Emergent geometric frustration and flat bands in twisted bilayer graphene

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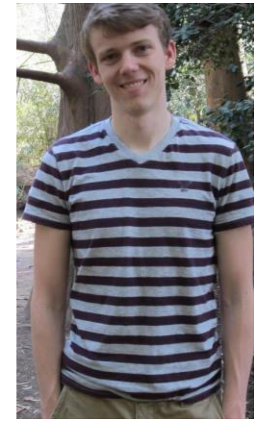
Acknowledgement

Markus Kindermann

Stephen Spitz



Steven Carter

- H. K. Pal, S. Spitz, M. Kindermann, Phys. Rev. Lett. 123, 186402 (2019)
- H. K. Pal, S. Carter, and M. Kindermann, arXiv:1409.1971

NSF, DMR-1055799

The gist

Twisted bilayer graphene

Small angles

Layers coupled—
flat bands

Large angles

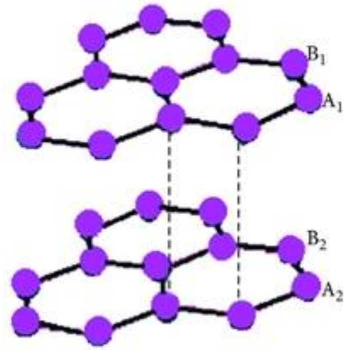
Layers decoupled—
no flat bands

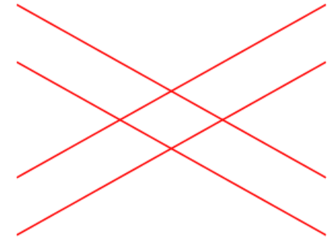
Layers coupled—
flat bands

Introduction

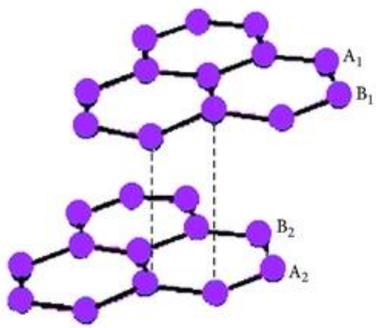
Twisted bilayer graphene

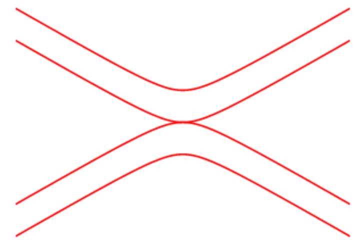
- AA



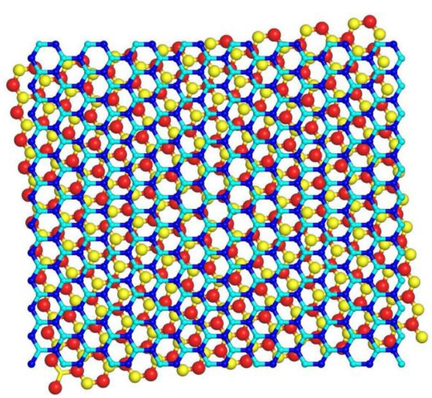


- AB





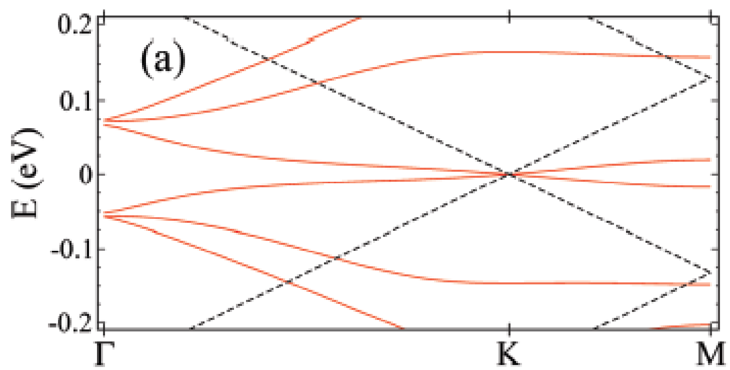
- Arbitrary angle

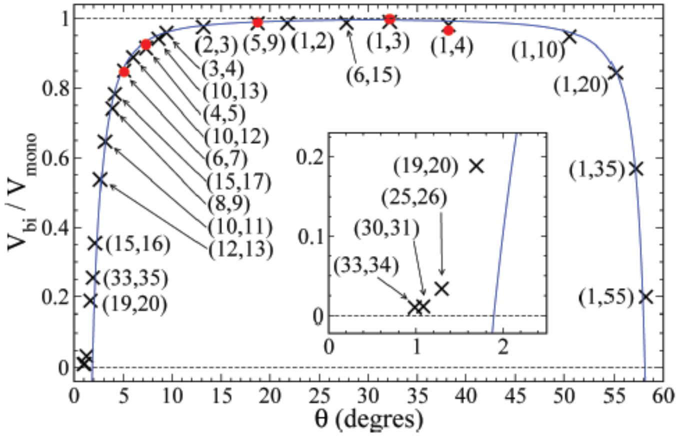


?

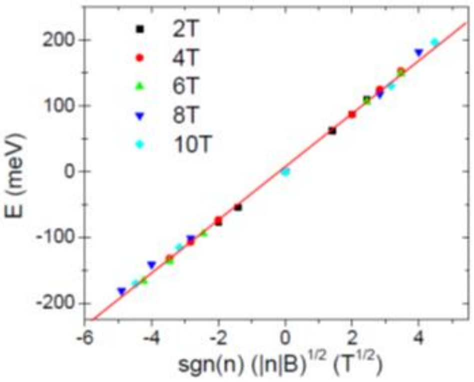
Current understanding

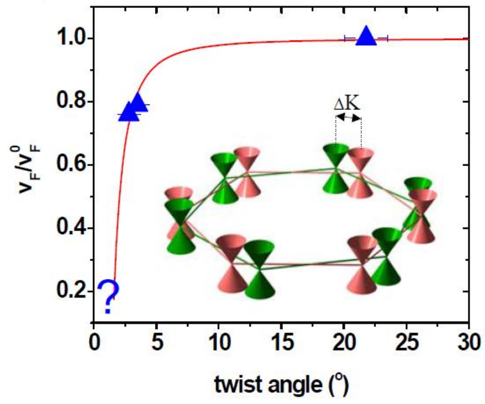
- Dirac cone preserved
- Velocity reduces at small angle but unaffected at large angle





Lopes dos Santos et al. ,PRL 99,256802 (2007); Laissardiere et al., Nano Lett. 10, 804 (2010)

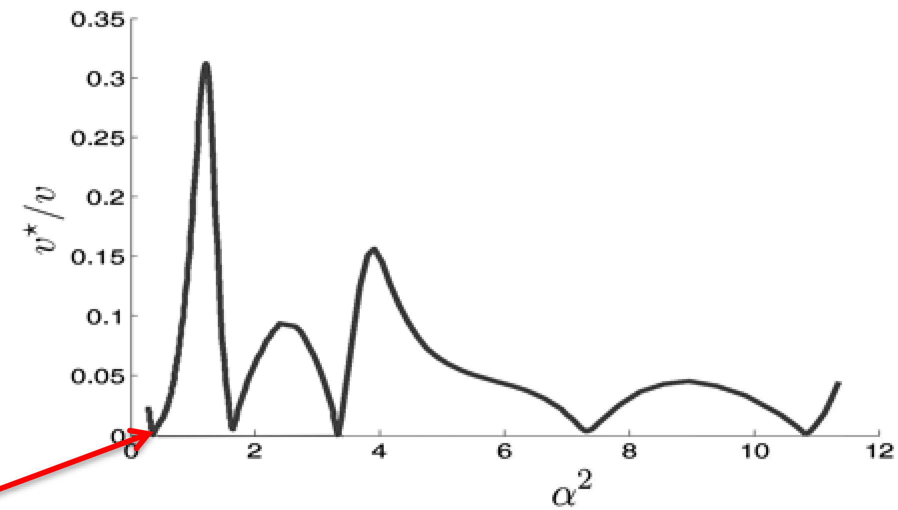




Luican, et al., PRL 106, 126802 (2011)

Current understanding (cont'd.)

