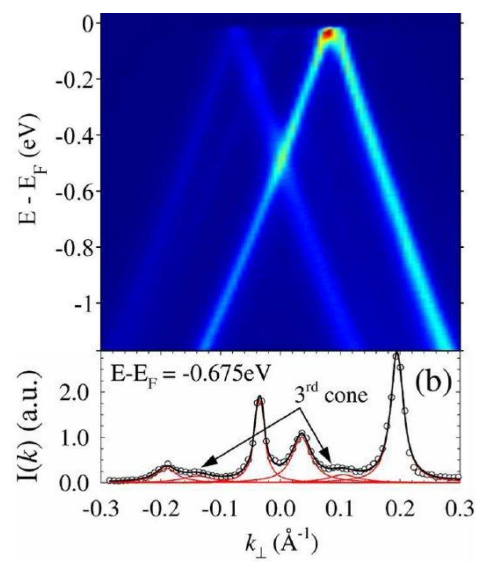
The interlayer coherence scale is large for a Bernal bilayer



Single layer **Bernal Bilayer**

but it is very small in faulted multilayers

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



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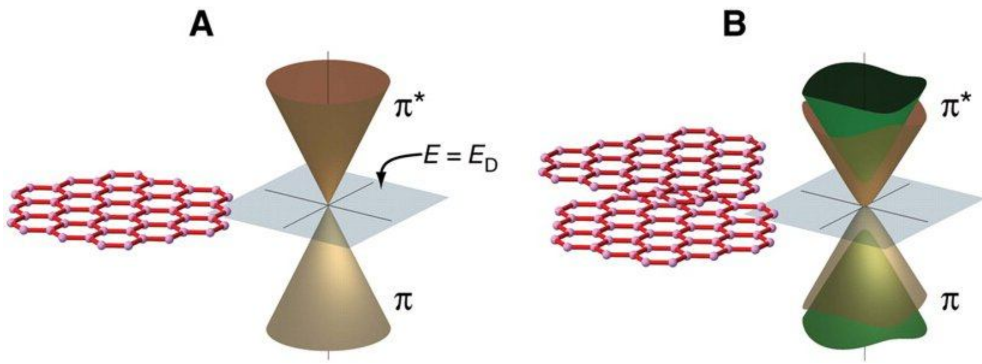
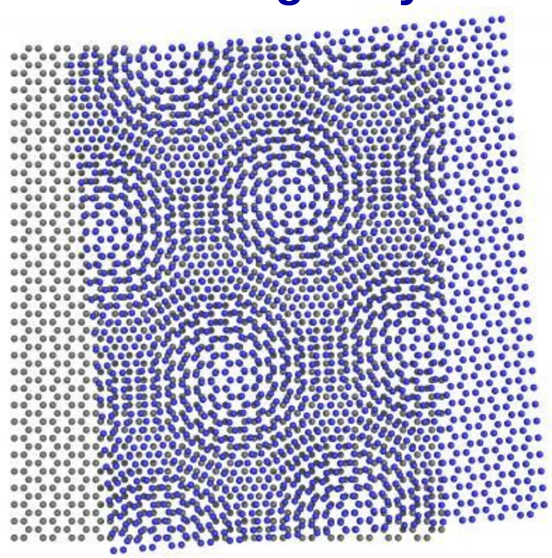
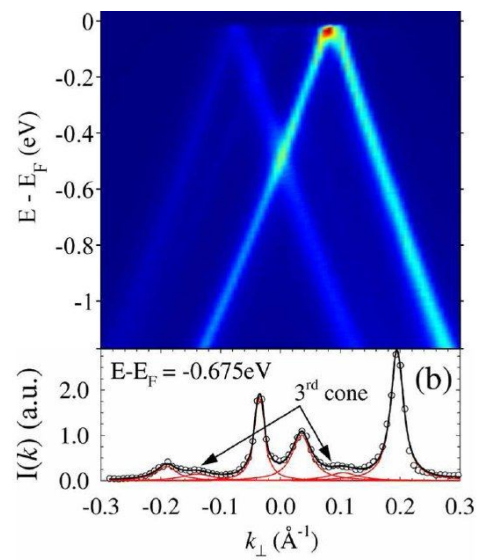


Single layer

Bernal Bilayer





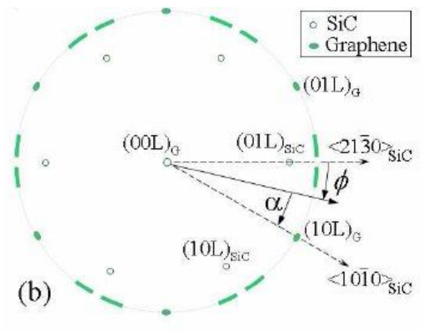
Some faulted graphene bilayers

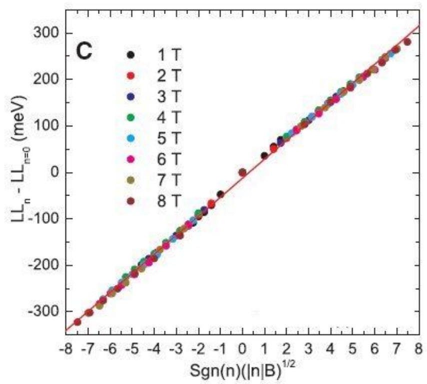
Epitaxial graphene on SiC $(000\bar{1})$

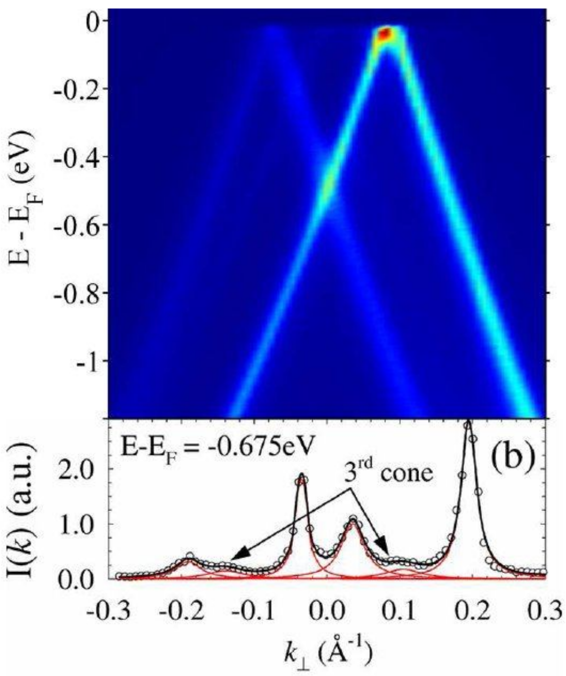
C. Berger *et al.* Science 312, 1191 (2006) (synthesis)

D.L. Miller *et al.* Science 324, 924 (2009) (Landau level spectroscopy)

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



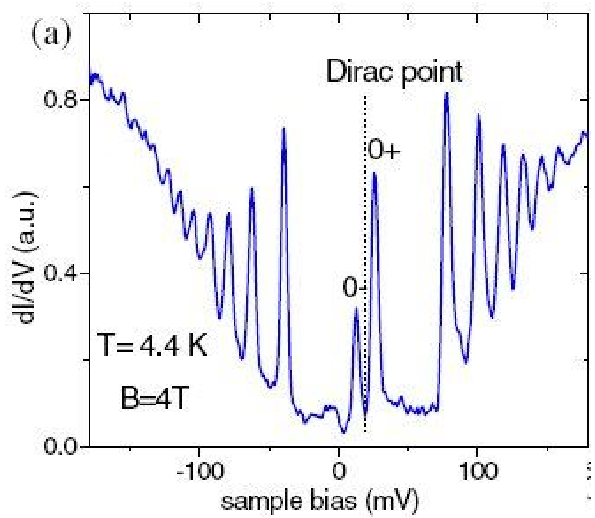




more faulted graphene bilayers

Graphene on Graphite

G. Li, A. Luican and E. Andrei, Phys. Rev. Lett. 102, 176804 (2009)
Landau level (Scanning Tunneling Spectroscopy)



Folded Exfoliated Graphene

H. Schmidt *et al.*, Appl. Phys. Lett. 93, 172108 (2009)

and some theory

Decoupling via Momentum Mismatch

J.M.B. Lopes dos Santos, N.M.R. Peres and A.H. Castro Neto
"Graphene Bilayer with a Twist: Electronic Structure"
Phys. Rev. Lett. 99, 256802 (2007)

S. Shallcross, S. Sharma and O.A. Pankratov:
"Quantum Interference at the Twist Boundary in Graphene"
Phys. Rev. Lett. 101, 056803 (2008)

Many Body Effects

H. Min *et al.*: "Room temperature superfluidity in graphene bilayers". Phys. Rev. B 78, 121401 (2008), etc.

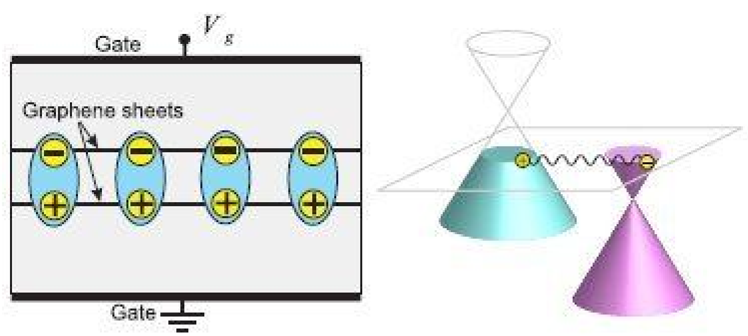
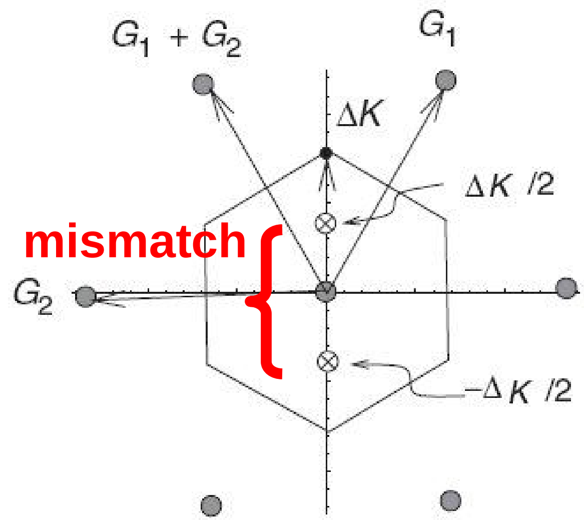


FIG. 1. (Color online) Excitonic condensate in a system of two spatially separated graphene layers. Electrons and holes in the layers are induced by applying the external gate voltage.

