Twist and Texture in Bilayer Graphene

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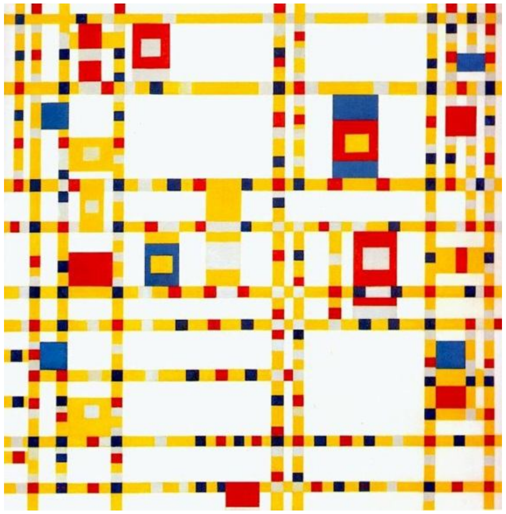
Topics for today

Some Background

<u>Part I</u>: Stacking <u>domains</u> and one-way boundary modes in BLG
Fan Zhang, Allan MacDonald, GM

<u>Part II</u>: Stacking <u>textures</u> in BLG
Xingting Gong, GM

<u>Part III</u>: Connect I & II
Zach Addison, Youngkuk Kim, GM



Broadway (Mondrian, 1943)

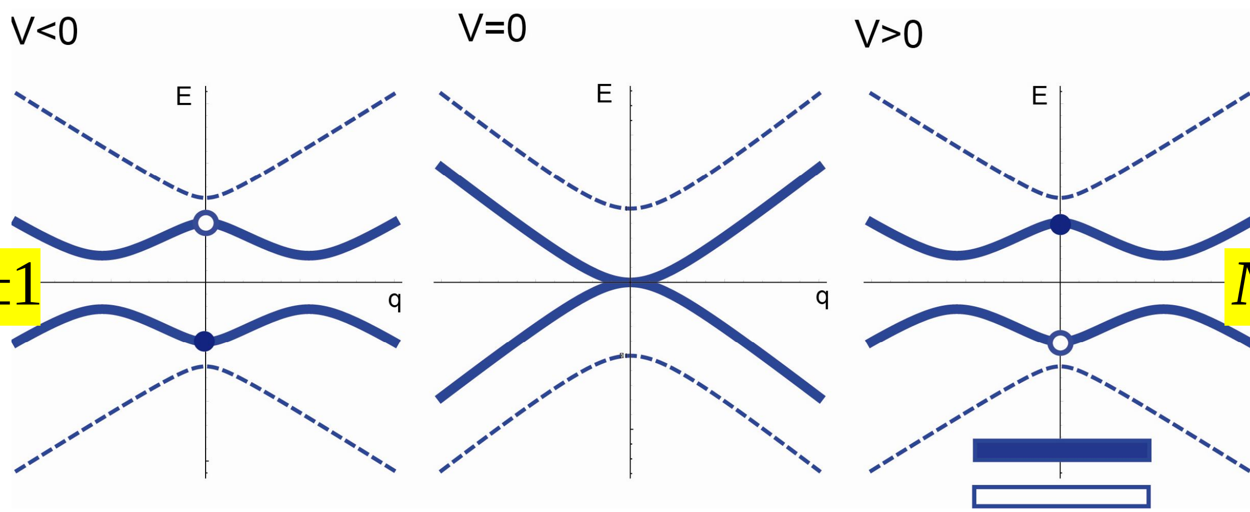
Starry Night (van Gogh, 1889)

Single-layer v. bilayer graphene

Single-layer graphene	Bilayer graphene
Massless Dirac Fermions	Touching massive (hyperbolic) bands
Un-gappable using smooth potentials (w/o spin orbit)	Gate tunable gap using interlayer bias
In-plane strain shifts Dirac point	Lifshitz transitions via trigonal warping/strain
(Weak) Interactions: qp velocity is weakly momentum-dependent	Interactions: competing insulating states from ordering spin, sublattice, valley and layer degrees of freedom
N/A	**All of the above depend on interlayer registry (shift, strain, twist)**

Gate-tunable gap in BLG

$N_{\pm} = \pm 1$



$N_{\pm} = \mp 1$

two band model: interlayer coupling gaps out one degree of freedom per layer

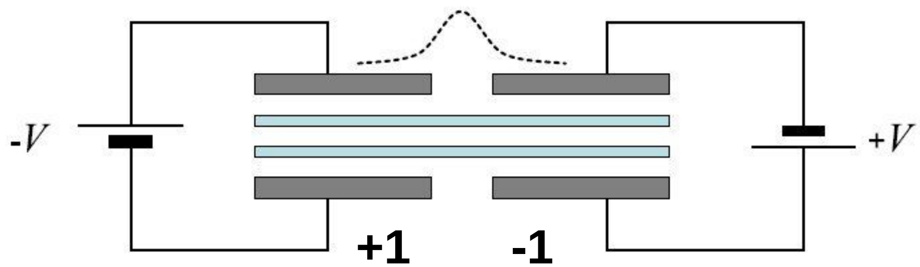
$$H_{\nu}(\mathbf{q}) = -\gamma\left(\left(q_x^2 - q_y^2\right)\sigma_x - \nu\left(2q_x q_y\right)\sigma_y\right) + \frac{V}{2}\sigma_z$$

producing a momentum space Berry curvature

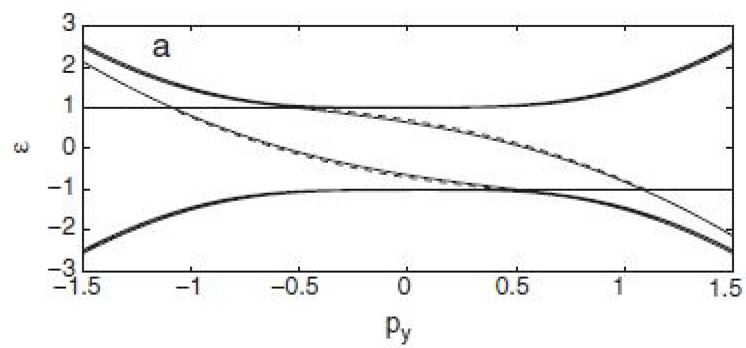
$$\Omega_{\nu}(\mathbf{q}) = -\nu\, V\, \gamma q^2 / \left(\gamma^2 q^4 + V^2/4\right)^{3/2}$$

$\Delta N=2$: <u>pairs</u> of valley-projected modes co-propagate along a bias switching edge

Bias reversal switches the sign of the "mass"



and gives a valley projected boundary spectrum

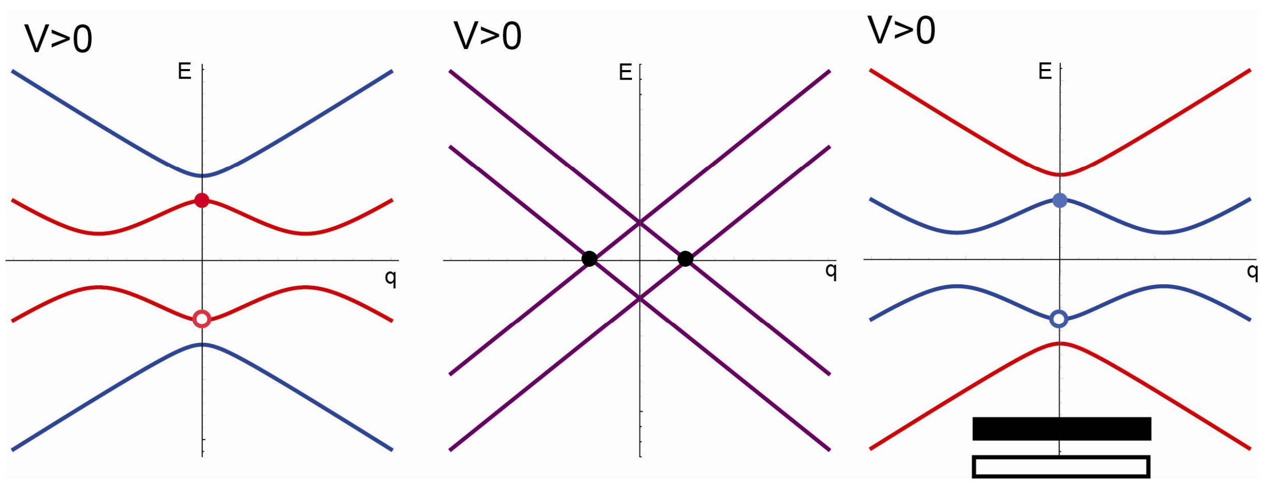


(Velocity-reversed partners are in the opposite valley)