- Magic angles: recurring zero velocity and localization (□□1/□)



Bistritzer and MacDonald, PNAS 108, 12233 (2011)

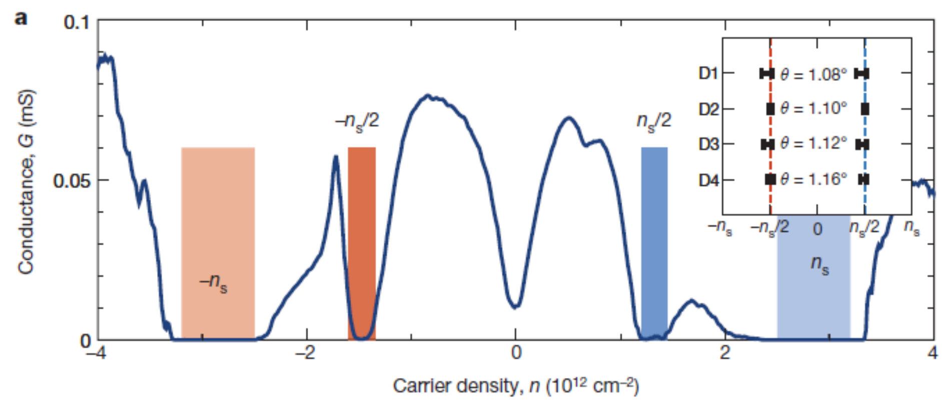
~ 1.08□

- Complete understanding of the small angle physics in non-perturbative regime is lacking – needs more work

H. K. Pal, arXiv : 1805.08803
G. Tarnopolsky, A. J. Kruchkov, and A. Vishwanath, Phys. Rev. Lett. 122, 106405 (2019)

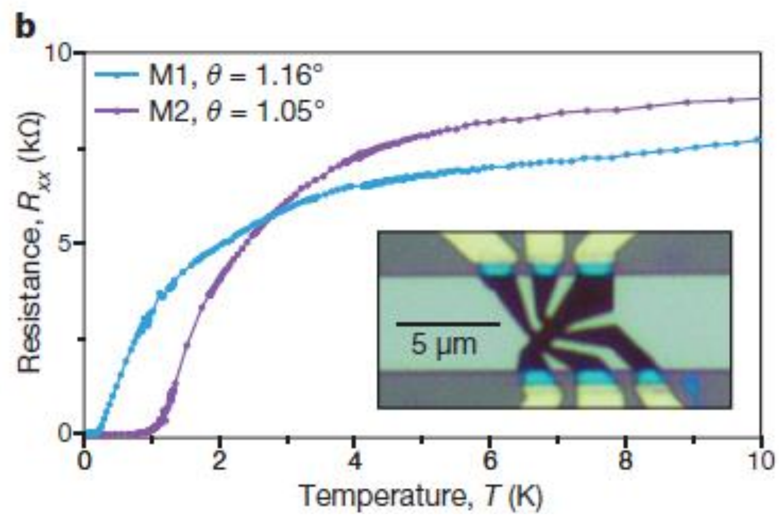
Experimental discovery of correlation effects

Correlated insulating phase at half-filling



Cao et al., Nature 556, 80 (2018)

Superconductor away from half-filling



Cao et al., Nature 556, 43 (2018)

Further experiments

Tuning superconductivity in twisted bilayer graphene

Matthew Yankowitz[1,*], Shaowen Chen[1,2,*], Hryhoriy Polshyn[3,*], Yuxuan Zhang[3], K. Watanabe[4], T. Taniguchi[4], David Graf[5], Andrea F. Young[3,†], Cory R. Dean[1,†]

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Superconductors, orbital magnets and correlated states in magic-angle bilayer graphene

Xiaobo Lu, Petr Stepanov, Wei Yang, Ming Xie, Mohammed Ali Aamir, Ipsita Das, Carles Urgell, Kenji Watanabe, Takashi Taniguchi, Guangyu Zhang, Adrian Bachtold, Allan H. MacDonald & Dmitri K. Efetov

Nature **574**, 653–657(2019) | Cite this article

Correlated insulating and superconducting states in twisted bilayer graphene below the magic angle

Emilio Codecido[1], Qiyue Wang[2], Ryan Koester[1], Shi Che[1], Haidong Tian[1], Rui Lv[1], Son Tran[1], Kenji Watanabe[3], Takashi Taniguchi[3], Fan Zhang[2,*], Marc Bockrath[1,*] and Chun Ning Lau[1,*]

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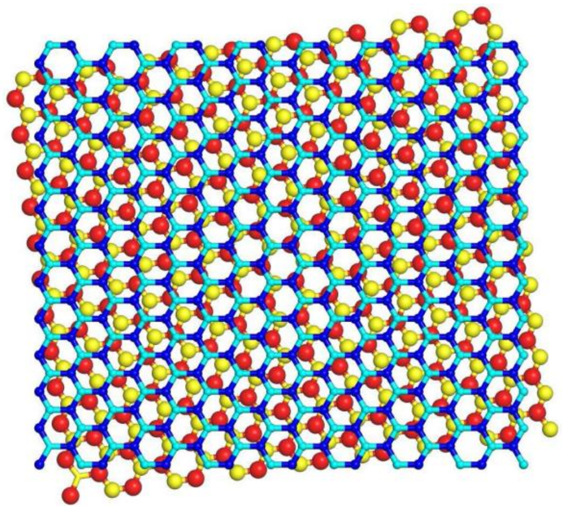
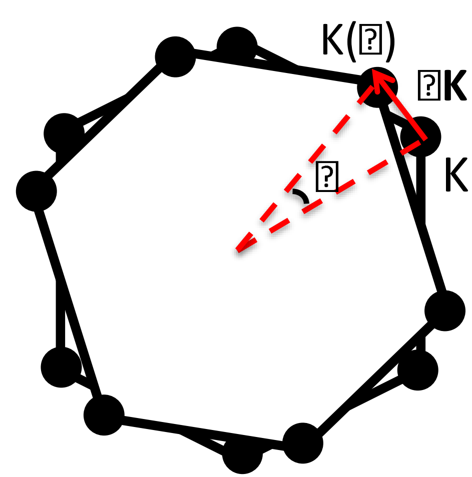
Long-wavelength theory





- Length scale: $|\Delta\boldsymbol{K}| = |\boldsymbol{K}(\theta) - \boldsymbol{K}| = 2K\sin(\theta/2)$
  Require: $|\Delta\boldsymbol{K}| \ll K$, i.e., ? << 1 (measured from AA or AB).

- Energy scales: interlayer coupling t and $v_F \Delta K$.

Long-wavelength theories (cont'd)

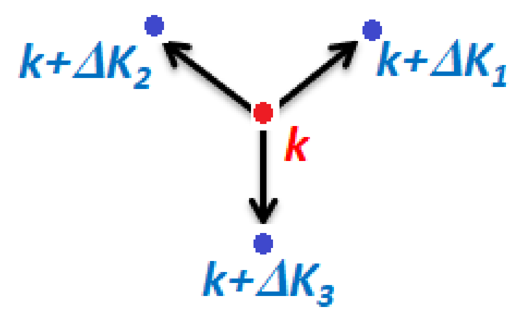
- Expand around K (K') point

$$H_1 = v_F \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} \sigma \cdot \mathbf{k} \psi_{\mathbf{k}}, \; H_2 = v_F \sum_{\mathbf{k}} \psi^\dagger_{\mathbf{k}} \sigma^\theta \cdot (\mathbf{k}) \psi_{\mathbf{k}},$$

$$H_{\text{int}} = \sum_{\mathbf{k},\mathbf{k}_\theta} \sum_{\alpha,\beta} \sum_{\mathbf{G},\mathbf{G}^\theta} \tilde{t}(\mathbf{k}+\mathbf{K}+\mathbf{G}) e^{-i\mathbf{G}\cdot\tau_\alpha} e^{i\mathbf{G}^\theta\cdot\tau^\theta_\beta}$$
$$\delta(\mathbf{k}^\theta - \mathbf{k} + \Delta\mathbf{K} + \mathbf{G}^\theta - \mathbf{G}) \psi^\dagger_{\mathbf{k}\alpha} \psi_{\mathbf{k}^\theta\beta},$$