Orthodoxy: *Layer decoupling comes from the momentum mismatch across a rotational fault*

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

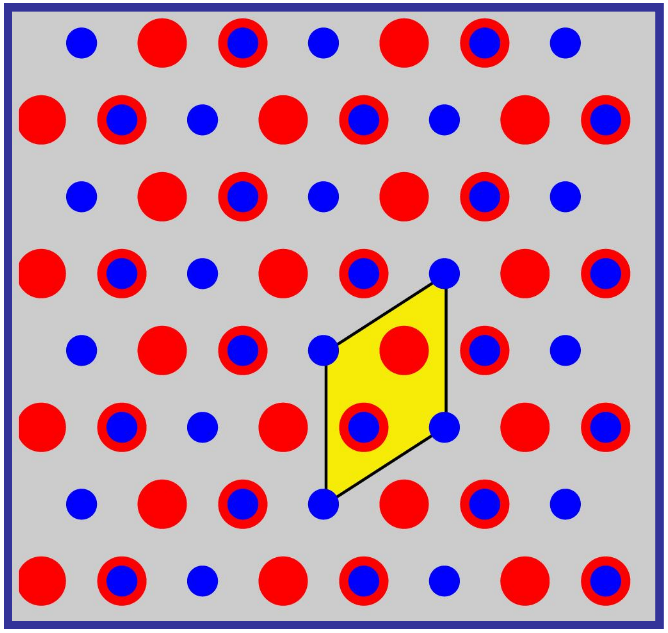
pseudo-spinor wf



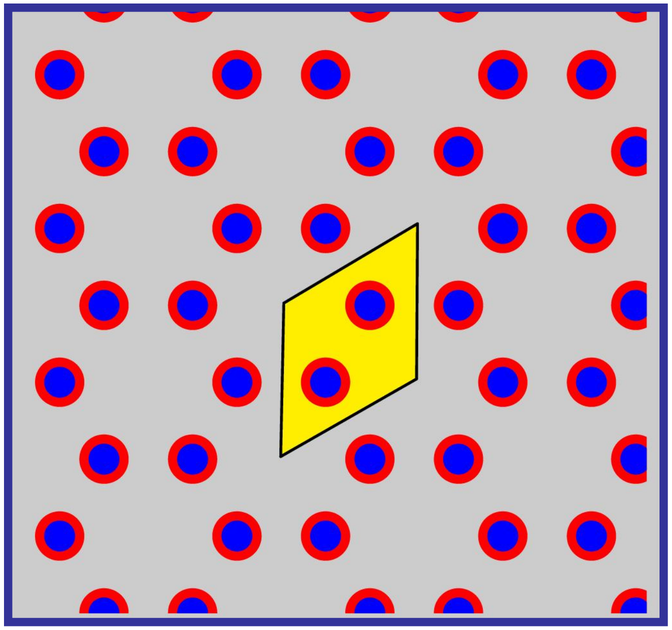
J.M.B. Lopes dos Santos, N.M.R. Peres and A.H. Castro Neto *Physical Review Letters* 99, 256802 (2007))

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

Highest Symmetry Bilayers

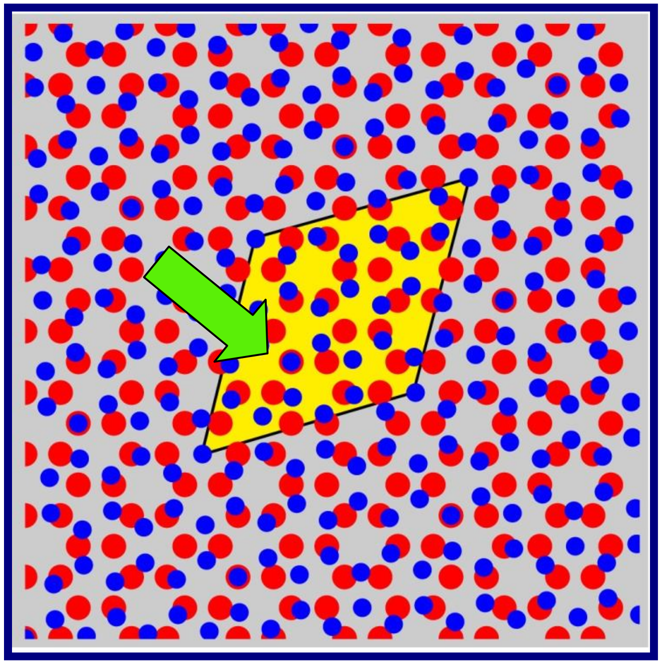


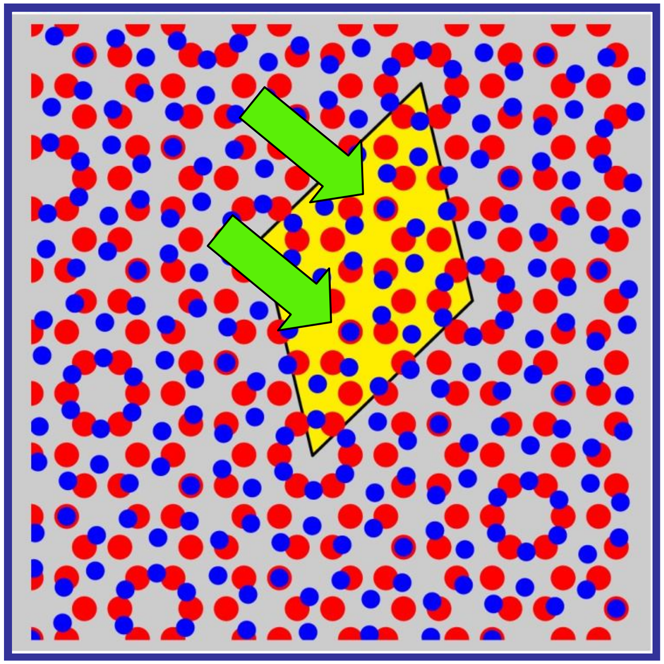
AB (Bernal) Stacking



AA Stacking

Rotationally Faulted Bilayers





32.204º **27.796º**

*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*

What is the smoothest density wave that matches the commensuration cell ?

Periodic on commensuration supercell
Maxima for "overlapping" sites
Minima for "misregistered" zones

$$n_\mu(\vec{r}) = \sum_{|\vec{G}_m|=G_1} \sum_\alpha e^{i\vec{G}_{\mu,m}\bullet(\vec{r}-\vec{\tau}_{\mu,\alpha})}$$ (real, lattice-symmetric)

$$n_{sc}(\vec{r}) = n_1(\vec{r}) + n_2(\vec{r})$$

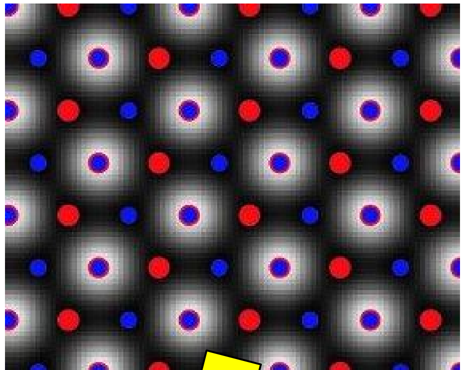
$$T_\ell(\vec{r}) = C_0 \exp\left[C_1 \left(n_1(\vec{r}) + n_2(\vec{r}) \right) \right]$$

Exponential suppression is misregistered regions.

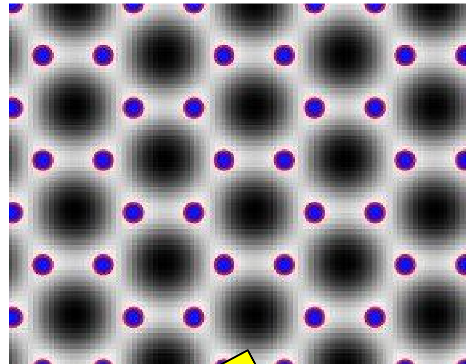
Nonlinear mixing of overlapping lattices: all G_s present.