Refs: I. Martin, Y.M. Blanter and A. Morpurgo, PRL **100**, 036804 (2008); G.E. Volovik *The Universe in a Helium Droplet* (Oxford, 2009)

Field-induced gap is also closed by interlayer slip

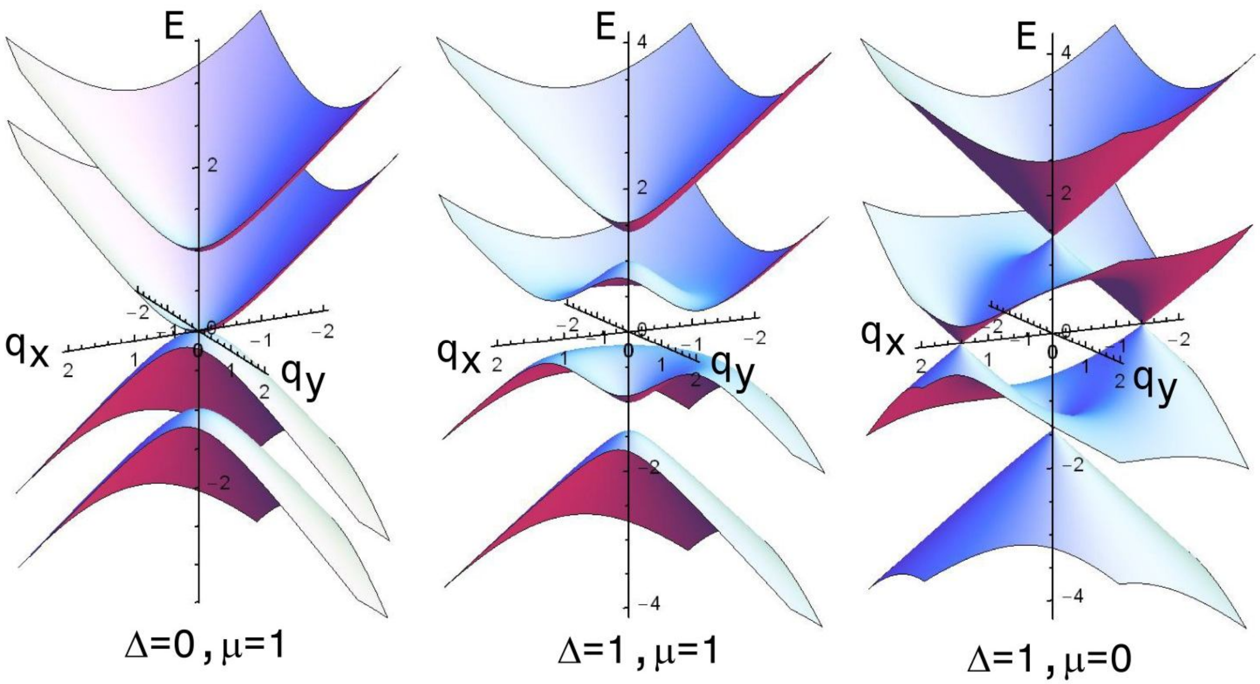
Keep V uniform but reverse the stacking order



four band model: valley-projected (ν): retains sublattice (σ) and layer (τ) degrees of freedom

$$H_{\nu}(\mathbf{q}) = \nu q_x \sigma_x + q_y \sigma_y + \frac{\gamma}{2}\left(\sigma_x \tau_x - \mu \sigma_y \tau_y\right) + \frac{V}{2}\tau_z$$

(Δ-μ)-induced gap closures

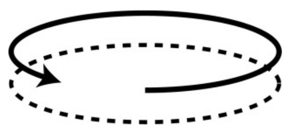


Unbiased ⟵ **Gapped BLG** ⟶ **Saddle point**

Slip-induced v. bias-induced walls

$$H_{\nu}[-\Delta,\mu]=\tau_x H_{\nu}[\Delta,-\mu]\tau_x$$

A loop integral of 2x2 matrix connection at large momentum gives the domain wall phase twist for occupied states:



$$\Psi_{\mu} \mapsto e^{i\mu\nu(1-\tau_z)\phi}\Psi_{\mu}$$

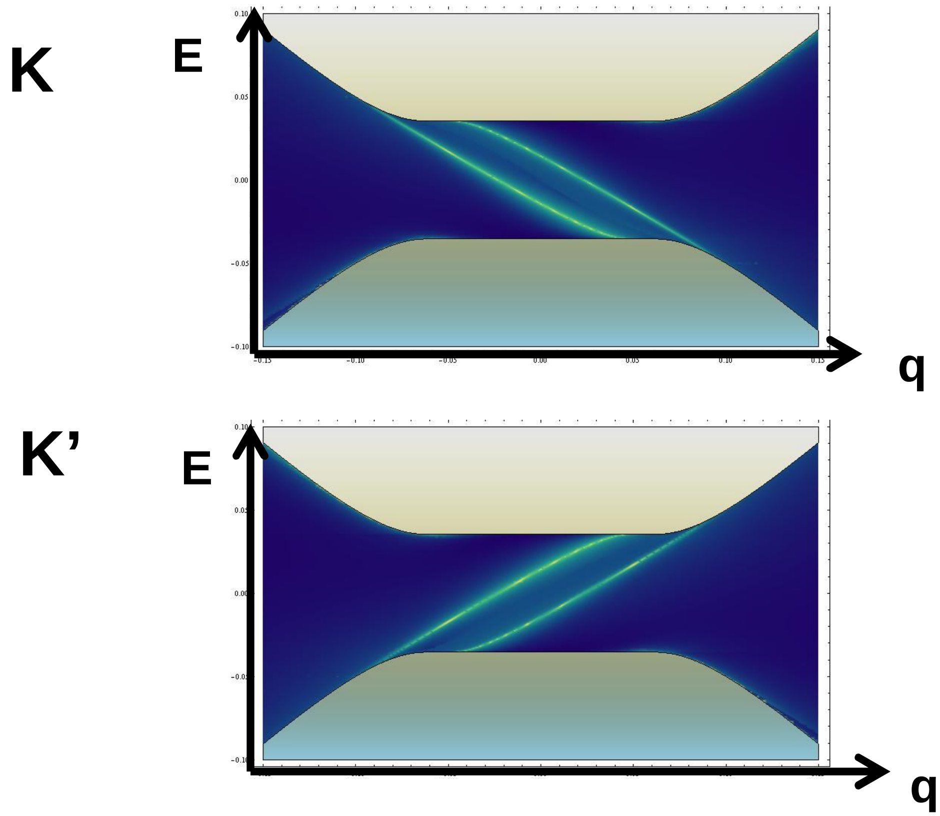
(registry switches: layer dependent twist)