- Lowest Fourier component $\tilde{t}(\mathbf{K}) = \gamma$

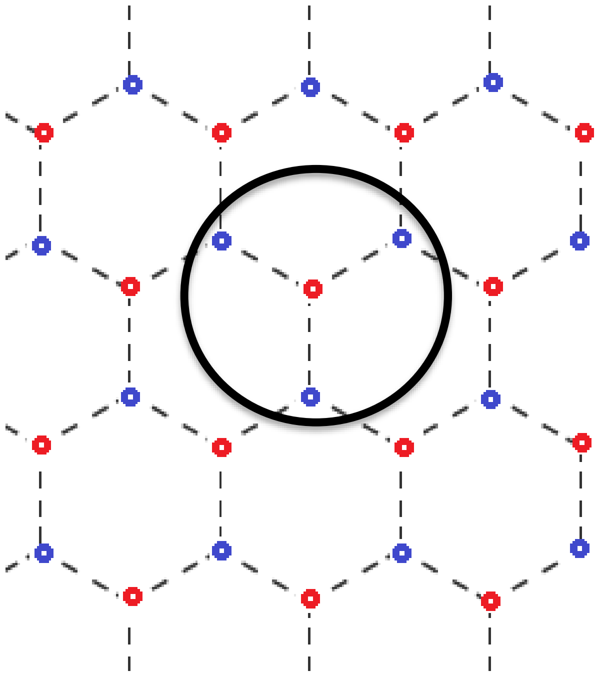
- Choose **G**, **G**$^\theta$ such that $|\Delta\mathbf{K}+\mathbf{G}^\theta-\mathbf{G}|=|\Delta\mathbf{K}|$



$$\delta(\mathbf{k}^\theta - \mathbf{k} + \Delta\mathbf{K} + \mathbf{G}^\theta - \mathbf{G}) \Rightarrow \delta(\mathbf{k}^\theta - \mathbf{k} + \Delta\mathbf{K}_n)$$

Lopes dos Santos et al. ,PRL 99,256802 (2007)

Long-wavelength theories (cont'd)



$$\frac{\gamma}{v_F \Delta K} < 1$$

$$H_k = \tilde{v}\, \boldsymbol{\sigma}.\boldsymbol{k}$$

$$\tilde{v} = v_F \left[1 - \left(\frac{\gamma}{v_F \Delta K}\right)^2\right]$$

- Small angle: Reduced velocity
- Large angle: velocity unchanged

The gist

Twisted bilayer graphene

Small angles

Layers coupled—
flat bands

Large angles

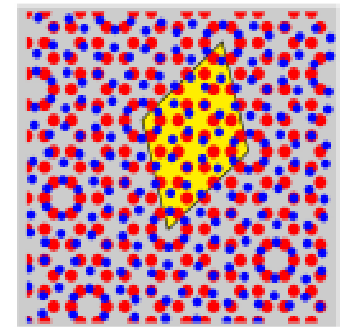
~~Layers decoupled—
no flat bands~~

Layers coupled—
flat bands

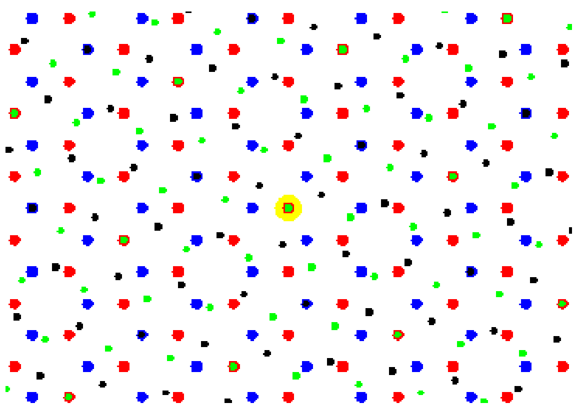
Our theory

Geometry

Mutually rotated graphene layers → Incommensurate / Commensurate

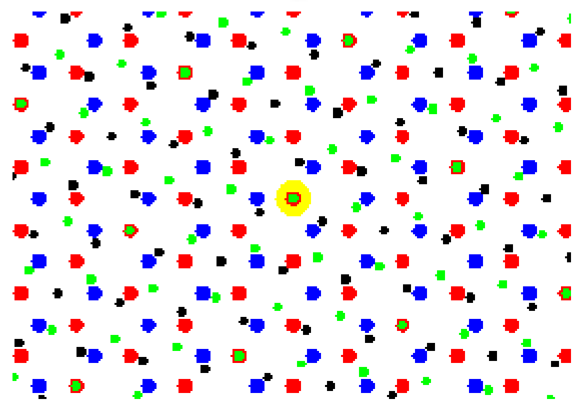


Commensuration



Sublattice even (SEE)
Both AA and BB match

➢ Similar to AA bilayer



Sublattice odd (SEO)
Only AA matches

➢ Similar to AB bilayer

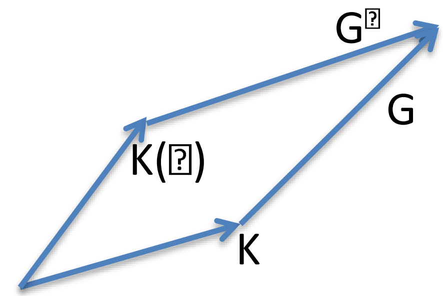
Mele, PRB 81, 161405R (2010)

Starting point: commensuration

$$H_{\text{int}} = \sum_{\mathbf{k},\mathbf{k}_\theta} \sum_{\alpha,\beta} \sum_{\mathbf{G},\mathbf{G}^\theta} \tilde{t}(\mathbf{k}+\mathbf{K}+\mathbf{G}) e^{-i\mathbf{G}\cdot\tau_\alpha} e^{i\mathbf{G}^\theta\cdot\tau^\theta_\beta}$$

$$\boxed{\delta(\mathbf{k}^\theta - \mathbf{k} + \Delta\mathbf{K} + \mathbf{G}^\theta - \mathbf{G})} \psi^\dagger_{\mathbf{k}\alpha} \psi_{\mathbf{k}^\theta \beta},$$

- Commensuration in real space implies commensuration in reciprocal space



- Choose **G**, **Gθ** such that **K + G = K(θ) + Gθ**

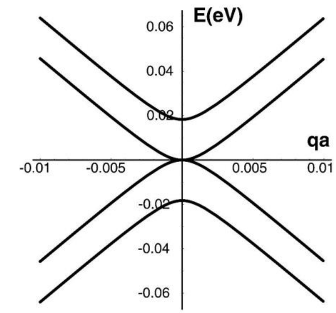
- Use higher Fourier component: $\tilde{t}(\mathbf{K}+\mathbf{G}) = \mathcal{V}$

$$\delta(\mathbf{k}^\theta - \mathbf{k} + \Delta\mathbf{K} + \mathbf{G}^\theta - \mathbf{G}) \;\Rightarrow\; \delta(\mathbf{k}^\theta - \mathbf{k})$$

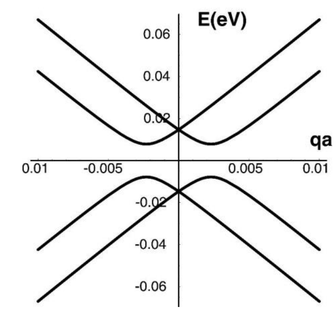
Mele, PRB 81,161405R (2010)

Commensuration effects

- Consequences
  - Introduces mass: curvature and, in some cases, gap
  - Energy scale: $\tilde{t}(\mathbf{K}+\mathbf{G}) = \mathcal{V}$ << □
  - Gap appreciable only at certain angles with small supercell



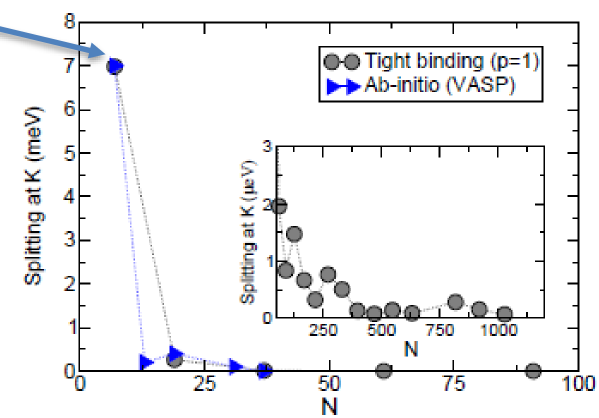
SEO



SEE

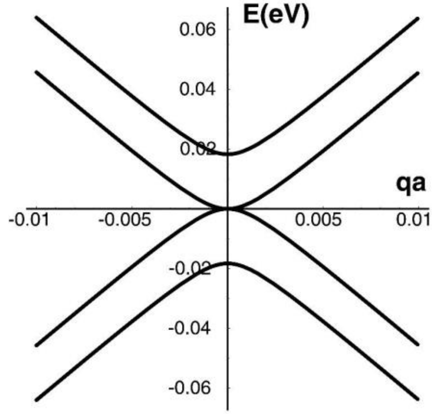
38.21□

- Numerical estimate of $\tilde{t}(\mathbf{K}+\mathbf{G}) = \mathcal{V}$

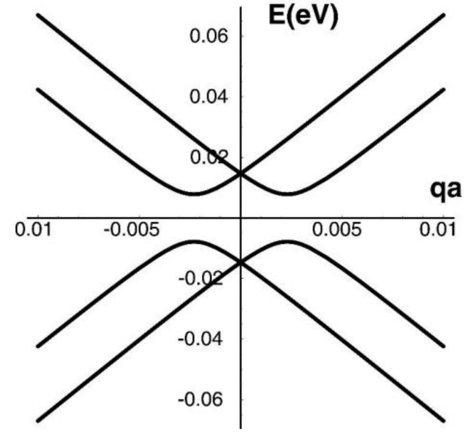


Shallcross et al., PRL 101, 056803 (2008)