Interlayer Potentials

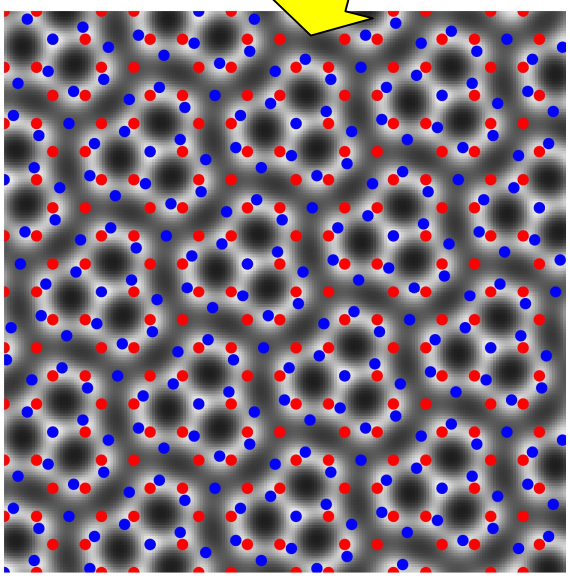
Bernal



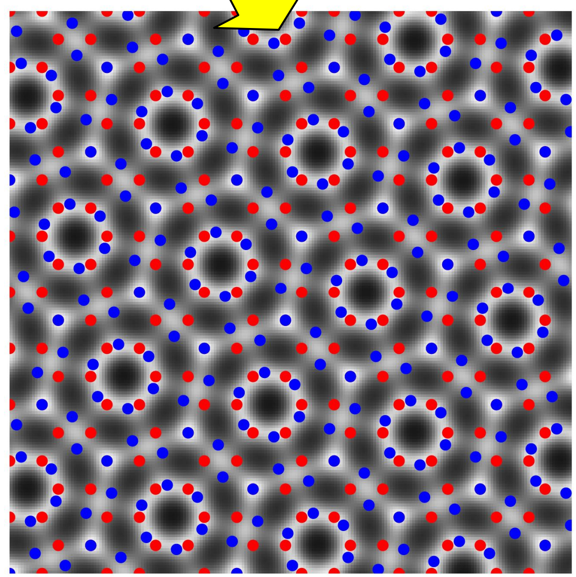
AA stacking



SE odd

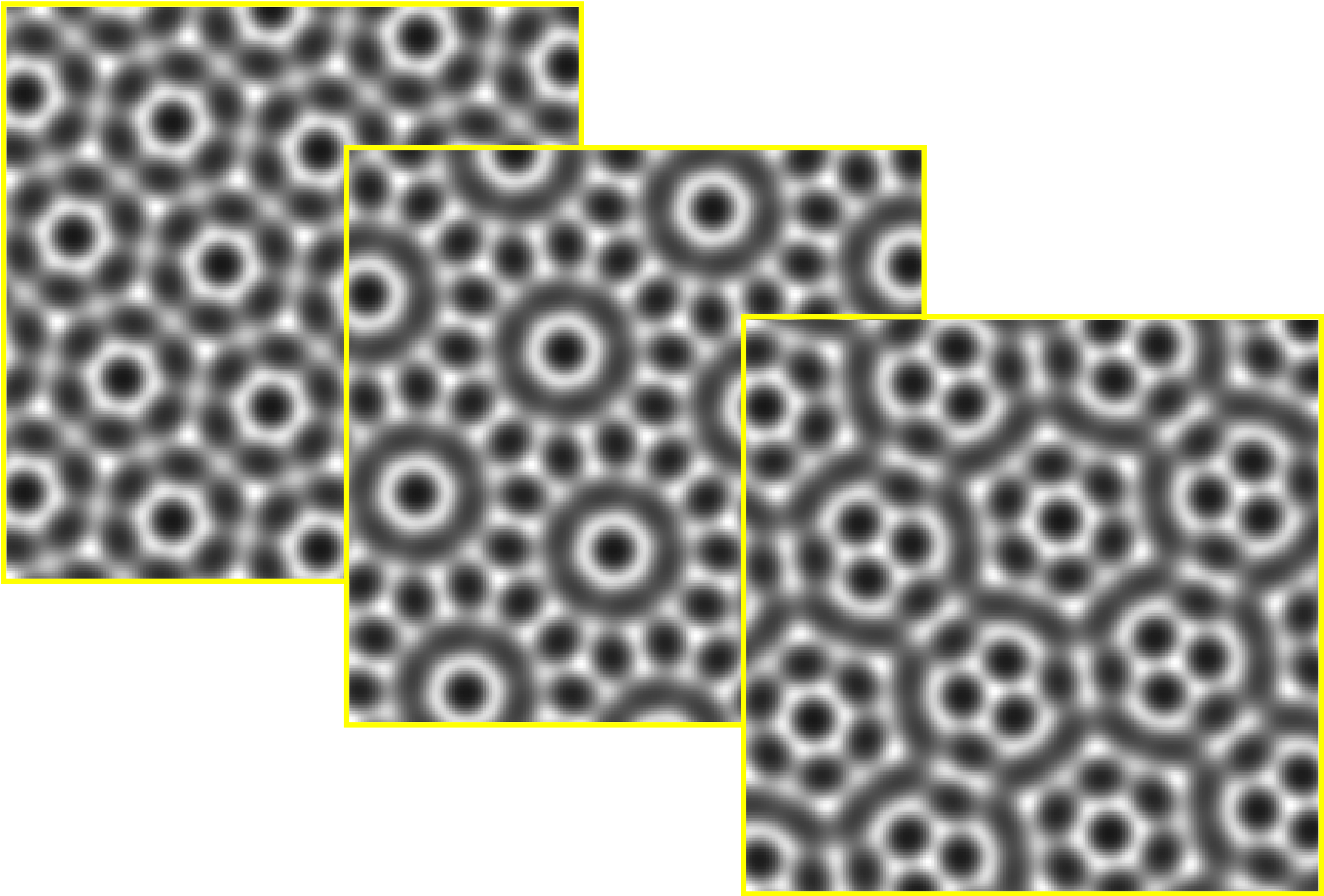


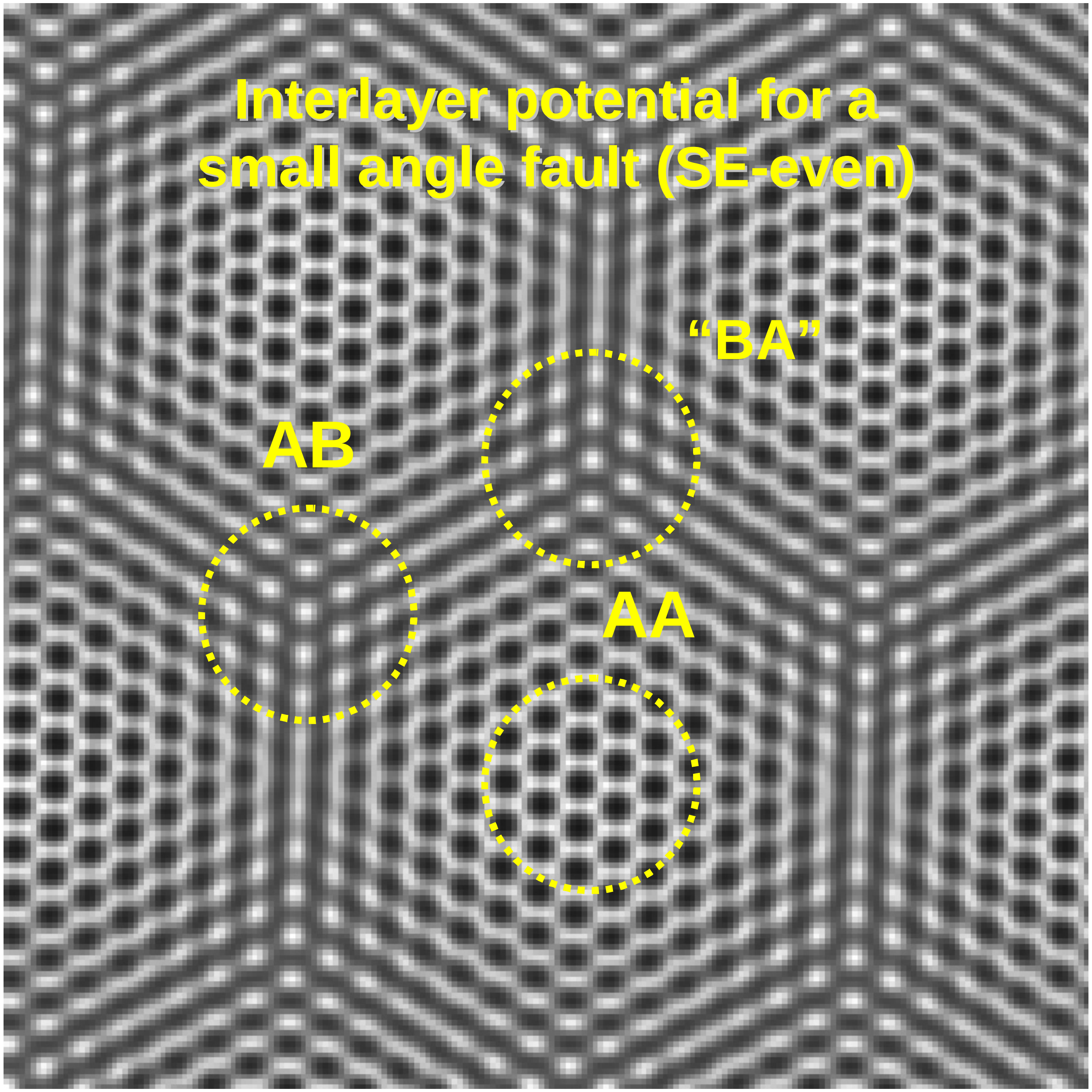
SE even

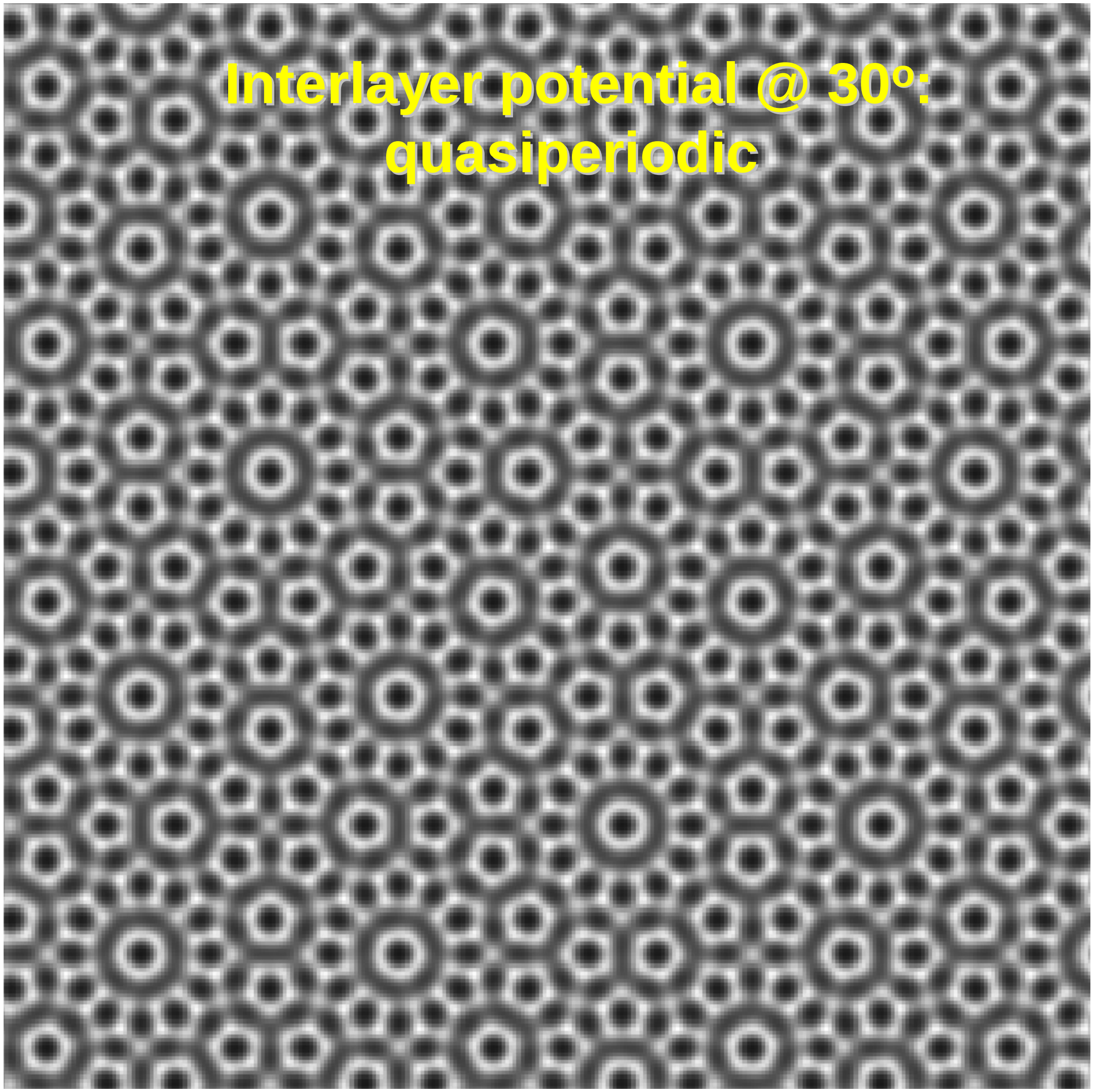


$30^{o} \pm 8.213^{o}$

More Interlayer Potentials
SE-even near 30°




Interlayer potential for a small angle fault (SE-even)
"BA"
AB
AA


Interlayer potential @ 30o:
quasiperiodic

Bilayer Hamiltonian in the pseudospin basis

SE even

$$\hat{H}_{even} = \begin{pmatrix} -i\hbar\tilde{v}_F\sigma_1 \bullet \nabla & \boxed{\hat{H}^{+}_{\text{int}}} \\ \left(\hat{H}^{+}_{\text{int}}\right)^{\dagger} & -i\hbar\tilde{v}_F\sigma_2 \bullet \nabla \end{pmatrix}$$

Interlayer &
<u>Intra</u>-valley
(two copies)

SE odd