$$\Psi_{\mu} \mapsto \mp\nu e^{i\mu\nu\phi}\Psi_{\mu}$$

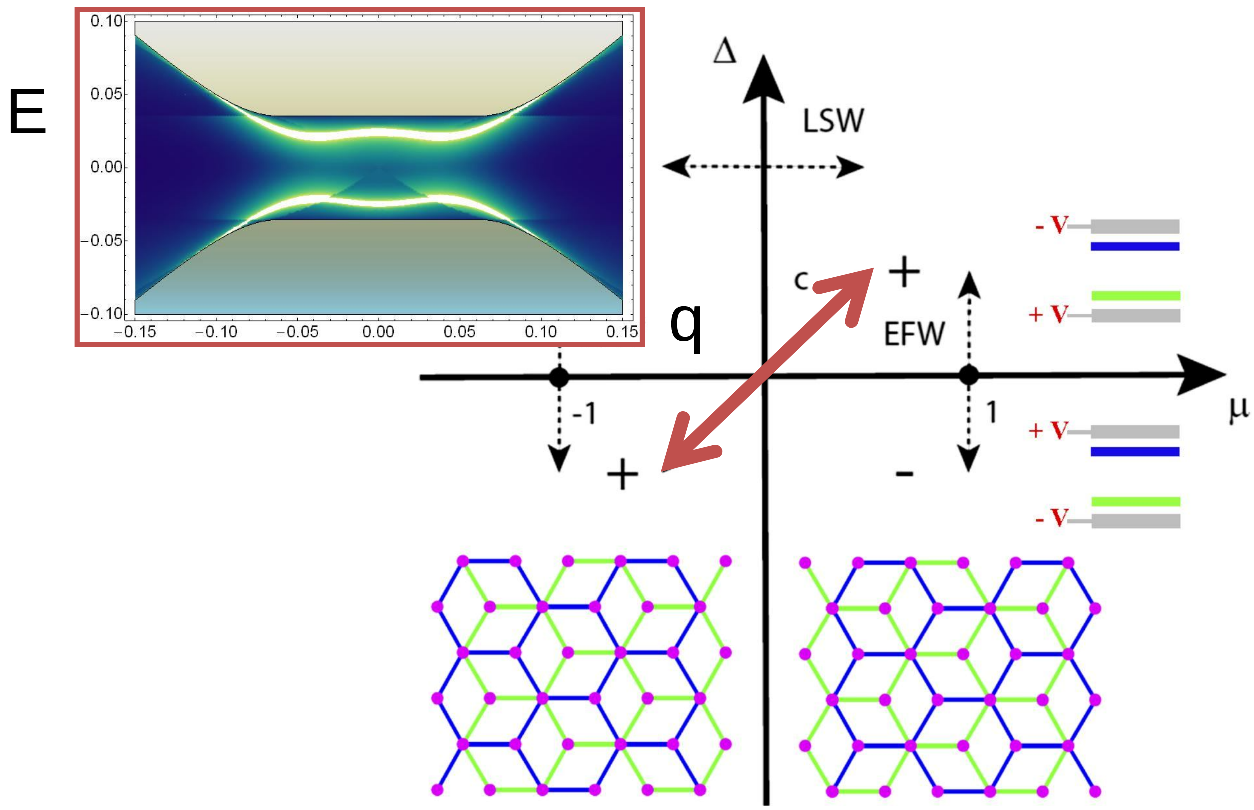
(bias switches: shared in both layers)

$$\boxed{N=\mu\nu}$$

Valley projected spectra for layer stacking walls



Fragile, fragiler, fragilest



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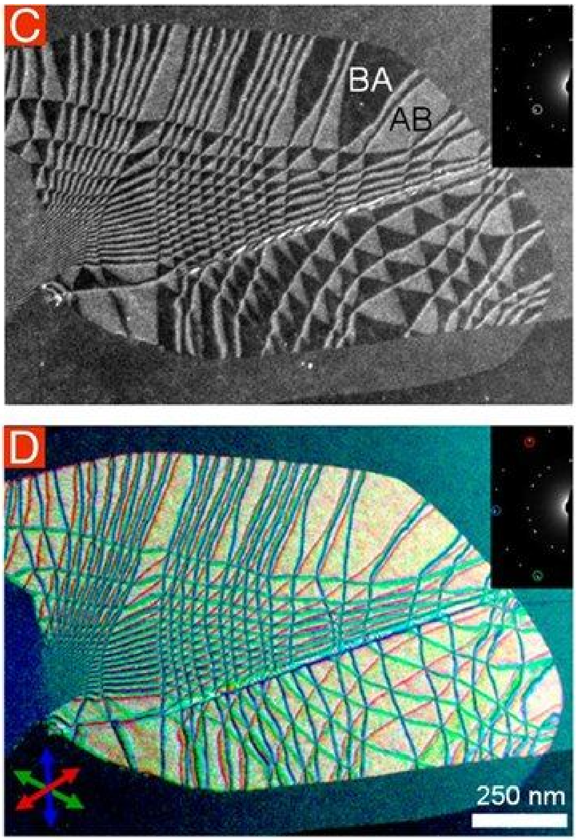
Dark field TEM on CVD-Bilayer graphene: stacking wall networks



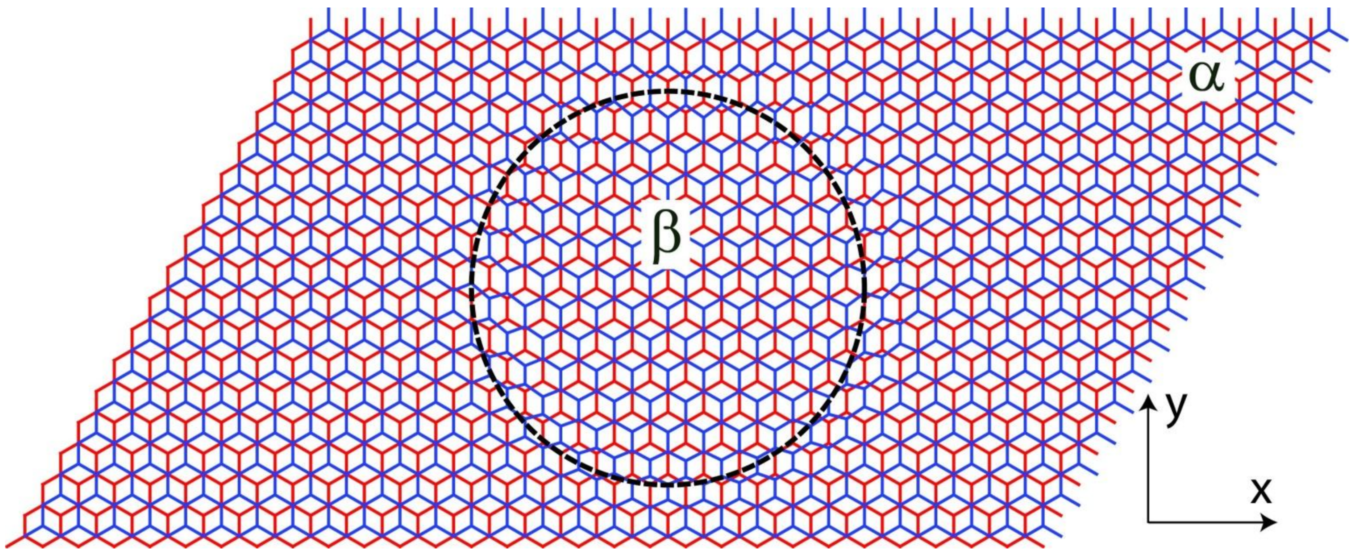
J.S. Alden et al (Cornell group) PNAS **110**, 1256 (2013)

Models for BLG discommensurations

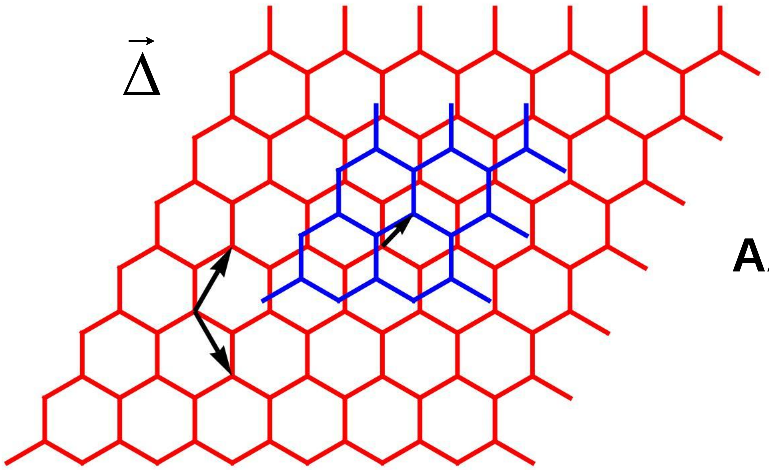
One dimension (simplest): Frenkel Kontorova model