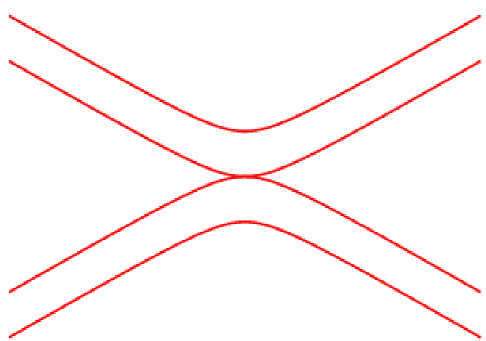
Commensuration effects (cont'd.)



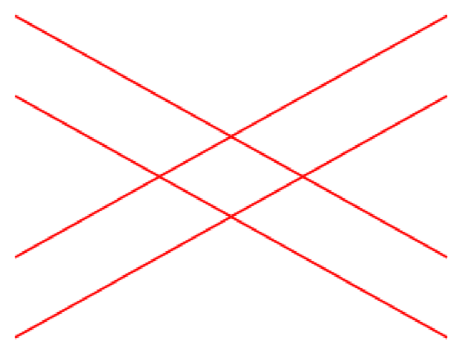
SEO



SEE



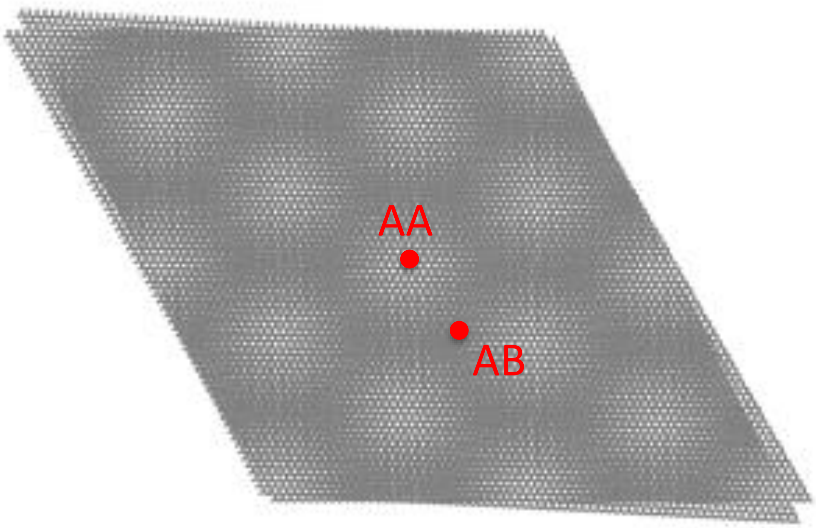
AB



AA

SE0 + SEE = [illegible]/3

Small vs. large angle



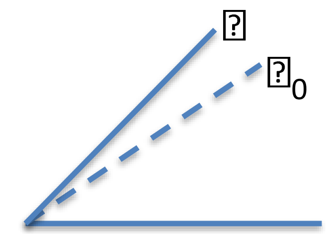
Small angle

Large angle

- ➢ Small angle from some commensuration

Theory at angle near commensuration

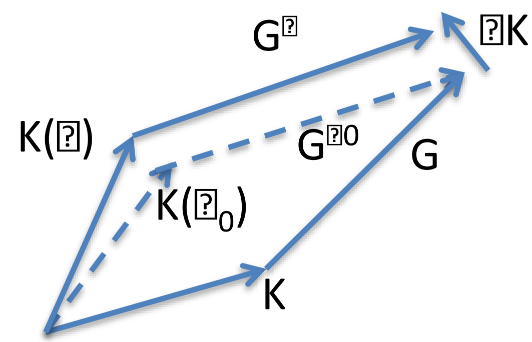
- Consider angle θ near commensuration θ_0
  - $\theta \sim 1$ but $\delta\theta = \theta - \theta_0 \ll 1$



- Formally try to expand around K point as before

$$H_{\rm int} = \sum_{\mathbf{k},\mathbf{k}_\theta} \sum_{\alpha,\beta} \sum_{\mathbf{G},\mathbf{G}^\theta} \tilde{t}(\mathbf{k}+\mathbf{K}+\mathbf{G}) e^{-i\mathbf{G}\cdot\tau_\alpha} e^{i\mathbf{G}^\theta\cdot\tau_\beta^\theta}$$
$$\delta(\mathbf{k}^\theta - \mathbf{k} + \Delta\mathbf{K} + \mathbf{G}^\theta - \mathbf{G}) \psi^\dagger_{\mathbf{k}\alpha} \psi_{\mathbf{k}^\theta\beta},$$

$$\delta(\mathbf{k}^\theta - \mathbf{k} + \Delta\mathbf{K} + \mathbf{G}^\theta - \mathbf{G}) \Rightarrow \boxed{\delta(\mathbf{k}^\theta - \mathbf{k} + \delta\mathbf{K})}$$



Formally same as before

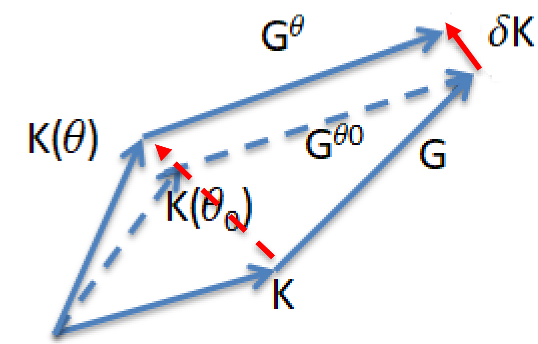
$$\delta K = 2|\mathbf{K}+\mathbf{G}|\sin(\delta\theta/2) \ll K$$
but $\Delta K = 2|\mathbf{K}|\sin(\theta/2) \sim K$

H. K. Pal, S. Carter, and M. Kindermann, arXiv:1409.1971

Theory at angle near commensuration(cont'd.)

- Expand around **K+G** instead of **K**
  1) Use □**K** and not □**K**
  2) Coupling energy scale reduced:

     use $\tilde{t}(\mathbf{K}+\mathbf{G}) = \mathcal{V}$ and not $\tilde{t}(\mathbf{K}) = \gamma$



- In real space:

$$H_{\text{int}}(\mathbf{r}) = \mathcal{V} \sum_n e^{i\delta\mathbf{K}_n\cdot\mathbf{r}} \begin{pmatrix} 1 & e^{-i\frac{2\pi}{3}(n-p)} \\ e^{i\frac{2\pi}{3}(n-l)} & e^{-i\frac{2\pi}{3}(l-p)} \end{pmatrix} e^{-i\sigma_z\theta/2}$$