$$\hat{H}_{odd} = \begin{pmatrix} -i\hbar\tilde{v}_F\sigma_1 \bullet \nabla & \boxed{\hat{H}^{-}_{\text{int}}} \\ \left(\hat{H}^{-}_{\text{int}}\right)^{\dagger} & i\hbar\tilde{v}_F\sigma_2^{*} \bullet \nabla \end{pmatrix}$$

Interlayer &
<u>Inter</u>-valley
(two copies)

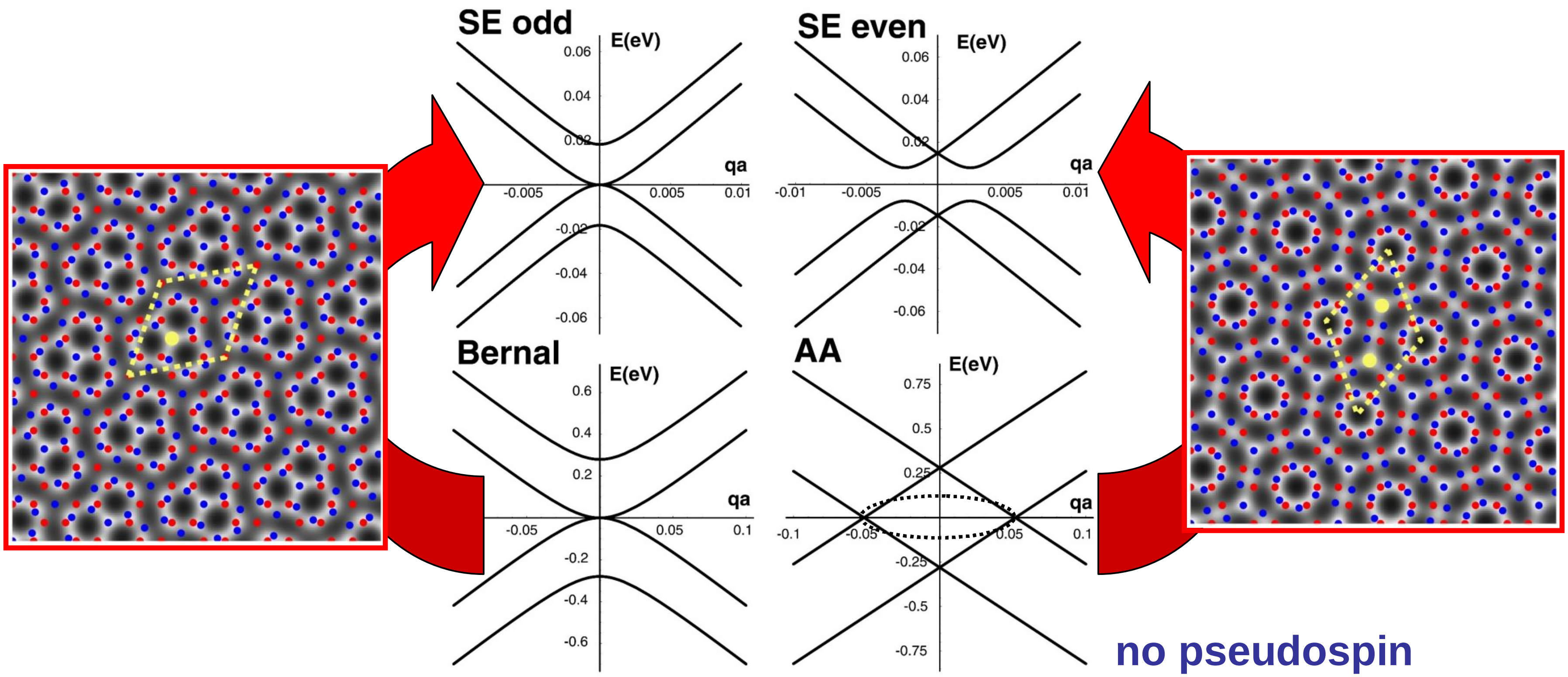
$$\hat{H}^{+}_{\text{int}} = V_{\ell} e^{i\vartheta} \begin{pmatrix} e^{i\varphi/2} & 0 \\ 0 & e^{-i\varphi/2} \end{pmatrix}$$

Transport on two sublattices via x-y pseudospin rotation

$$\hat{H}^{-}_{\text{int}} = V_{\ell} e^{i\vartheta} \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}$$

Transport on the dominant (eclipsed) sublattice

Two types of low energy physics



no pseudospin rotation in AA stacking

Topics for today:

I. Introduction: what, where, why

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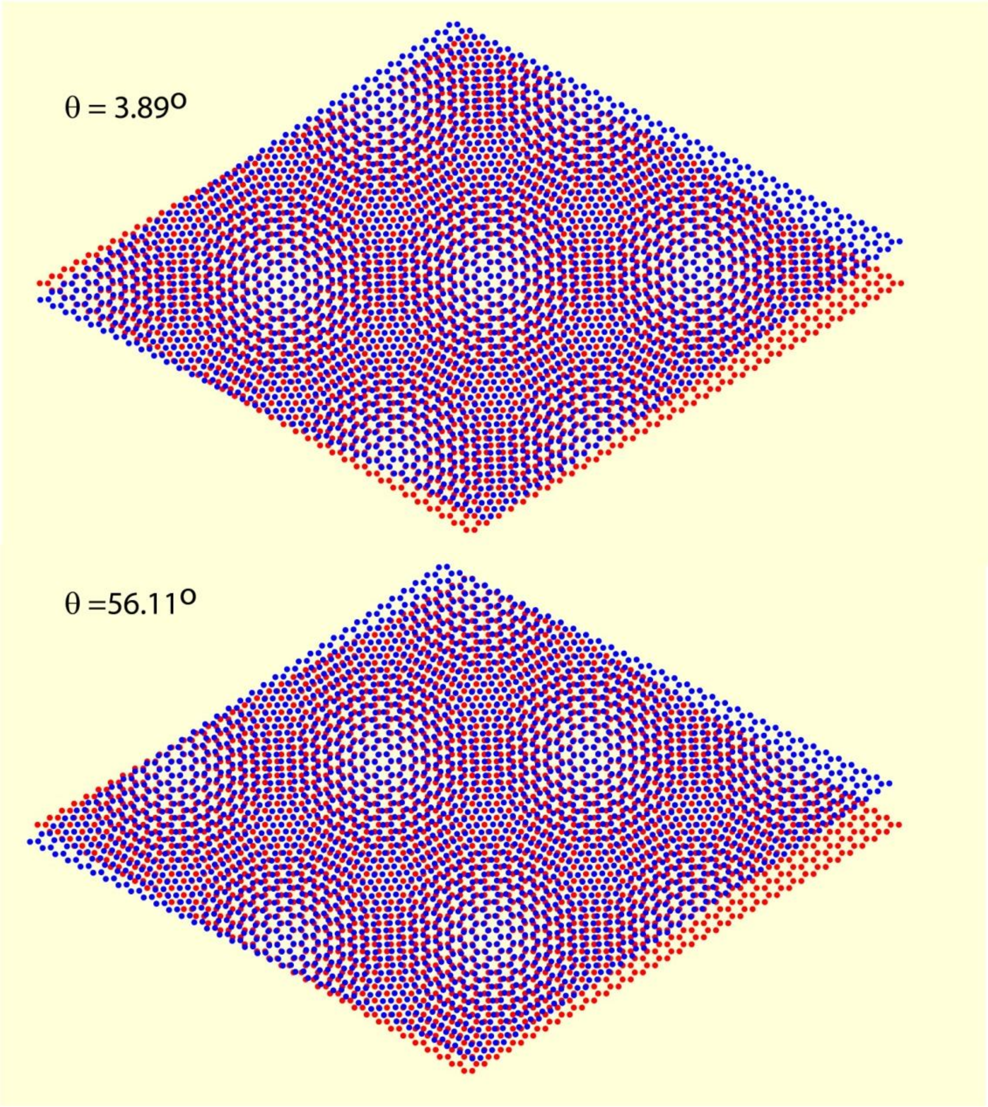
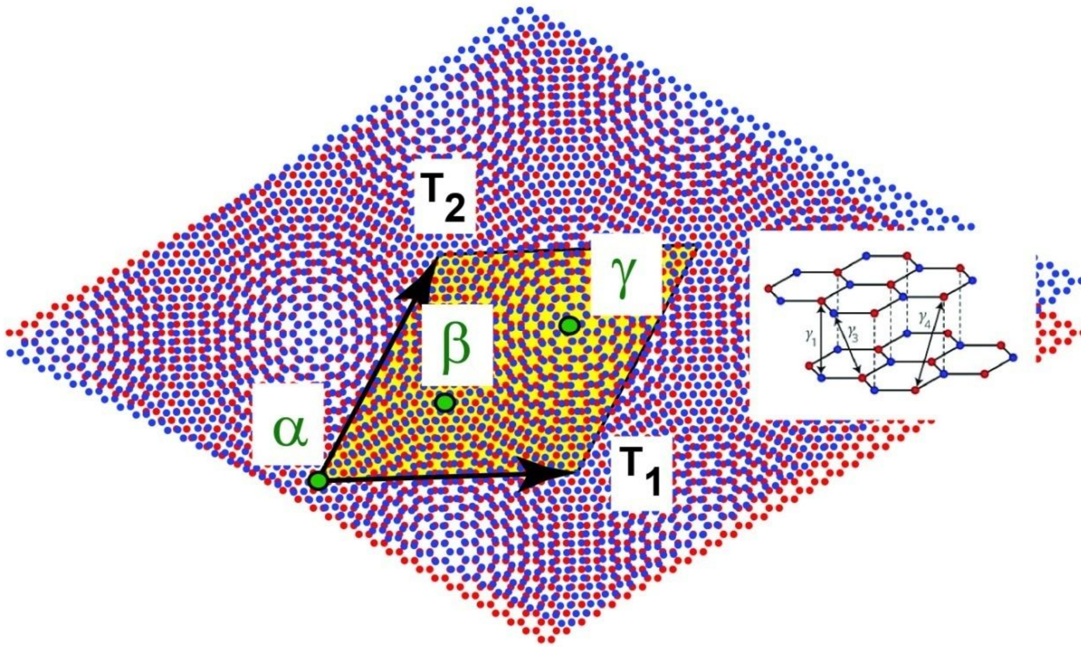
IV. "Compensated" class near a topological transition