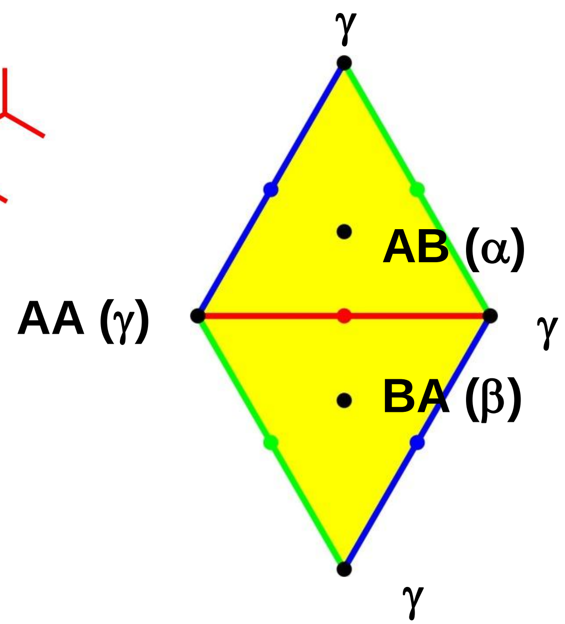
BLG version: A.M. Popov, I.V. Lebedeva, A.A. Knizhnik, Y.A. Lozovik, B.V. Potapkin
Phys. Rev. B 84, 045404 (2011)

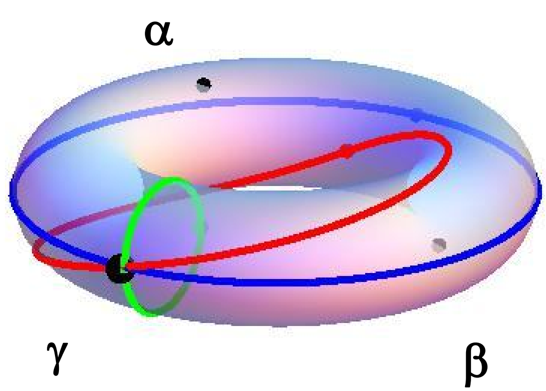
Two dimensions (simplest): Domain wall loop



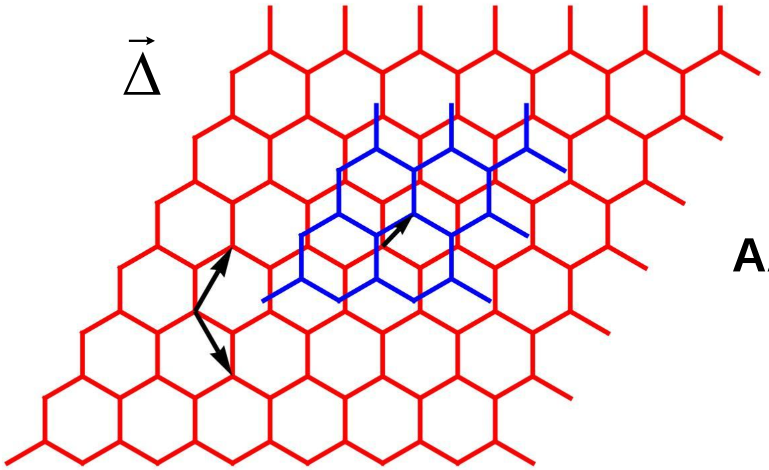
Interlayer registry = 2D Vector with PBC

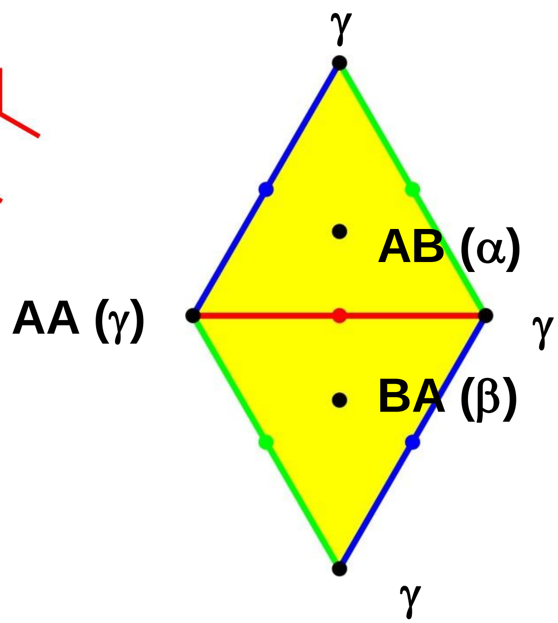


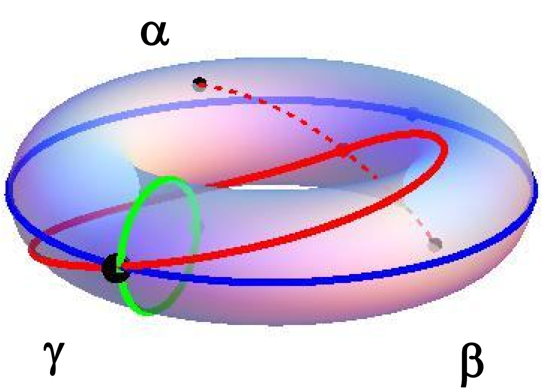




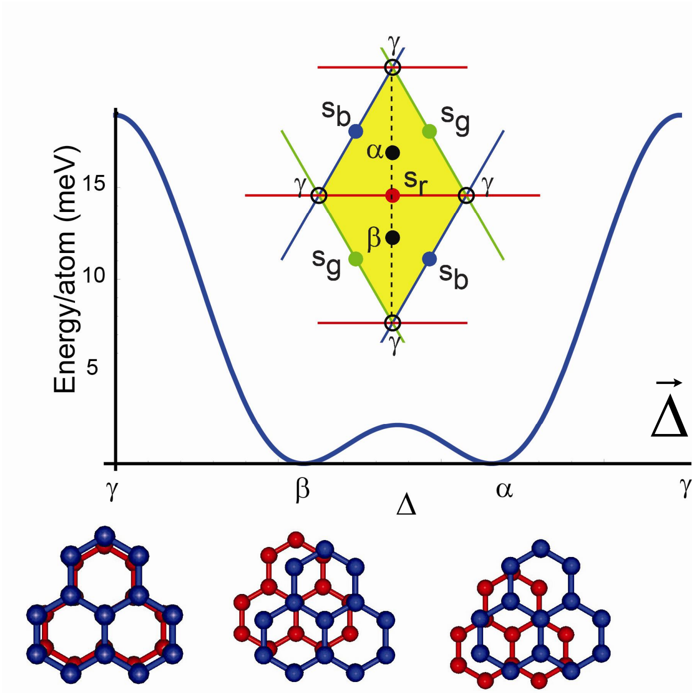
Interlayer registry = 2D Vector with PBC







Elastic and Commensuration Energies



$$U_c\left[\vec{\Delta}(\mathbf{r})\right] = \int d^2\mathbf{r}\, u_c\left(\vec{\Delta}(\mathbf{r})\right)$$

$$u_{el} = \frac{\lambda+\mu}{2}\left|\nabla \bullet \vec{\Delta}\right|^2 + \frac{\mu}{2}\frac{\partial \Delta_i}{\partial r_j}\frac{\partial \Delta_i}{\partial r_j}$$

(Energy/Area)

$$\frac{U_{el}}{U_c} \gg 10^2$$

i.e. elastic interactions dominate the weak commensuration potential

Minimal textures:
optimally smooth Δ fields satisfying the BC

$$\Delta(\infty) = \Delta_\alpha, \Delta(0) = \Delta_\beta$$

$$\Delta = \Delta_x + i\Delta_y$$
$$z = x + iy$$

$$\nabla \bullet \vec{\Delta} = 2\,\mathrm{Re}\left\{\frac{\partial \Delta}{\partial z}\right\} \qquad \frac{1}{2}\left(\frac{\partial \Delta_x}{\partial x} - \frac{\partial \Delta_y}{\partial y}\right) = \mathrm{Re}\left\{\frac{\partial \Delta}{\partial \bar{z}}\right\}$$

$$\nabla \times \vec{\Delta} = 2\,\mathrm{Im}\left\{\frac{\partial \Delta}{\partial z}\right\} \qquad \frac{1}{2}\left(\frac{\partial \Delta_y}{\partial x} + \frac{\partial \Delta_x}{\partial y}\right) = \mathrm{Im}\left\{\frac{\partial \Delta}{\partial \bar{z}}\right\}$$

$\partial \Delta / \partial z = 0$**:** **Anti-analytic functions**:
divergenceless and harmonic(minimally strained)