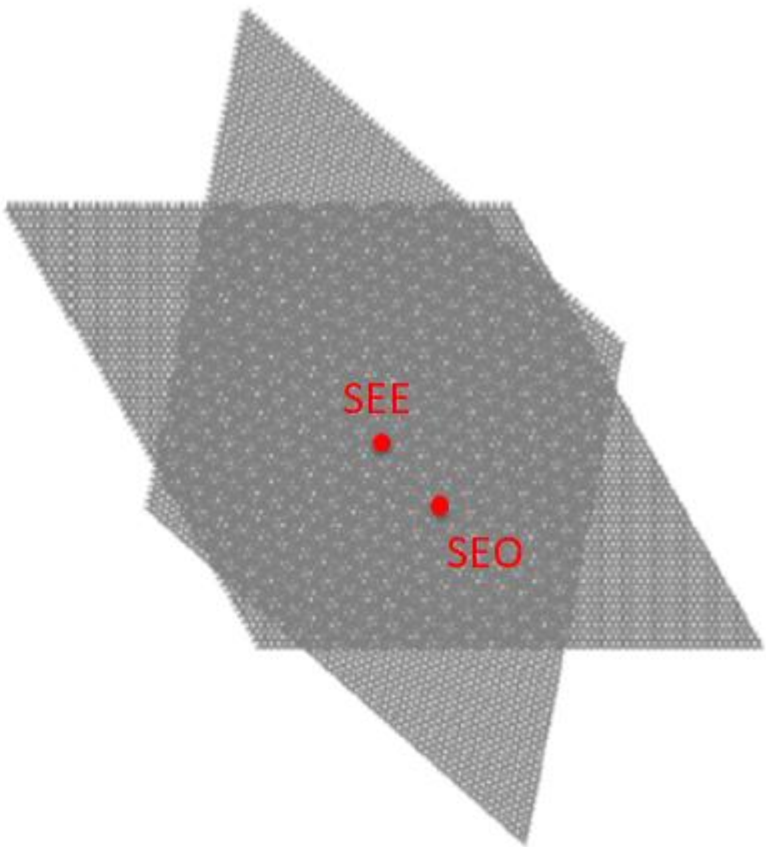
Here $\mathbf{G} = l_1\mathbf{b}_1 + l_2\mathbf{b}_2$, $\mathbf{G}^{\theta_0} = p_1\mathbf{b}_1^{\theta_0} + p_2\mathbf{b}_2^{\theta_0}$

and $l = l_1 + l_2,\ p = p_1 + p_1$

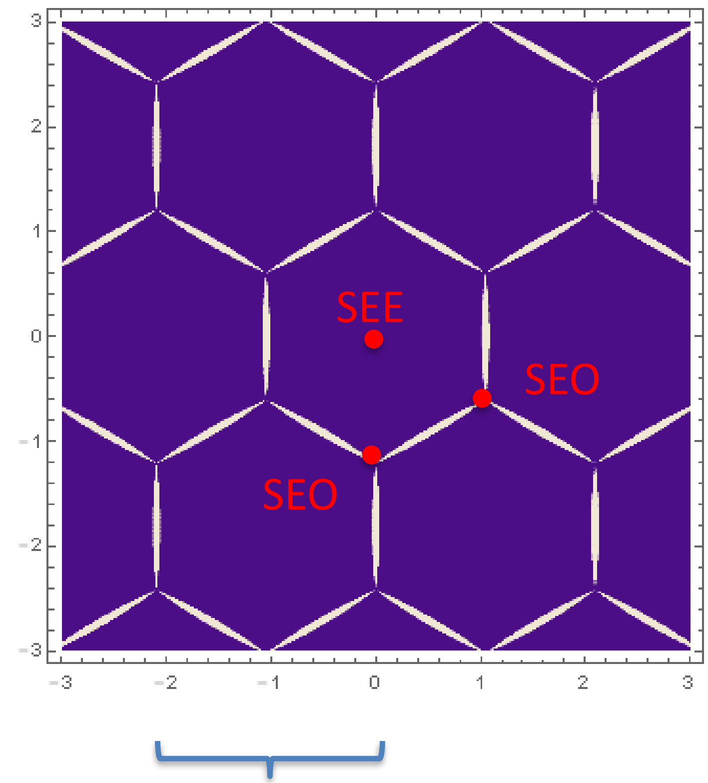
- Reduces to small angle theory at □=0

System at large angles: local gaps

Real space (Non-perturbative limit: □/v_F□K >> *1*)



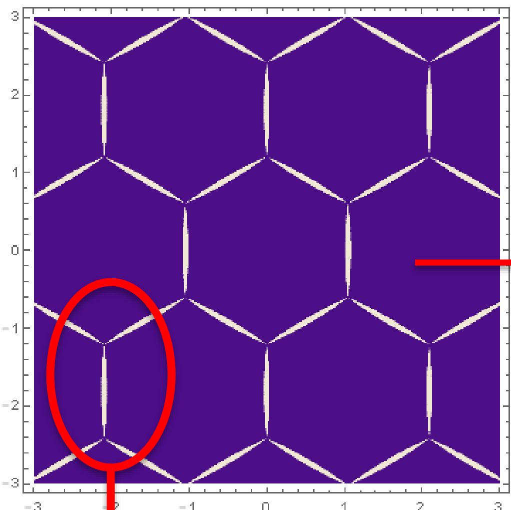
Near $\theta_0 = 38.21^\circ$



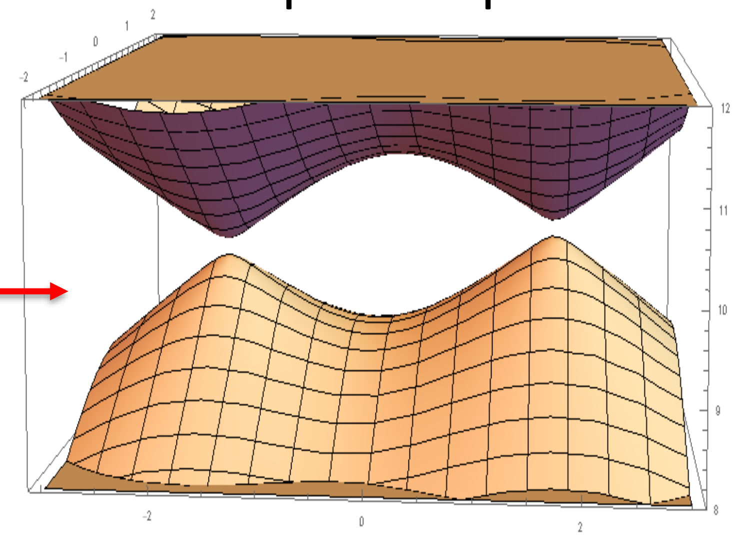
~1/□K

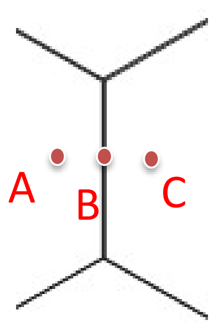
Local gaps

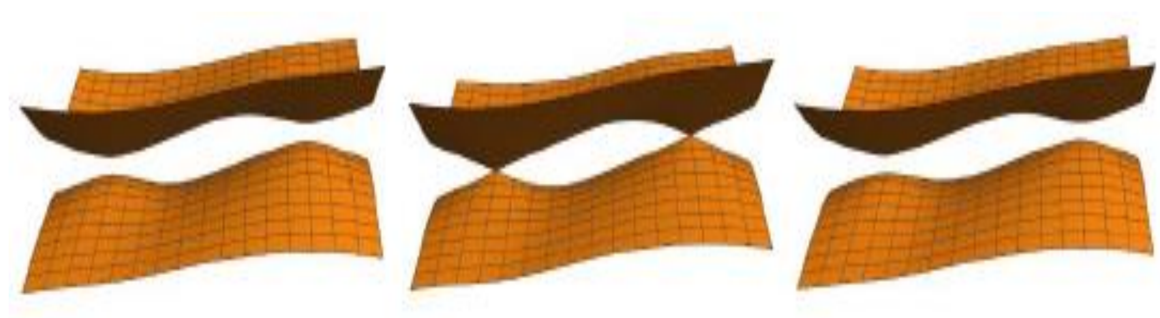
Real space



Reciprocal space







A B C

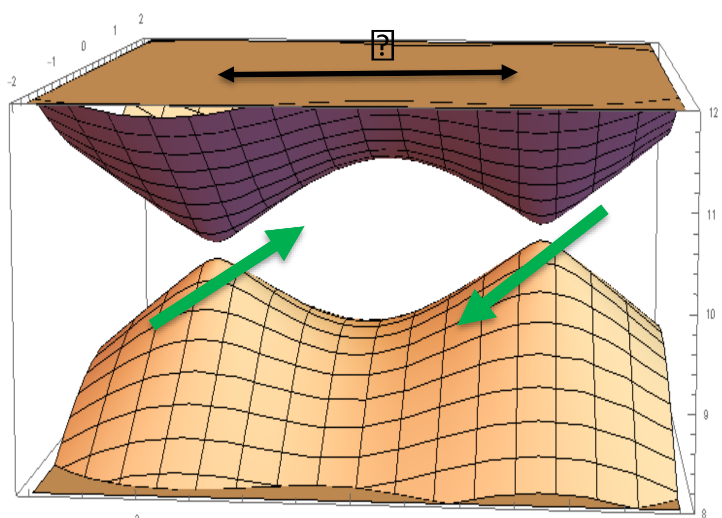
Counter-propagating chiral modes

- Effective low-energy physics

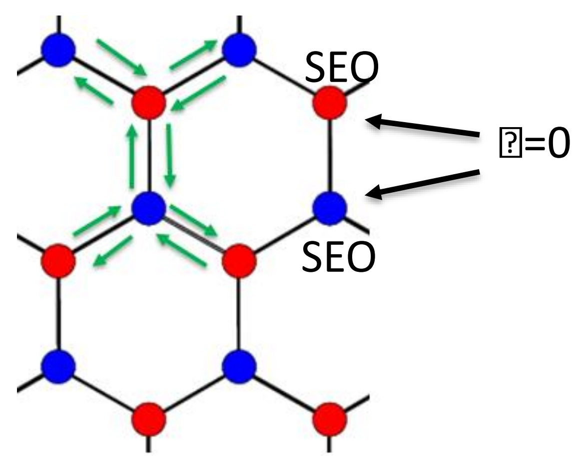
$$h_\nu = g_\nu(\mathbf{k}) \cdot \sigma$$