V. "Uncompensated" new topological state in twisted FLG's

Small angle partners



Spatially modulated coupling



$$2\times 2 \text{ Matrix Coupling: } \hat{T}(\vec{r}) = \hat{t}_0 + \sum_{n=1}^{6} \hat{t}_n \, e^{i\vec{G}_n \bullet \vec{r}}$$

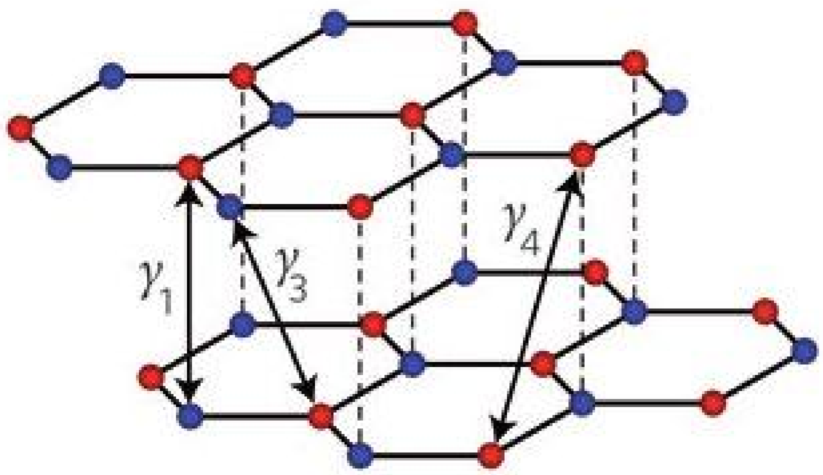
with expansion coefficients

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

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

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

Slonczewski-Weiss-McClure model

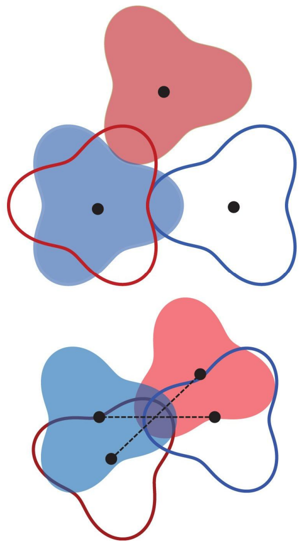


SWMcC model contains a (strong) threefold lattice anisotropy

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: γ_1 = 390 meV, $\gamma_3 = \gamma_4 = 0$. Model II: γ_1 = 390 meV, γ_3 = 315 meV and γ_4 = 44 meV.

Slonczewski-Weiss-McClure model



reflects a threefold anisotropy of its lattice Wannier states

Coefficient	Parameterization	I	II
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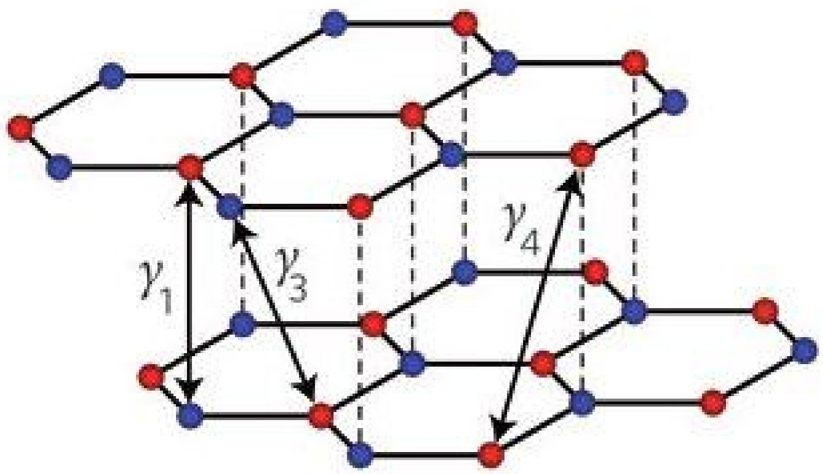

isotropic two center tight binding model

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c_{aa}	$\gamma_4 + (\gamma_1 - \gamma_3)/3$	130.0	69.0
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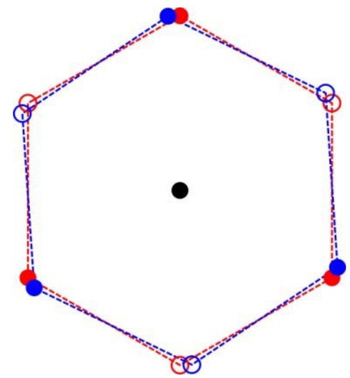
Model I: q=0 term in K-point basis

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

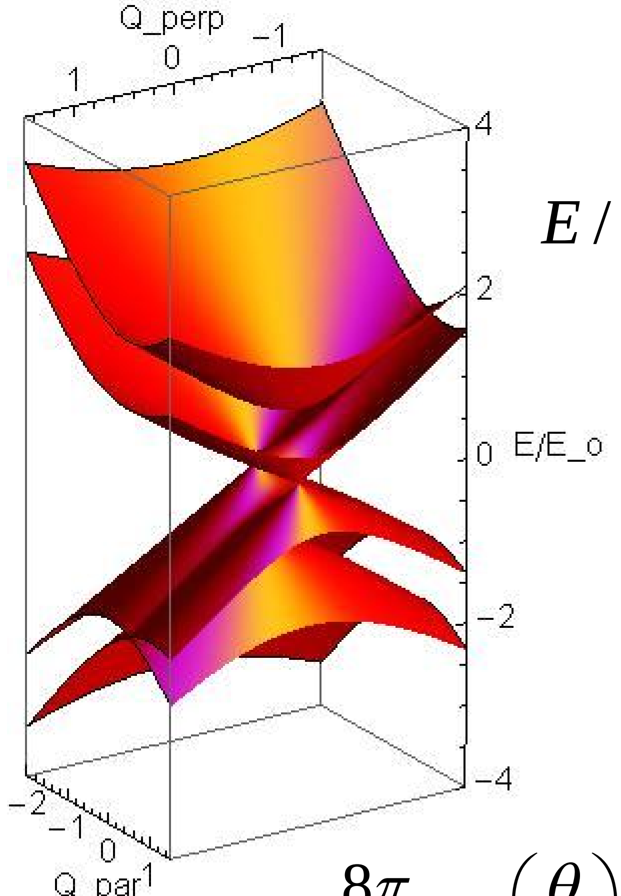
$$T_1 = w\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$



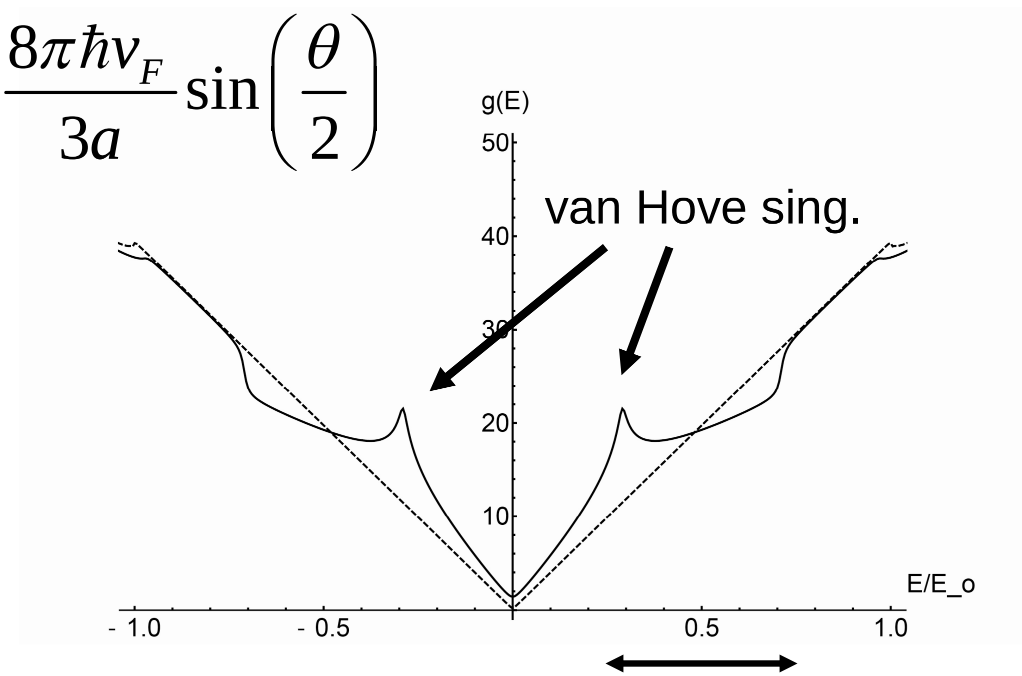
$$T_2 = w\begin{pmatrix} z & 1 \\ \bar{z} & z \end{pmatrix} \qquad T_3 = w\begin{pmatrix} \bar{z} & 1 \\ z & \bar{z} \end{pmatrix}$$