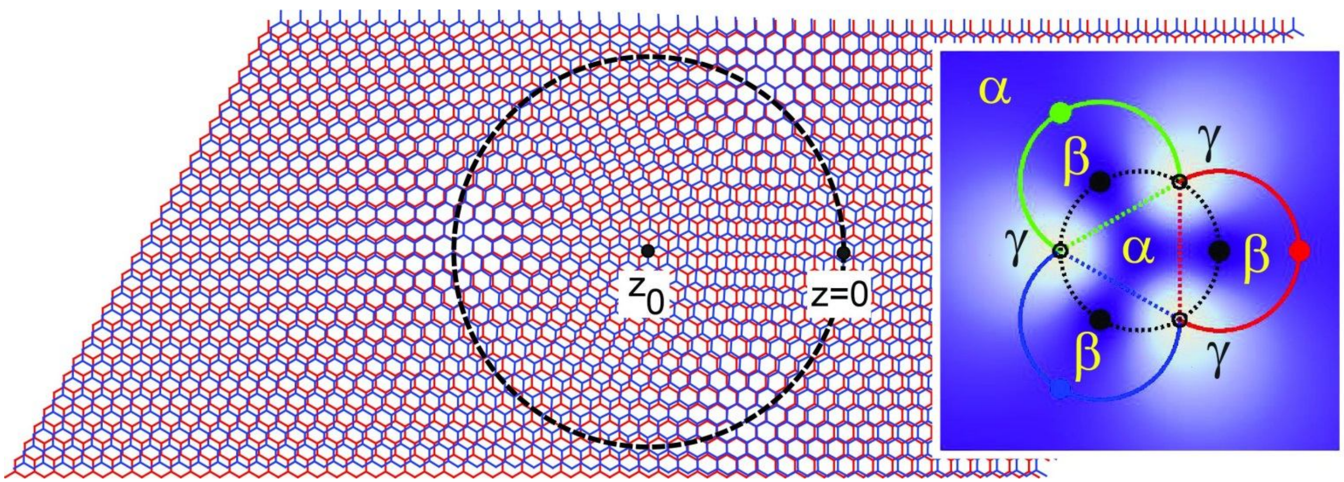
Smoothest single-valued anti-analytic form

$$\Delta^{>}(\bar{z}) = \Delta_\alpha + (\Delta_\beta - \Delta_\alpha)\frac{\bar{z}_o}{\bar{z}_o - \bar{z}}$$

pole at z_o

This matches an interior solution

$$\Delta^{<}(z) = \Delta_\alpha + (\Delta_\beta - \Delta_\alpha)\frac{z_o - z}{z_o}; \left|z_o - z\right| < \left|z_o\right|$$



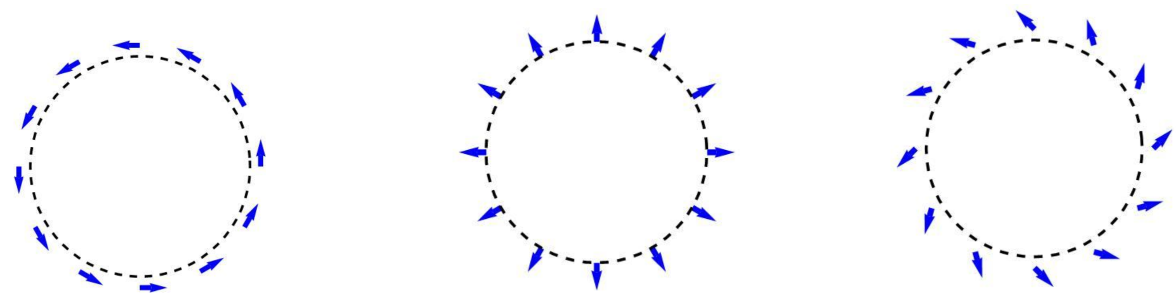
Force Distribution in a Minimal Texture

Exterior: divergenceless and harmonic (minimally strained)

Interior: divergenceless (transverse) and strain free

No body forces in exterior or interior regions, but **they are nonzero on the matching curve** (layer forces and moments compensate)

Boundary force distribution:



$\operatorname{Im} z_o = 0$ $\operatorname{Re} z_o = 0$

Elastic Energies

Minimal texture:

$$U_{\mathbf{elastic}} = 2\pi(\lambda+\mu)\left[\operatorname{Re}\Delta_{\alpha\beta}\right]^2 + \frac{\pi}{2}\mu\left|\Delta_{\alpha\beta}\right|^2$$

interior: dilation/compression

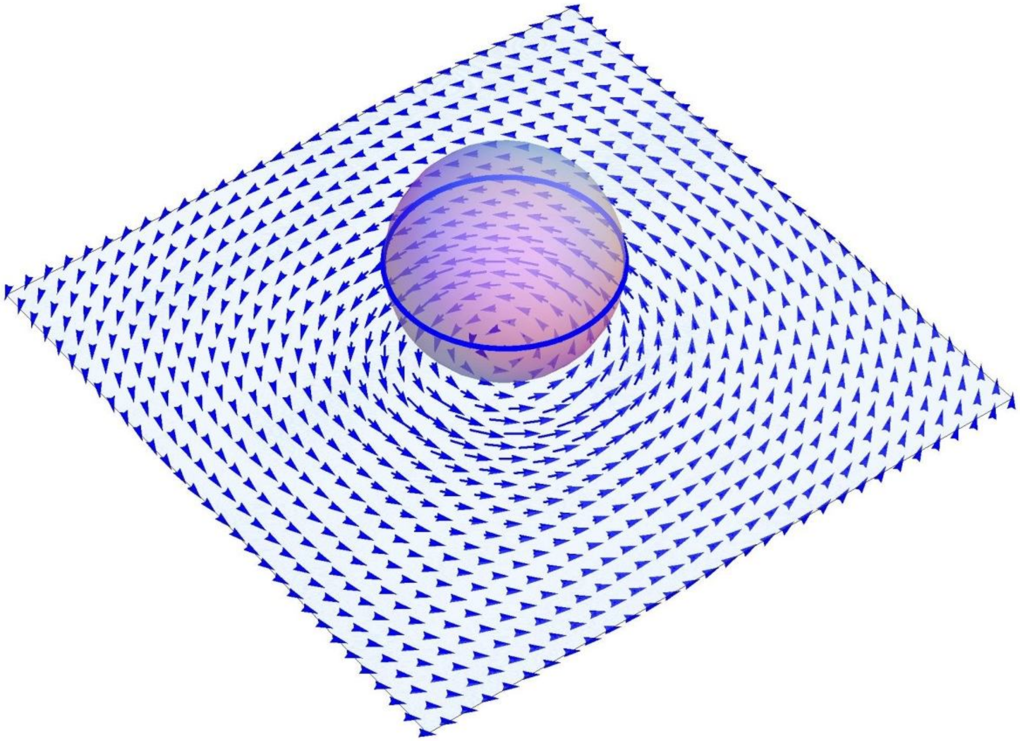
exterior: orthorhombic and/or shear strain

Domain wall: $U_{\mathbf{wall}} = 2\pi\gamma R$ (line tension γ)

$U_{\mathbf{wall}} > U_{\mathbf{elastic}}$ for R>5 nm (the minimal solution is favored)

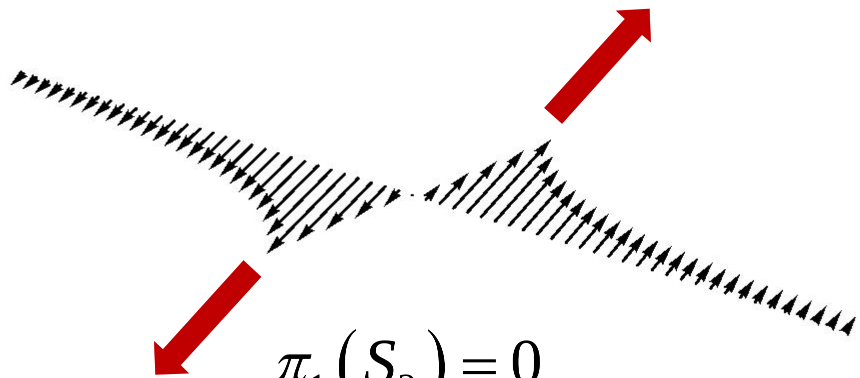
Texture is planar projection of the baby skyrmion