$$N_3 = \int d\mathbf{k}\mathbf{g}.(\partial_{k_x}\mathbf{g} \times \partial_{k_y}\mathbf{g})/4\pi|\mathbf{g}|^3$$

$$N_3^A - N_3^C = \pm 1$$

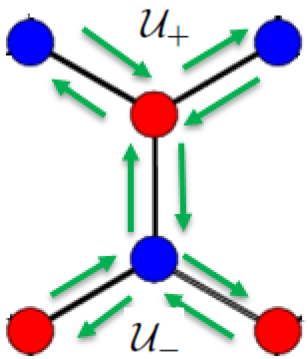


Reciprocal space



Real space

Network model



- Unitary scattering matrix for each scattering center
- Obey the symmetries of Hamiltonian:
  - C_3 symmetry around node
  - Mirror reflection along line joining nodes
  - Point reflection at midpoint of line joining nodes

$$\mathcal{U}_+ = \mathcal{U}_- = \cancel{e^{i\varphi}} \begin{pmatrix} \alpha & \beta e^{i\lambda} & \beta e^{i\lambda} \\ \beta e^{i\lambda} & \alpha & \beta e^{i\lambda} \\ \beta e^{i\lambda} & \beta e^{i\lambda} & \alpha \end{pmatrix}$$

one parameter model !

$$\alpha = 1/\sqrt{1+8\cos^2\lambda} \text{ and } \beta = -2\cos\lambda/\sqrt{1+8\cos^2\lambda}.$$

Network model: energy spectrum

- Use Bloch's theorem
- Exact analytical solution for the eigenstates!

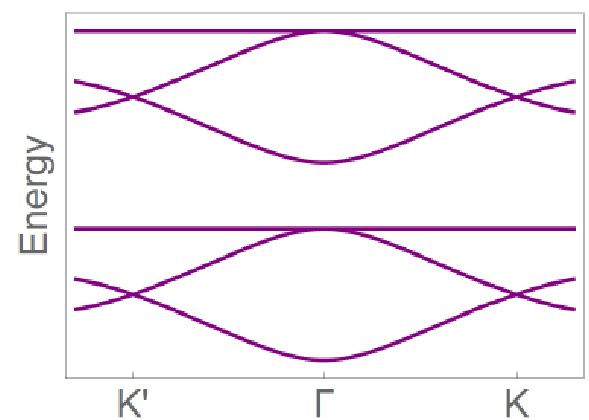
$$\varepsilon_1(\mathbf{k}) = \begin{cases} \lambda \pm \frac{1}{2}\cos^{-1}\left[\frac{(2c_{\mathbf{k}}-1)(1+\cos 2\lambda)-1}{(5+4\cos 2\lambda)}\right], & \text{dispersive} \\ \tan^{-1}\left[\frac{\sin 2\lambda}{2+\cos 2\lambda}\right], & \text{Flat} \end{cases}$$

$$\varepsilon_2(\mathbf{k}) = \varepsilon_1(\mathbf{k}) + \pi, \qquad \text{Periodic}$$

$c_{\mathbf{k}} = \sum \cos(\mathbf{k}_n \cdot \mathbf{r})$, $\mathbf{k}_n$ is vector $\mathbf{k}$ rotated by $2n\pi/3$

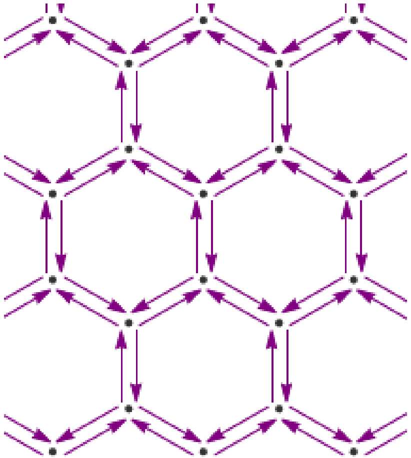
Features:

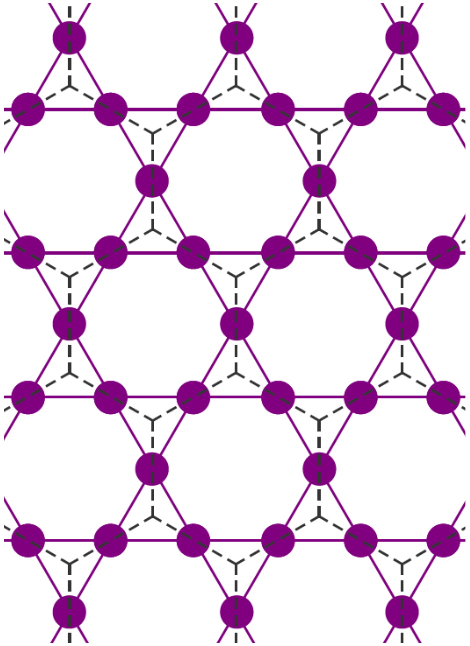
- Dirac points and flat band.
- Degeneracy at Γ and K points in the superlattice BZ.
- Reminiscent of Kagome lattice!



Emergent Kagome lattice

- Similarity with Kagome lattice not accidental
- In the limit of strong backscattering at each scattering center, states get localized on each link
- Think of a TB model with lattice points on each link
- The emergent lattice is indeed Kagome!
- Origin of flat bands is, therefore, geometric frustration

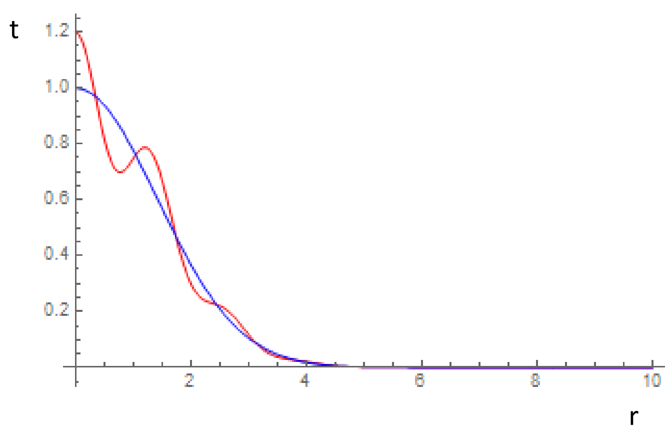


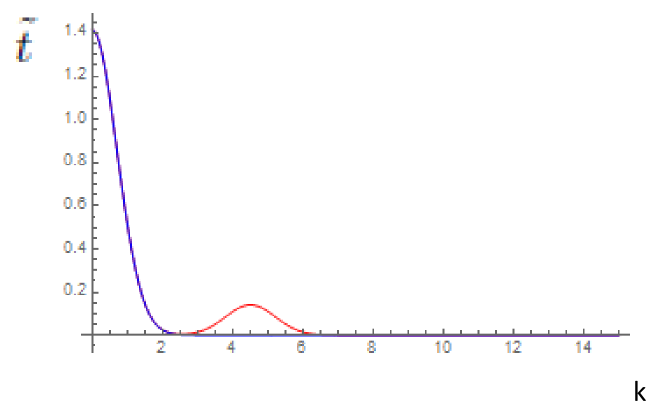


Numerical confirmation

- Localization length scales as v_F/□ □ 700 lattice constants
- In order to see localized modes, we need □ 10^6 atoms
- Numerical calculation is challenging!
- Trick: use artificial coupling between the layers such that □ is enhanced
- Recall: $\tilde{t}(\mathbf{K}+\mathbf{G}) = \mathcal{V}$