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

Canonical (isotropic) picture



$$E \Big/ \frac{8\pi\hbar v_F}{3a}\sin\left(\frac{\theta}{2}\right)$$



$$q \Big/ \frac{8\pi}{3a}\sin\left(\frac{\theta}{2}\right)$$

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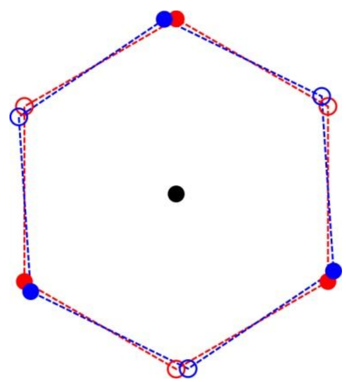
Model II q=0 term in K-point basis

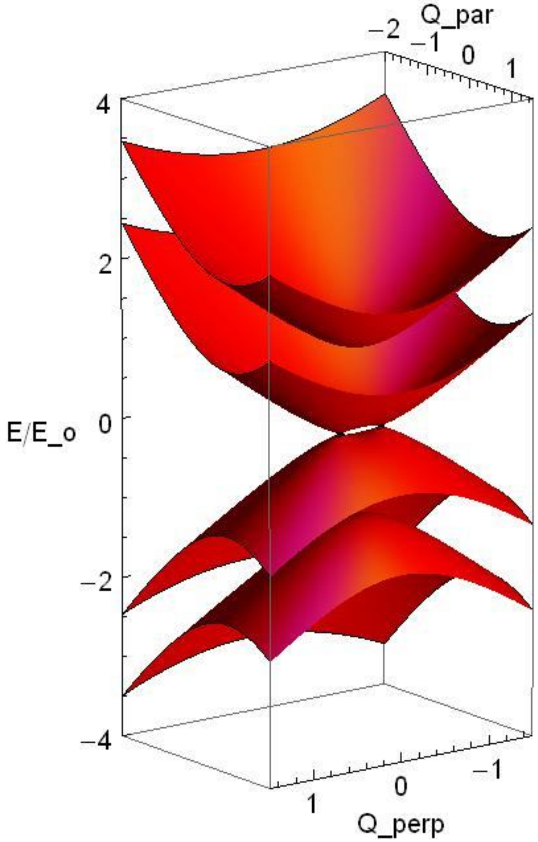
$$T_1 = w\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \rightarrow c_{ab}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} = c_{ab}\sigma_x\tau_x$$

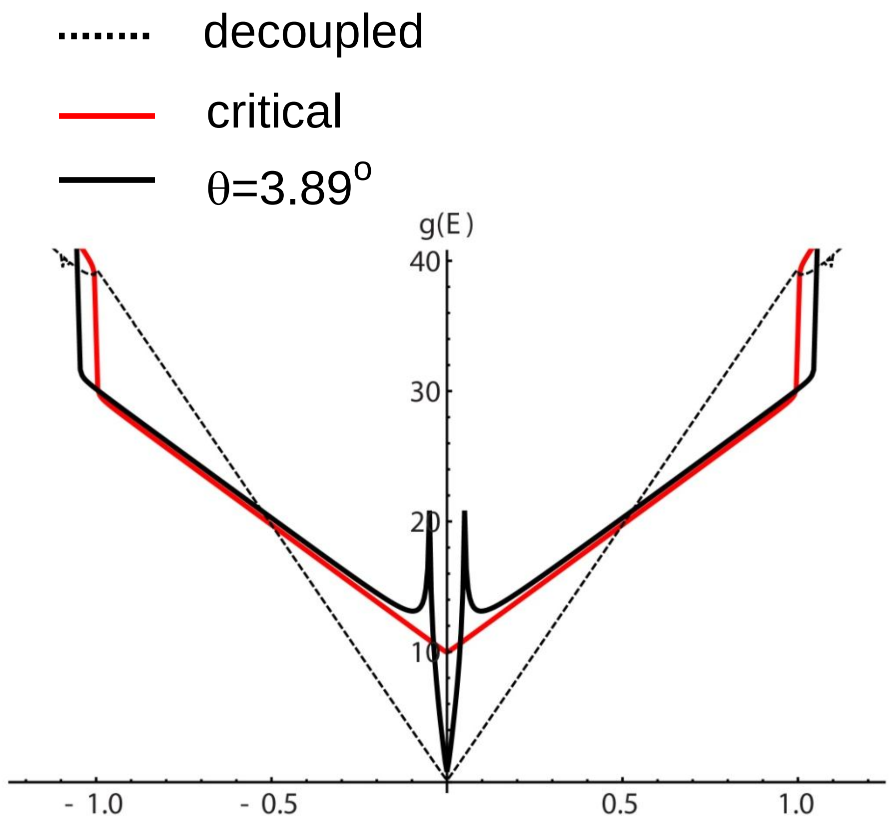


$$T_2 = c_{ab}\begin{pmatrix} 0 & 1 \\ \bar{z} & 0 \end{pmatrix}$$

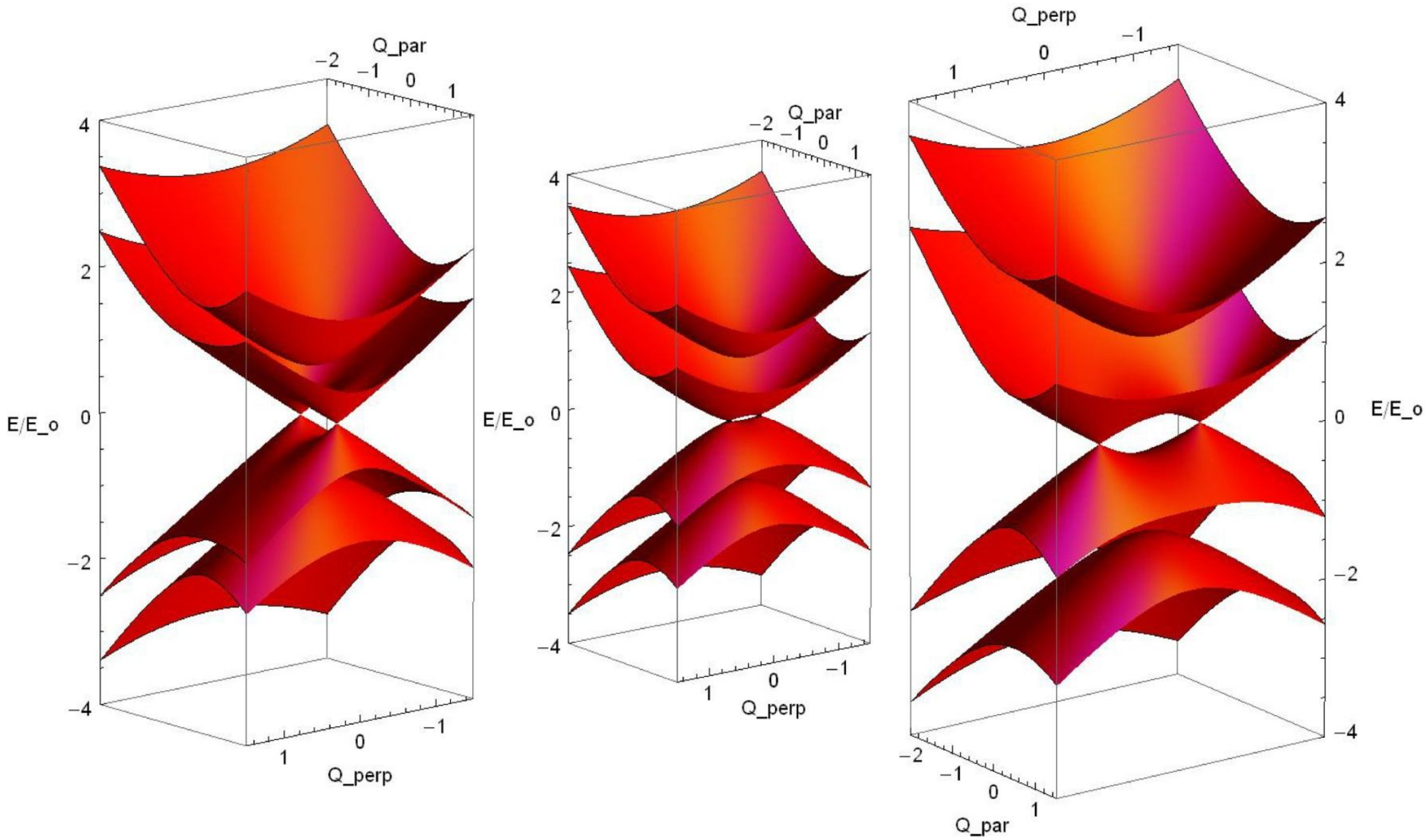
$$T_3 = c_{ab}\begin{pmatrix} 0 & 1 \\ z & 0 \end{pmatrix}$$

Model I: coupled layer spectra





Decrease rotation angle



increasing c

Topological Transition

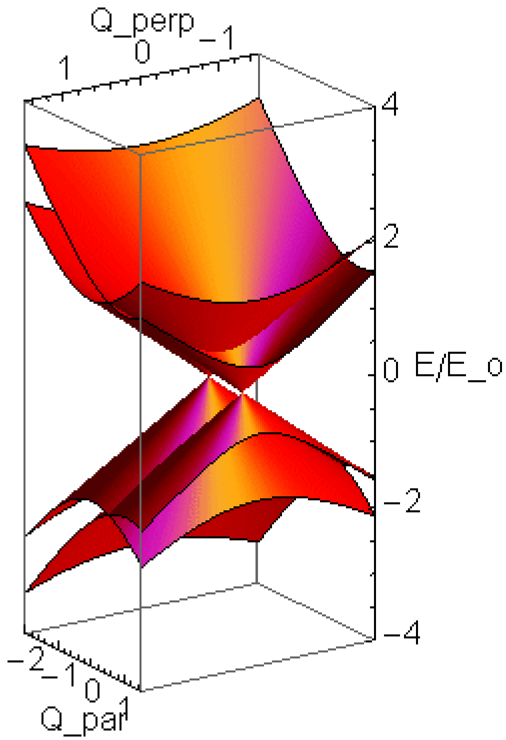
$$H = \begin{pmatrix} \sigma \bullet (-i\nabla) & \tilde{c}\sigma_x \\ \tilde{c}\sigma_x & \sigma \bullet (-i\nabla - (1)\,\hat{e}_{\Delta K}) \end{pmatrix}$$