$$\hat{n}(z) \to \left(\vec{n}_\perp, n_z\right) \to \vec{n}_{xy}$$

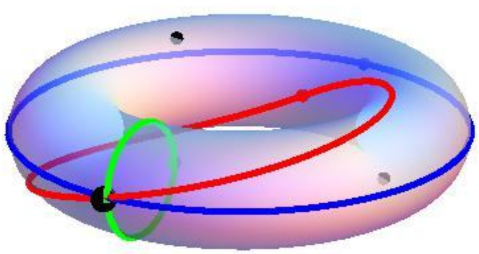


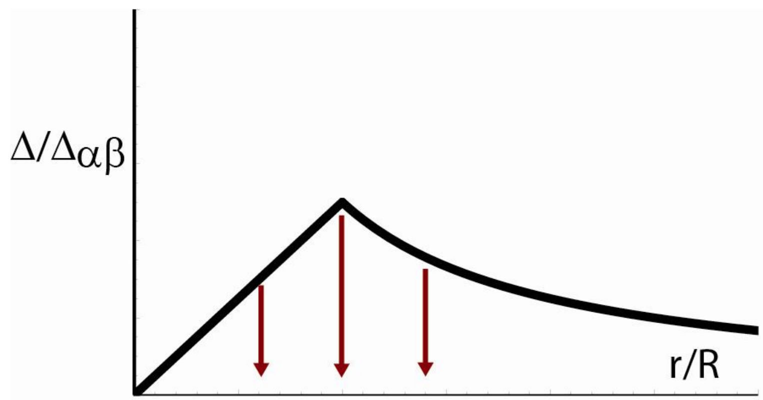
$$\frac{1}{2}\int d^2\mathbf{r}\ \nabla\hat{n}\bullet\nabla\hat{n} \Leftrightarrow \frac{1}{2}\int d^2\mathbf{r}\ \nabla\vec{n}_\perp \bullet\nabla\vec{n}_\perp$$

Topology lost (and found): unstable and stable stacking textures



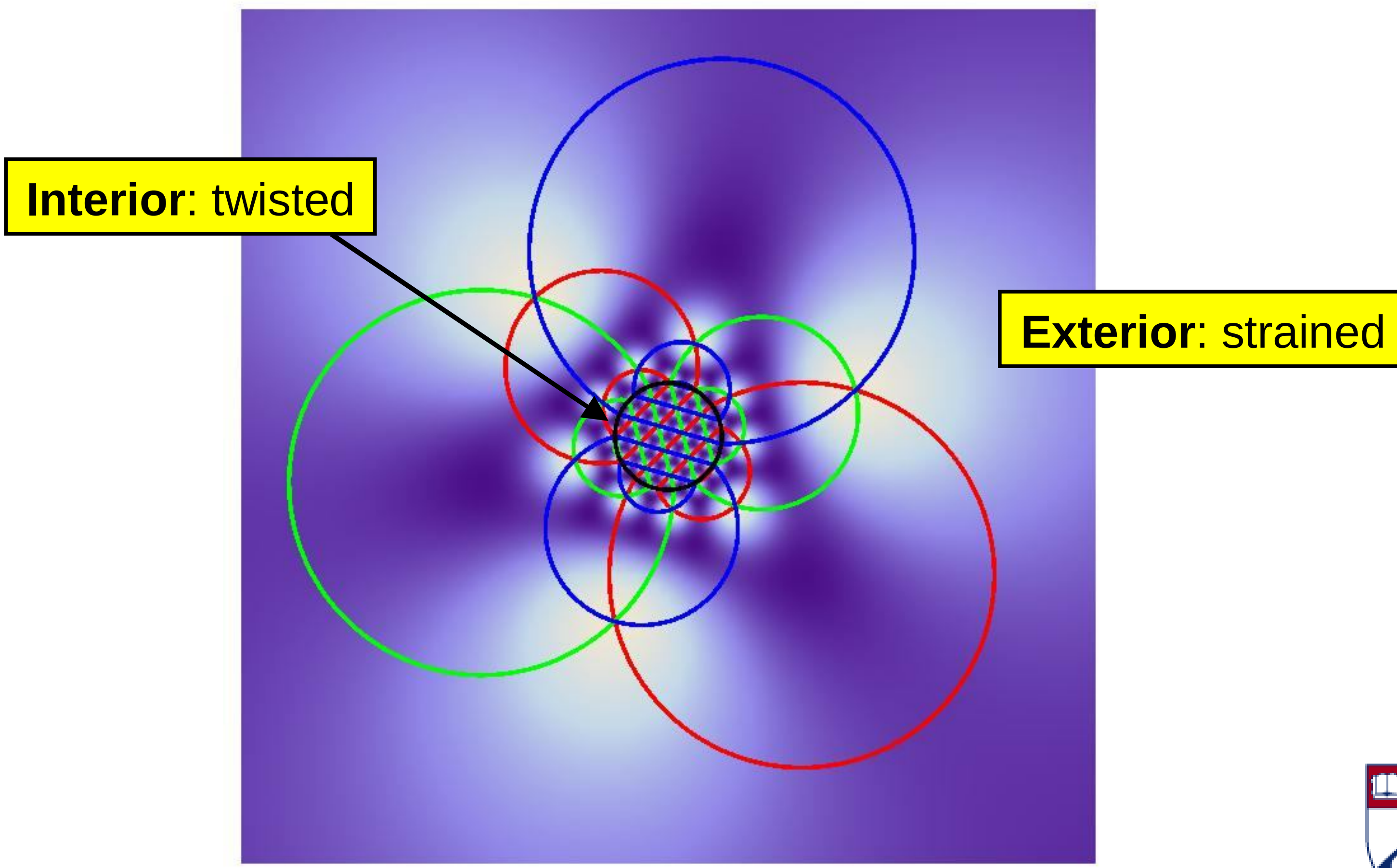
$$\pi_1\left(S_2\right)=0$$





Case I: Exterior (relative shift @ boundary)

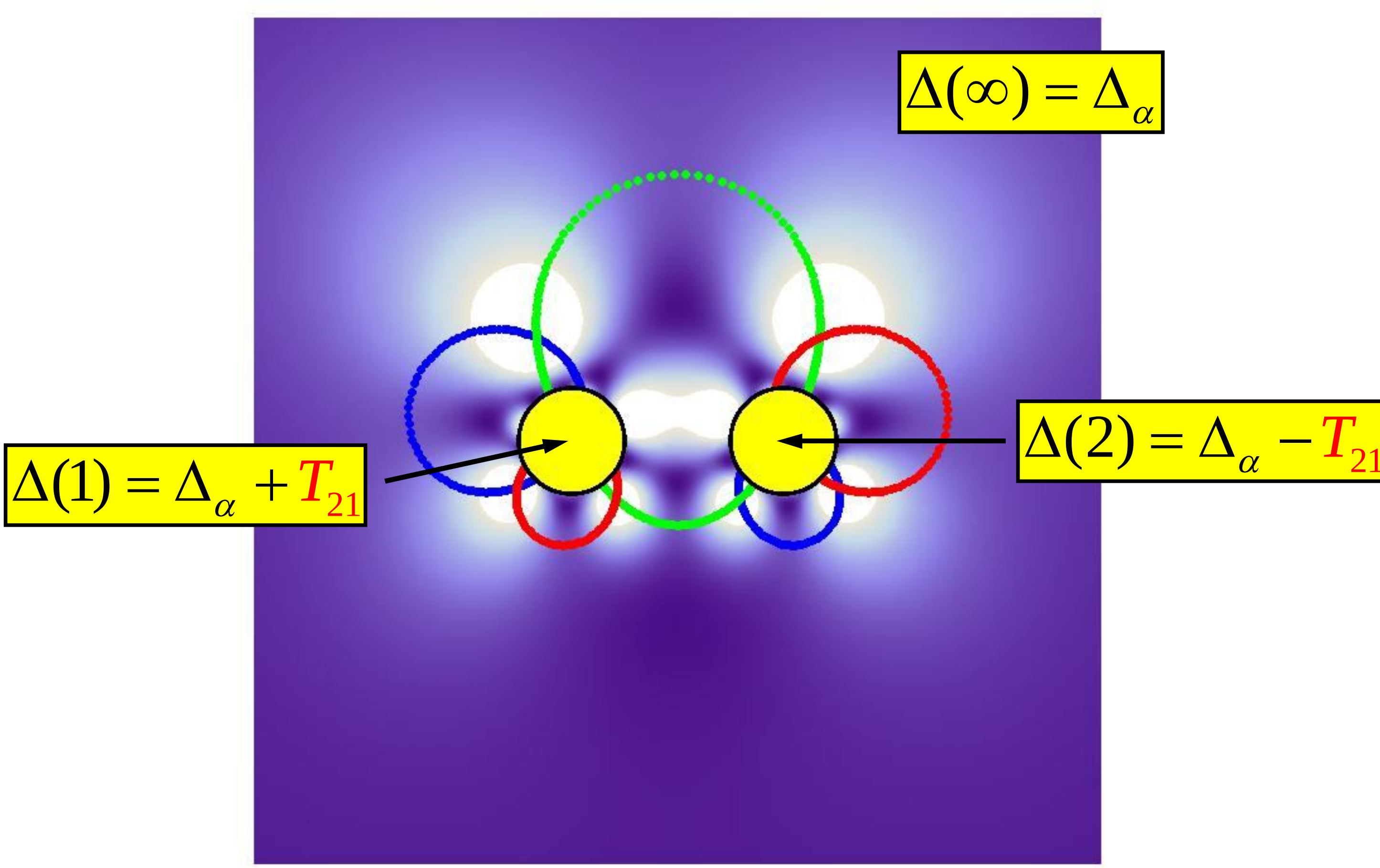
$$\Delta^{>} = \Delta_{\alpha} + \left(\Delta_{\beta} - \Delta_{\alpha} + T_{lm}\right)\frac{\bar{z}_o}{\bar{z}_o - \bar{z}}$$