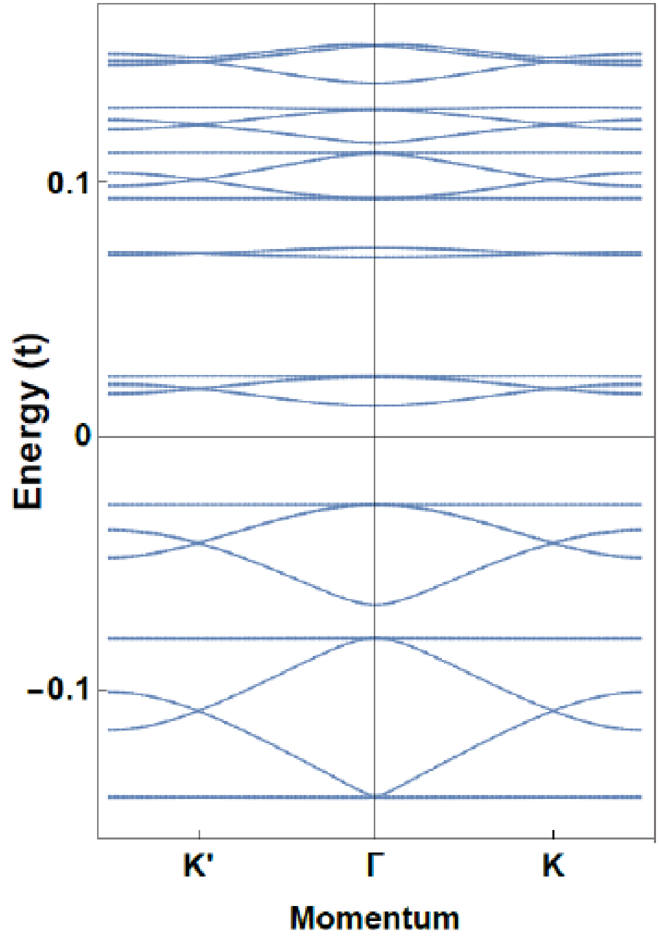
$$t_{\perp}^{art}(\mathbf{r}_i, \mathbf{r}_j) = t_1 J_0(G\delta r)\theta_{\mathrm{H}}(\delta r - l_0)$$

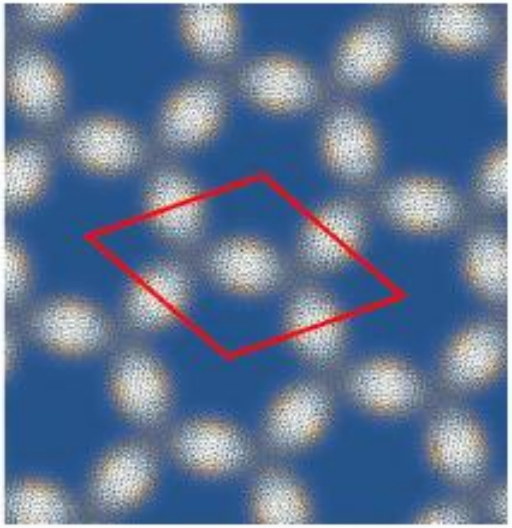




Numerical confirmation

- Tight-binding calculation near commensuration
- Choose □= 38.546□ near commensuration at 38.213□
- Lattice contains □ 10^4 atoms





H. K. Pal, S. Spitz, M. Kindermann,
Phys. Rev. Lett. 123, 186402 (2019)

Summary and Outlook

The gist

Twisted bilayer graphene

Small angles

Layers coupled—
flat bands

Large angles

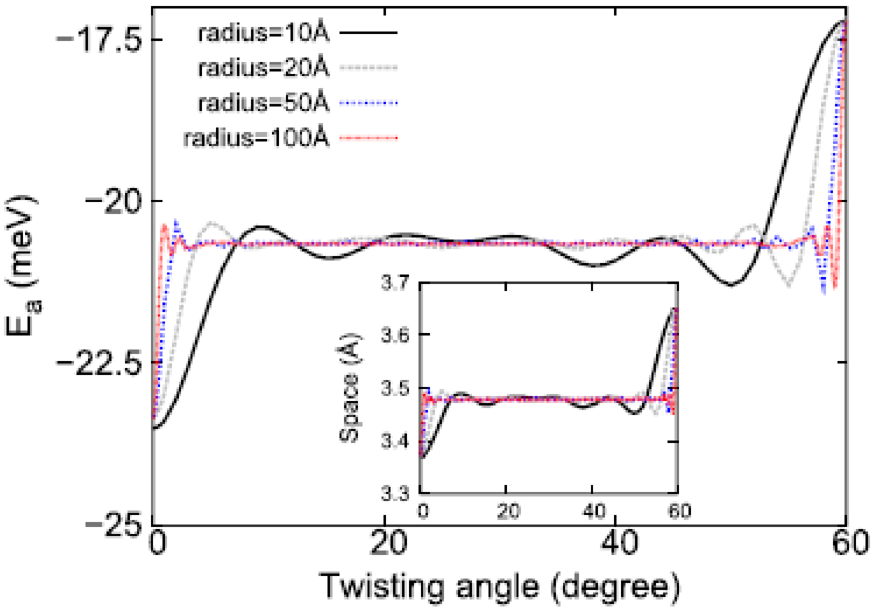
- Layers coupled—flat bands
- Different from small angles
  - Commensuration
  - Topology
  - ➢ Emergent frustration
- Look near 38.21°
- New correlation effects?

Thank you

Extras

Extras

- DFT calculation showing no preference for any particular angle



JOURNAL OF APPLIED PHYSICS 113, 194304 (2013)

Small angle vs large angle: comparison

- Flat bands are thus present at both large and small angles.
- But the underlying physics is very different in the two cases

Large angle

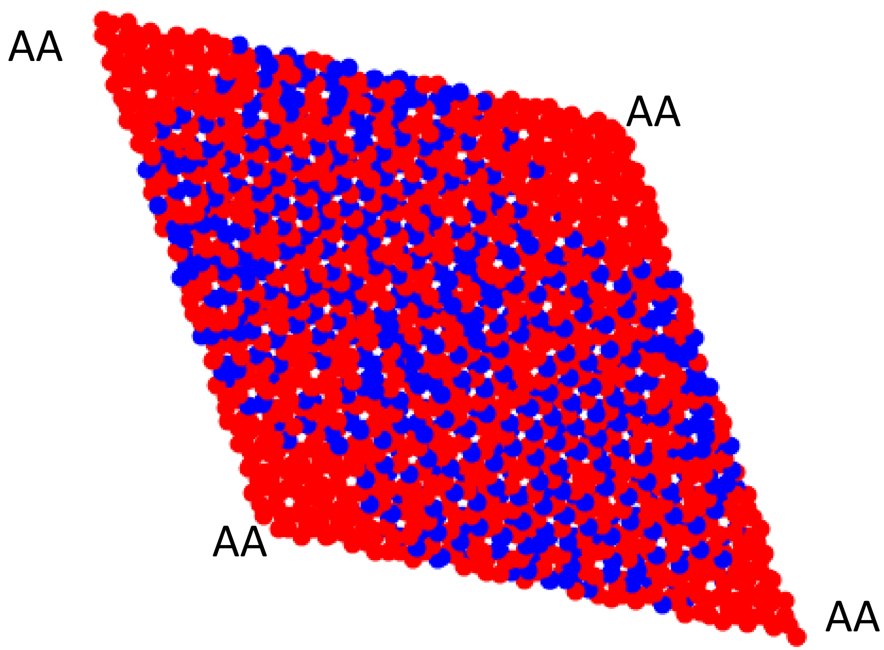
- Flat band persistent at non-perturbative regime
- Arises due to geometric frustration
- Electrons localized along AB-BA directions. AA regions gapped