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

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

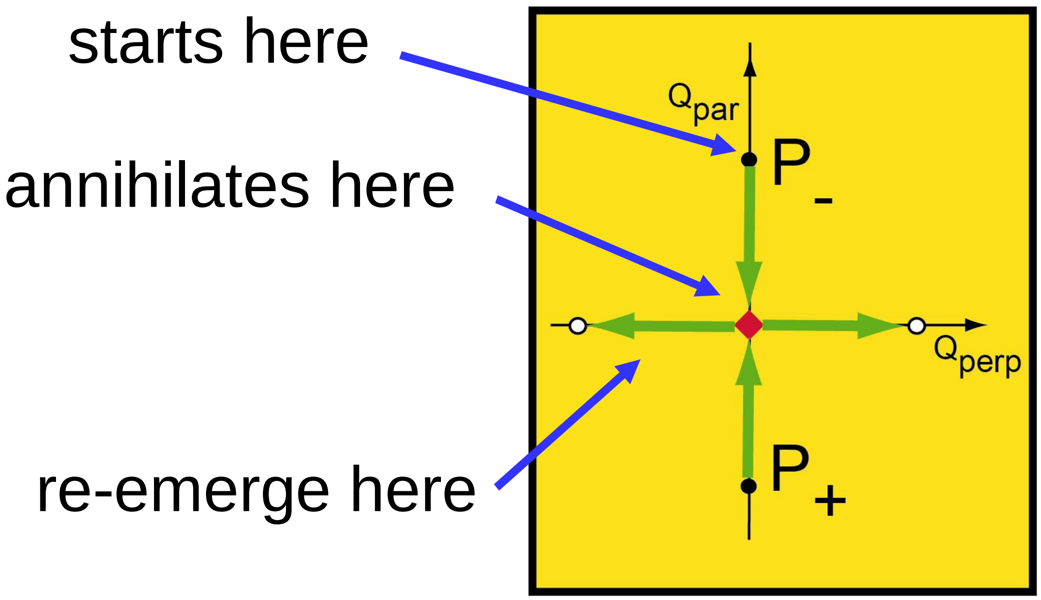
"Compensated" (opposite helicities)

Evolution of Dirac points

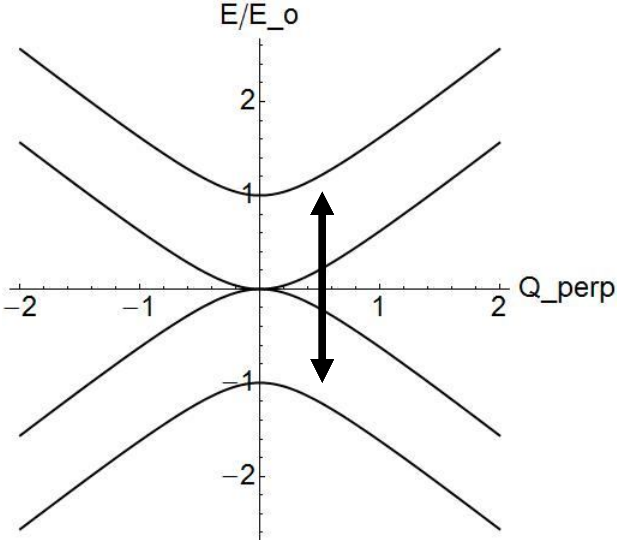


Decrease angle: increase coupling strength

Spectral reconstruction



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



Pair annihilation for compensated DP’s

Converge/collapse/diverge with increasing c

Comments:

The SWMcC model contains a (large) threefold lattice anisotropy

Breakdown of first generation models :

Relativistic (linear) bands → Massive (curved) bands

Dirac point annihilation and regeneration.

Gauge potential from twisted neighbor

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➡ V. "Uncompensated" new topological state in twisted FLG's

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 (+)

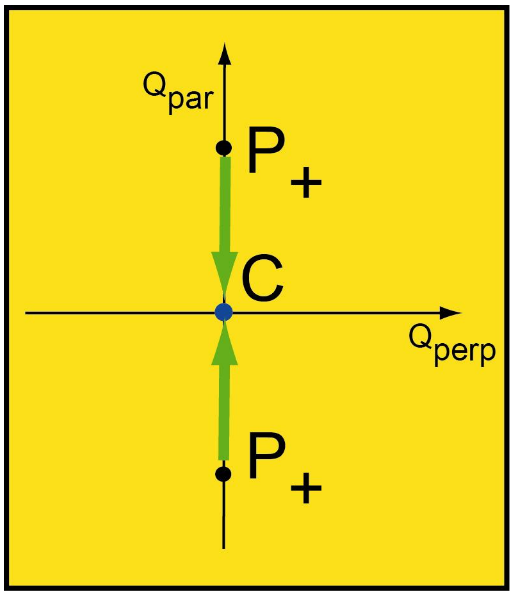
Topological Transition

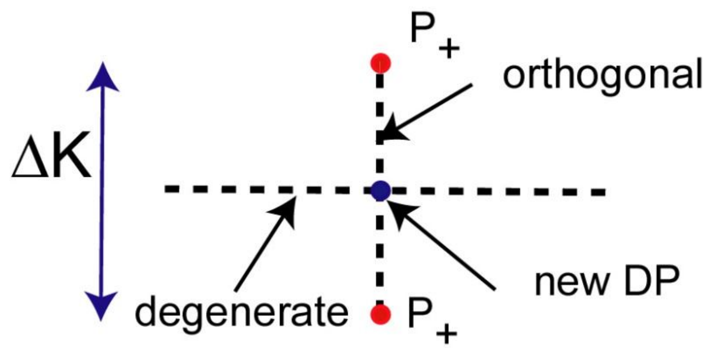
$$H = \begin{pmatrix} \sigma \bullet (-i\nabla) & \tilde{c}\, I \\ \tilde{c}\, I & \sigma \bullet (-i\nabla + \hat{e}_{\Delta K}) \end{pmatrix}$$

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

"Uncompensated" (same helicity)

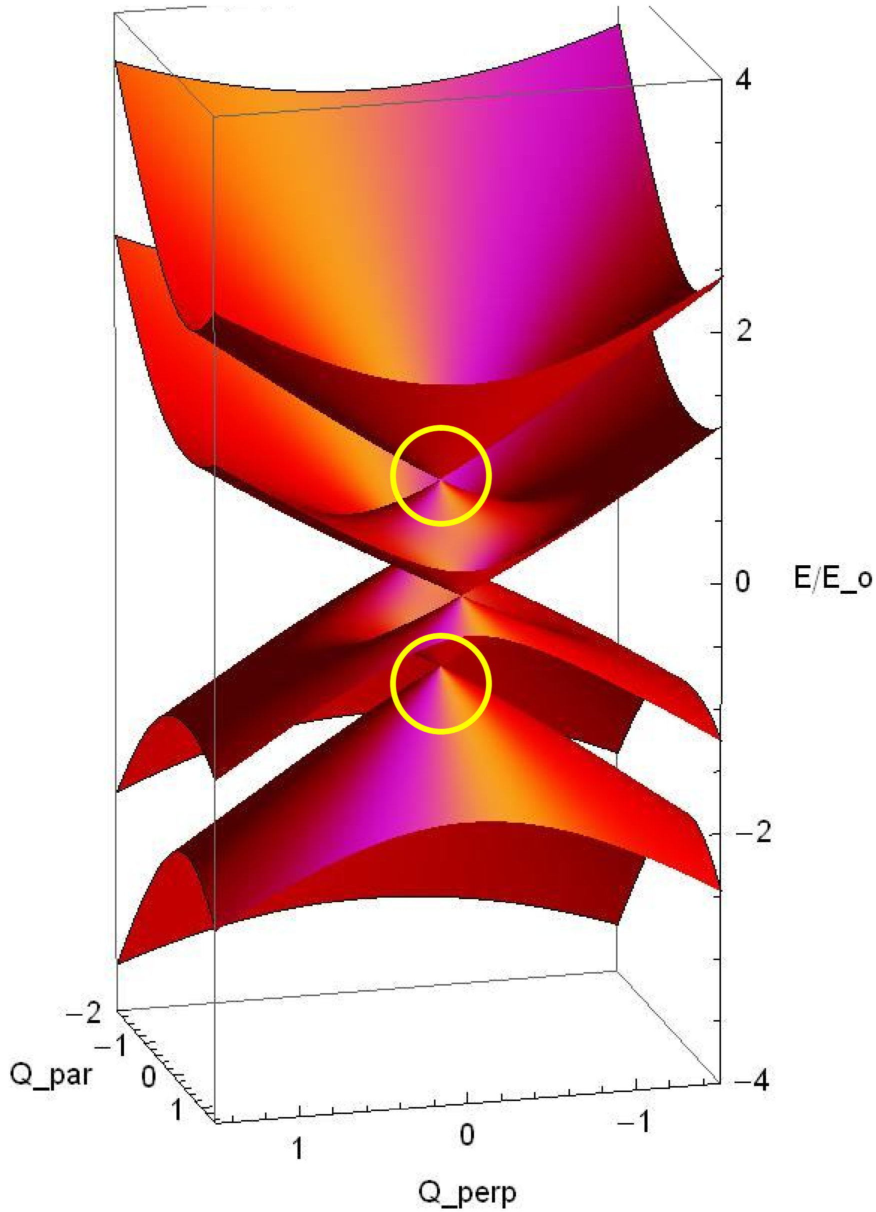
Symmetry-protected crossing



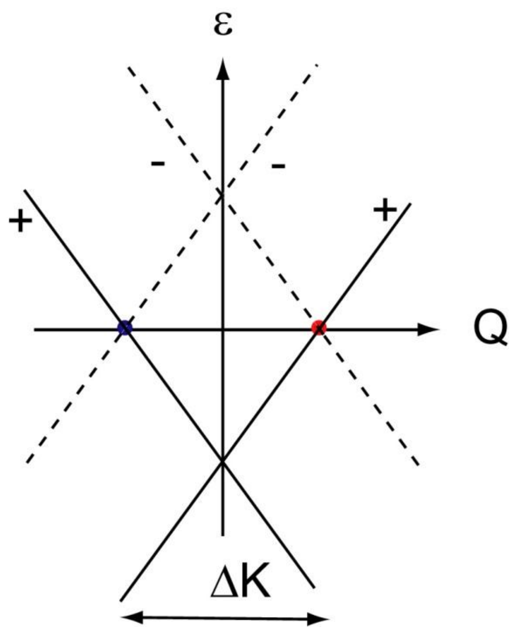


Bilayer version of absence of backscattering

Symmetry-protected intersection

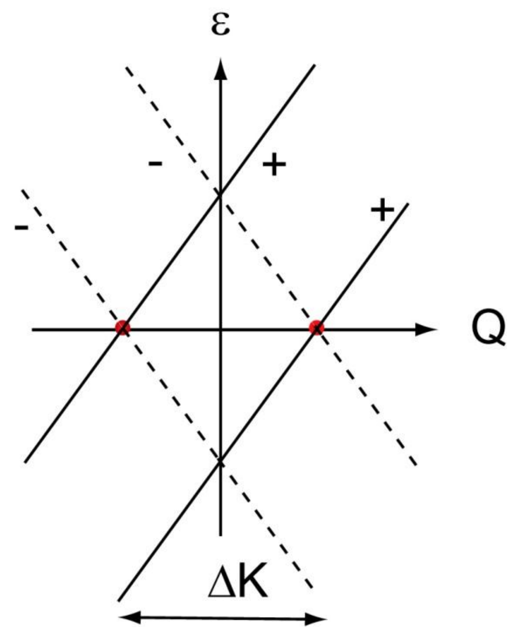


Helicity eigenstates



compensated

hybridized cones



uncompensated

symmetry-protected

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)

Signatures of the uncompensated state

SYMMETRY-PROTECTED BAND CROSSING

SECOND GENERATION DIRAC POINTS: DEGENERATE AT DISCRETE POINTS (NOT LINES)[1].