Case II: Interior (relative shift @ origin)

$$\Delta(0) = \Delta(\infty) + T_{lm}$$

This is impossible for a single defect!



Comment

The elastic energy of this texture is extremely low. It realizes a **lower bound** on the elastic energy for an interlayer displacement field subject to the boundary conditions.

The commensuration (Peierls) energy is not optimized.

Commensuration Energies

$$U_c \sim \frac{1}{2}\kappa\left|\Delta - \Delta_{\alpha(\beta)}\right|^2$$

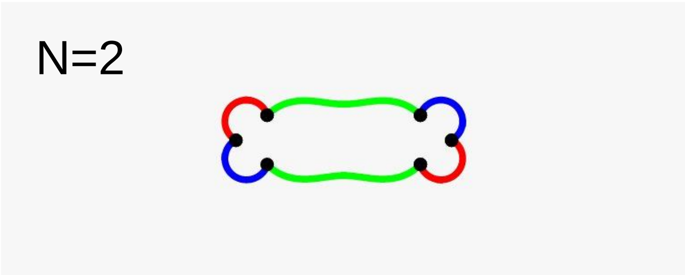
Power law relaxation of minimal texture leaves a large area **incompletely relaxed** and has a high commensuration energy.

1. (naïve): $$U_c \sim \left|\Delta_{\beta\alpha}\right|^2 \log R_c$$

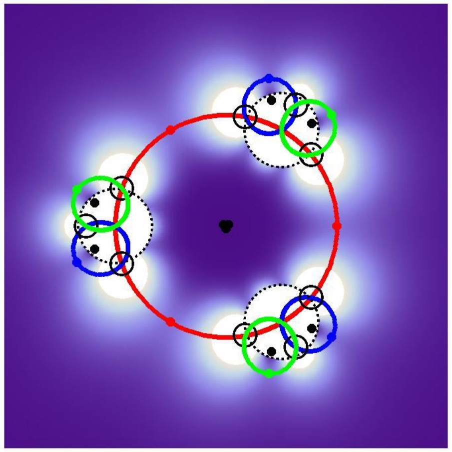
2. (better): Link defects in N-mers to compensate the far field commensuration energy penalty

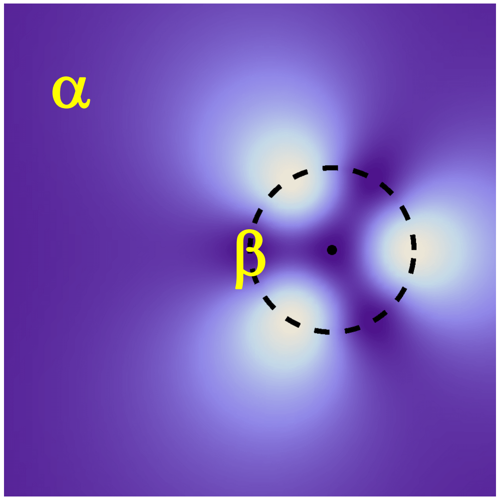
N-mers that compensate far field energy

N=2



N=3





Domain wall: string of point defects
Wall network: condensation of strings

Commensuration Energy

$$U_c = \frac{1}{2}\kappa\left|\Delta - \Delta_{\alpha(\beta)}\right|^2$$

Algebraic relaxation of texture is problematic
for the commensuration energy

1. (naïve): $$U_c \sim \left|\Delta_{\beta\alpha}\right|^2 \log R_c$$

2. (better): Link defects in N-mers to compensate the far field commensuration energy penalty

3. (best): Mass from commensuration potential

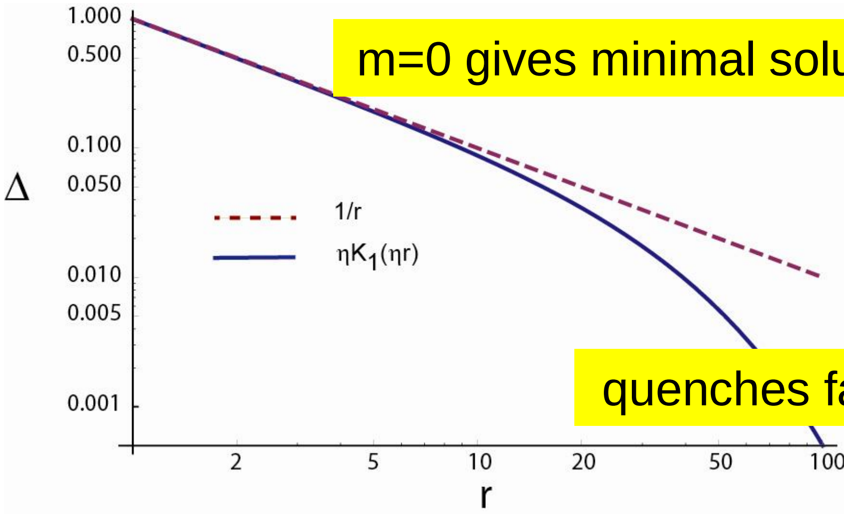
Massive Solutions

$$\vec{f} = (\lambda + 2\mu)\nabla^2\vec{\Delta} - (\lambda + \mu)\nabla\times\nabla\times\vec{\Delta} - \kappa\,\vec{\Delta} = 0$$