Small angle

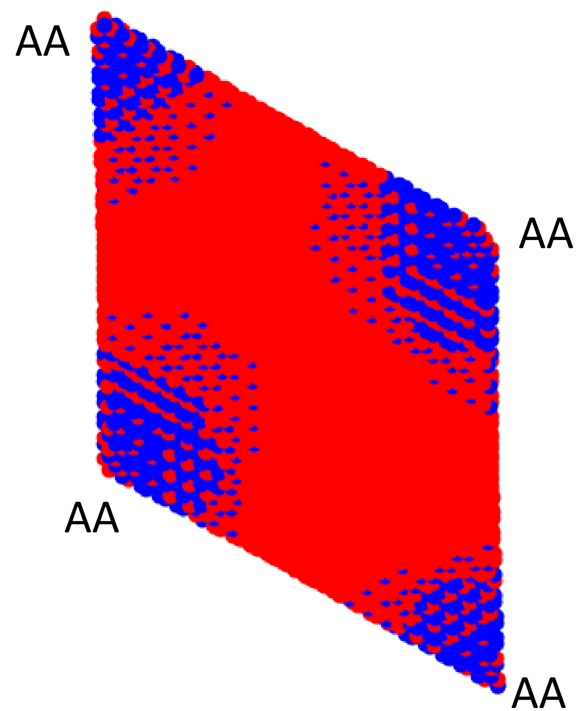
- Recurring flat bands at magic angles
- (?) Probably, particle-in-a- box-like confinement
- Electrons localized in AA regions gapped

Small angle vs large angle: localization

- Localization patterns at large and small angles are complementary



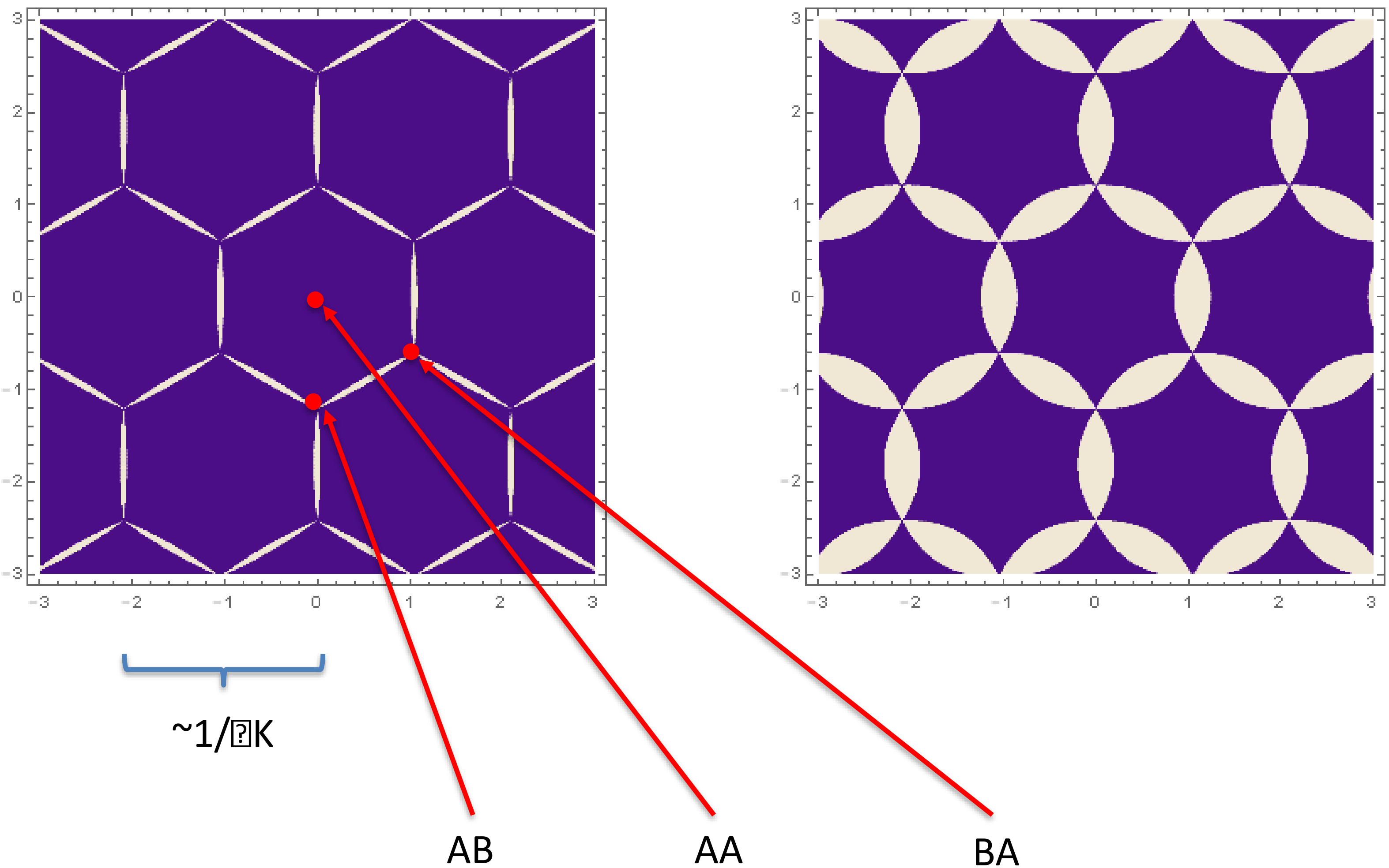
Near 38.2°



Near 0°

System at large angles: local gaps

Real space (Non-perturbative limit: □/v_F□K >> *1*)



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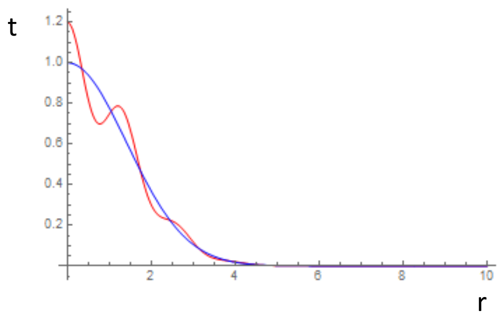
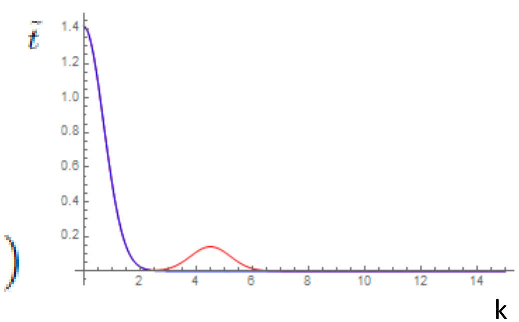


$$t_{\perp}^{art}(\mathbf{r}_i, \mathbf{r}_j) = V(\mathbf{r}_i - \mathbf{r}_j) + \eta g(\mathbf{r}_i - \mathbf{r}_j)$$



$$V(\mathbf{r}_i, \mathbf{r}_j) = t_0 e^{-(|\mathbf{r}_i - \mathbf{r}_j|/l_0)^2}$$

$$g(\mathbf{r}_i - \mathbf{r}_j) = t_1 e^{-(|\mathbf{r}_i - \mathbf{r}_j|/l_1)^2} \cos(|\mathbf{K}+\mathbf{G}||\mathbf{r}_i - \mathbf{r}_j|)$$

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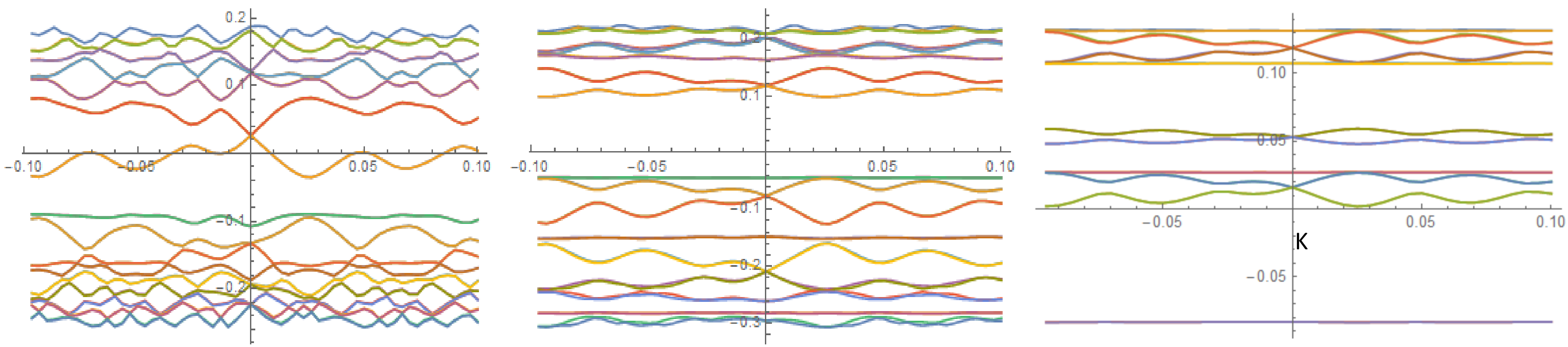

⍰ increasing