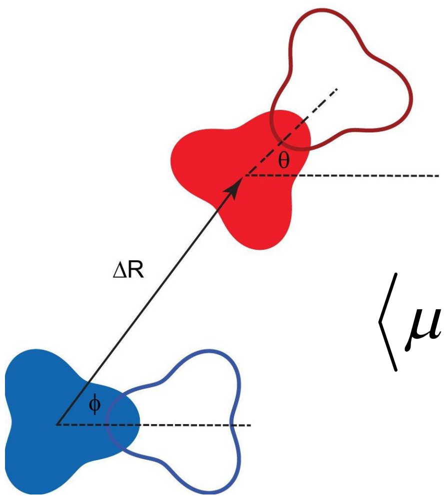
NO PERTURBATIVE VELOCITY RENORMALIZATION

EXTENDED (STRONGER) VAN HOVE SINGULARITY

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

[1] ARPES pending

Matrix elements with threefold anisotropy



$$A(B): \quad \mu = 0(1)$$

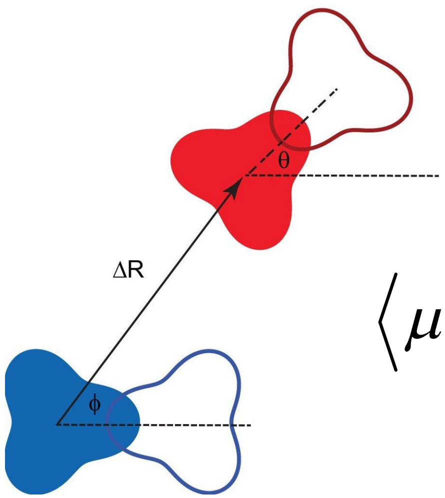
$$\left\langle \mu, 0, \vec{R} \left| h \right| \nu, \theta, \vec{R}' \right\rangle = h \int d^2 q \, e^{i\vec{q}\cdot(\vec{R}-\vec{R}')} \sum_{m=0,3,6} \Gamma_{m;\mu,\nu}(\vec{q})$$

$$\Gamma_{0;\mu,\nu} = f_0^2(q) + \frac{(-1)^{\mu+\nu} \lambda^2}{2} f_3^2(q) \cos(3\theta)$$

$$\Gamma_{3;\mu,\nu} = i\lambda \, f_0(q) \, f_3(q) \left[(-1)^{\mu} - (-1)^{\nu} \right] \cos\left(3(\phi_q - \alpha - \theta) \right)$$

$$\Gamma_{6;\mu,\nu} = \frac{(-1)^{\mu+\nu} \lambda^2}{2} f_3^2(q) \cos\left(6(\phi_q - \alpha - \theta/2) \right)$$

Matrix elements with threefold anisotropy



$$A(B): \quad \mu = 0(1)$$

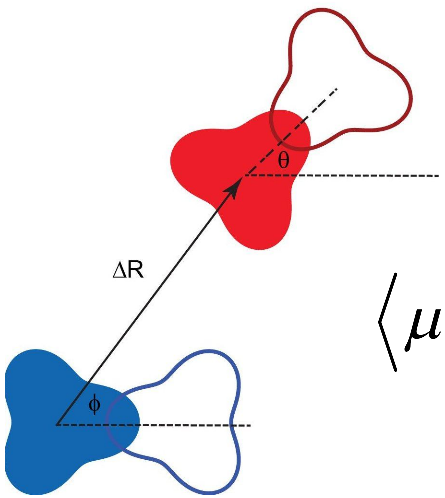
$$\left\langle \mu, 0, \vec{R} \left| h \right| \nu, \theta, \vec{R}' \right\rangle = h \int d^2 q \, e^{i\vec{q}\cdot(\vec{R}-\vec{R}')} \sum_{m=0,3,6} \Gamma_{m;\mu,\nu}(\vec{q})$$

Bernal anisotropy comes from $m = 3$

$$\Gamma_{3;\mu,\nu} = i\lambda \, f_0(q) \, f_3(q) \left[(-1)^{\mu} - (-1)^{\nu} \right] \cos\left(3(\phi_q - \alpha - \theta) \right)$$

Favors compensated class (SWMcC)

Matrix elements with threefold anisotropy



$$A(B): \quad \mu = 0(1)$$

$$\left\langle \mu, 0, \vec{R} \left| h \right| \nu, \theta, \vec{R}' \right\rangle = h \int d^2 q \, e^{i\vec{q}\cdot(\vec{R}-\vec{R}')} \sum_{m=0,3,6} \Gamma_{m;\mu,\nu}(\vec{q})$$

But an average over bond directions gives $m = 0$

$$\Gamma_{0;\mu,\nu} = f_0^2(q) + \frac{(-1)^{\mu+\nu} \lambda^2}{2} f_3^2(q) \cos(3\theta)$$

Relevant to **low angle twists** & favors uncompensated class

Comments:

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

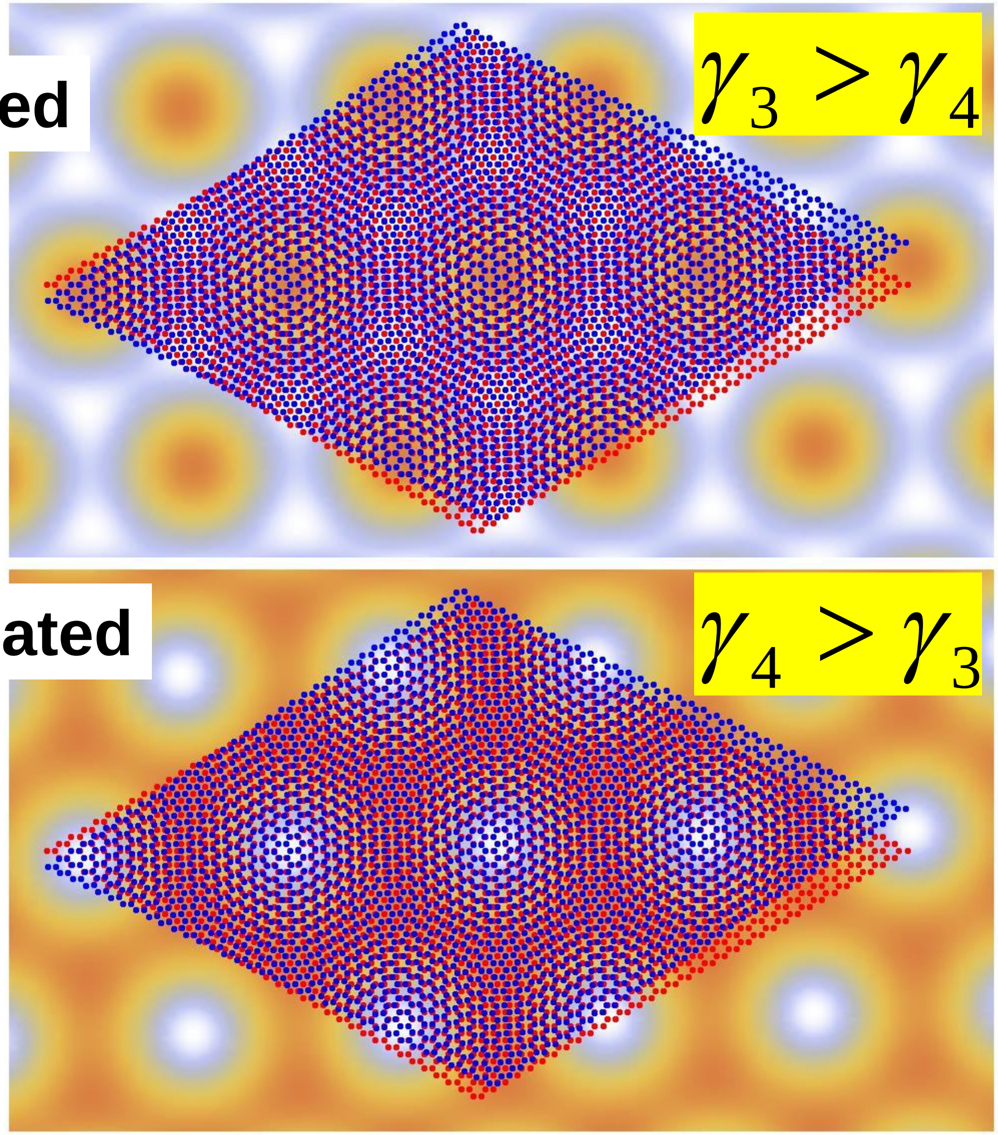
Interlayer hybridization prevented by pseudospin orthogonality at <u>discrete symmetry-protected second generation</u> Dirac singularities.

The Fermi velocity in U-class is unrenormalized (in weak coupling)

Geometrical class from anisotropy

compensated

uncompensated



Prospects:

- ***Topological analysis of (n>2) multilayers***
  (topological semimetals)
- ***Transport in vertically-integrated FLG's***
  (birefringence in ballistic transport ?)
- ***Narrow band physics at small angles***

Theory Collaborators:

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