e.g. for longitudinal solution $\vec{\Delta} = -\nabla\psi$

$$-\nabla\left(\nabla^2\psi - \eta_L^2\psi\right) = 0$$

$$\psi(\zeta) = \sum_m c_m K_m\left(\eta_L|\zeta|\right)\cos m\phi$$

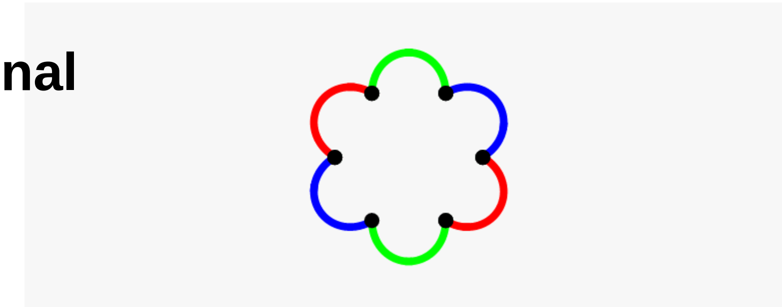


m=0 gives minimal solution in near field

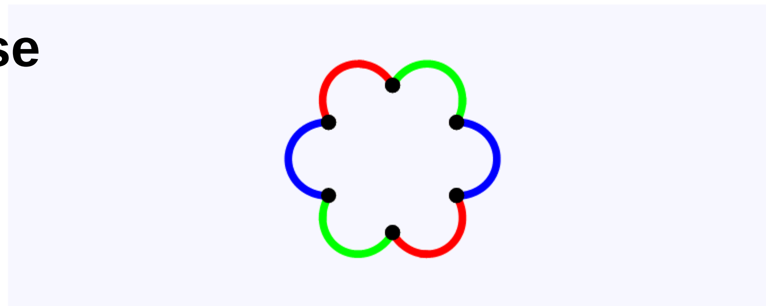
quenches far field energy

Dissociation of m=1 solutions

Longitudinal

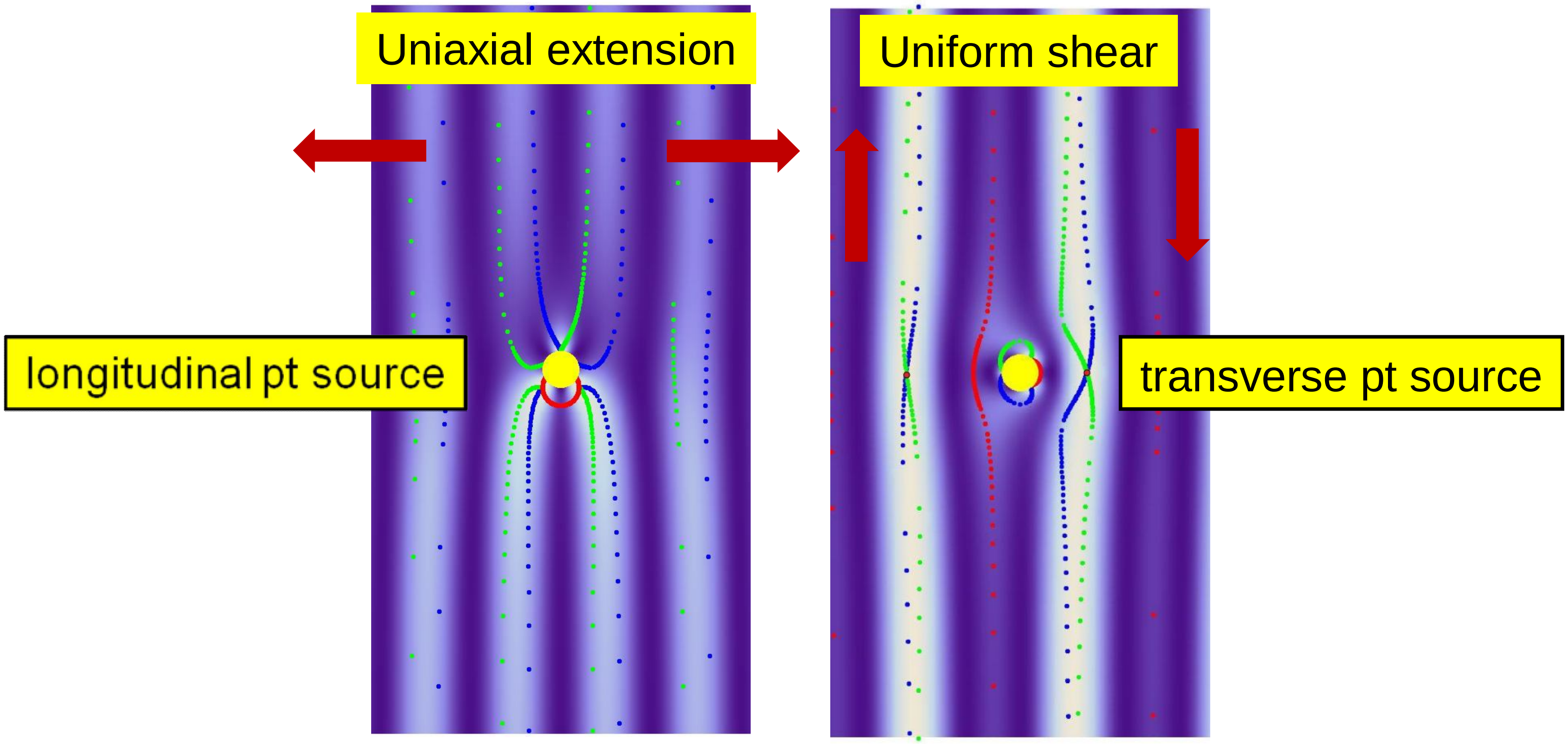


Transverse



Elastic dipole is bound for pure longitudinal solution unbound for transverse solution

Can be used to screen a uniformly strained background



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→ **<u>Part III</u>: Connect I & II**
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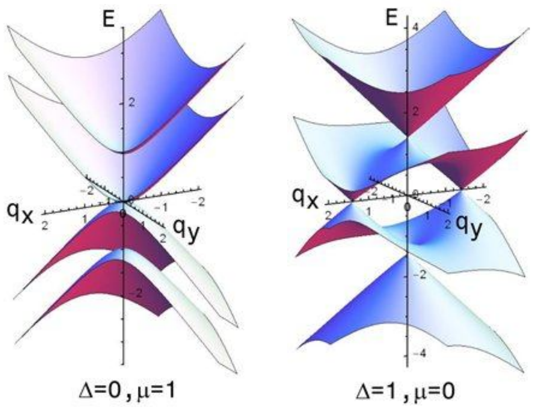
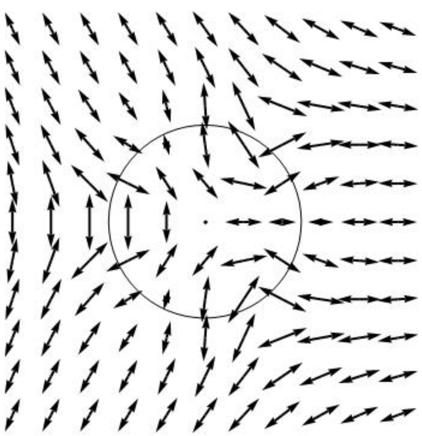
Key Results from Parts I-II

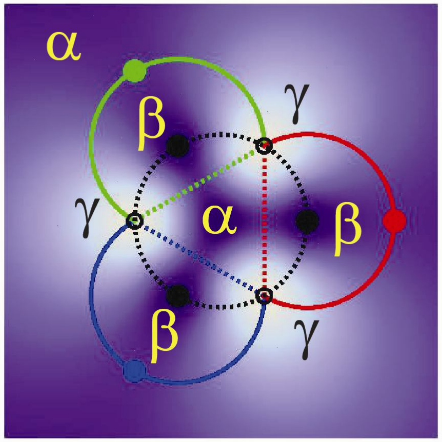
Part I



Interlayer slip fissions the contact point

Part II



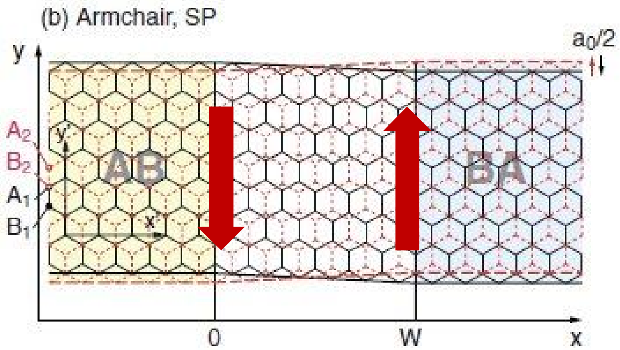


Minimal 2D textures spreads entire Δ domain over the plane

Signatures in spectroscopy, scattering and transport
(Zach Addison)

Prior results (not ours) for 1D variant

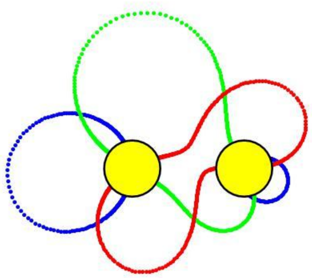
Transmission across a straight boundary



Boundary-specific transmittance for 1D wall (M. Koshino, PRB **88**, 115409 (2013)

Stacking boundaries and transport in bilayer Graphene (San-Jose et al, arXiv:1311.1483)

Transmission along boundary



Valley-polarized currents in walls that bridge AA regions (San-Jose and Prada, PRB **88**, 121408 (2013)

Valley-polarized one-way channels along the critical lines:
Strain engineering of topologically confined channels.

Collaborators

Zachary Addison, Xingting Gong, Charlie Kane, Youngkuk Kim, Allan MacDonald, Andrew Rappe, Vivek Shenoy, Ben Wieder, Fan Zhang

Domain wall states**:** PNAS **110**,10546 (2013)
Stacking textures: Phys. Rev. B **89**, 121415 (2014)

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