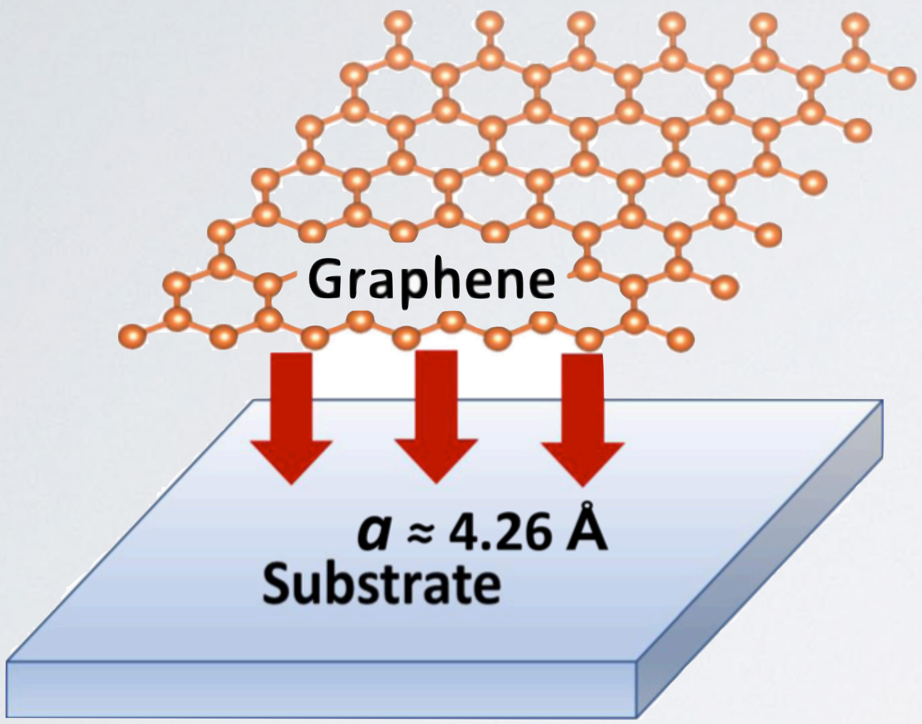
The realization of Moiré flat bands in monolayer graphene and the generalized non-Hermitian 2D Nielsen-Ninomiya theorem



The Main Building in RIKEN Wako Campus

Ching-Kai Chiu
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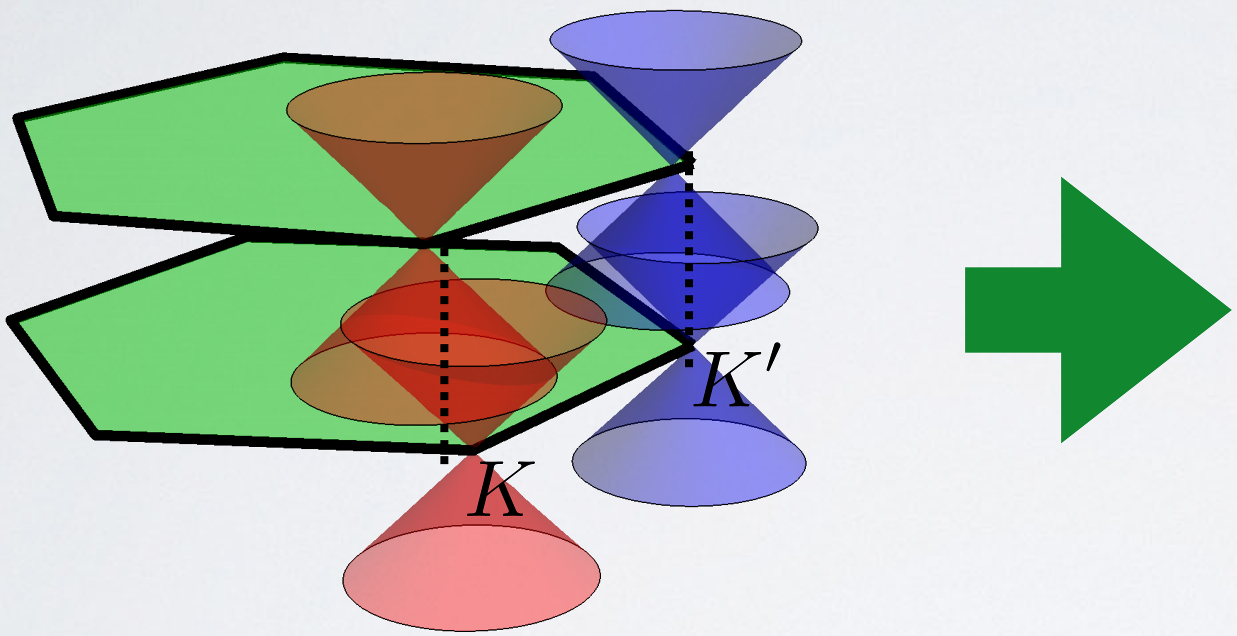
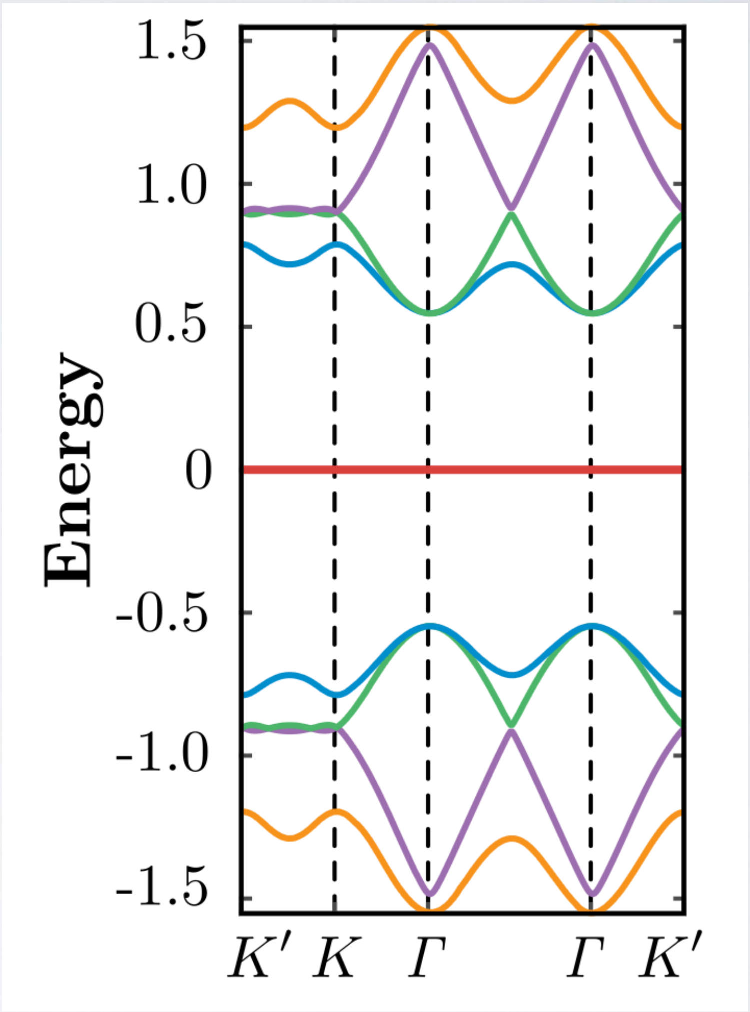
Two Questions related to twisted bilayer graphene

Flat bands stems from the coupling of two Dirac cones in different graphene layers





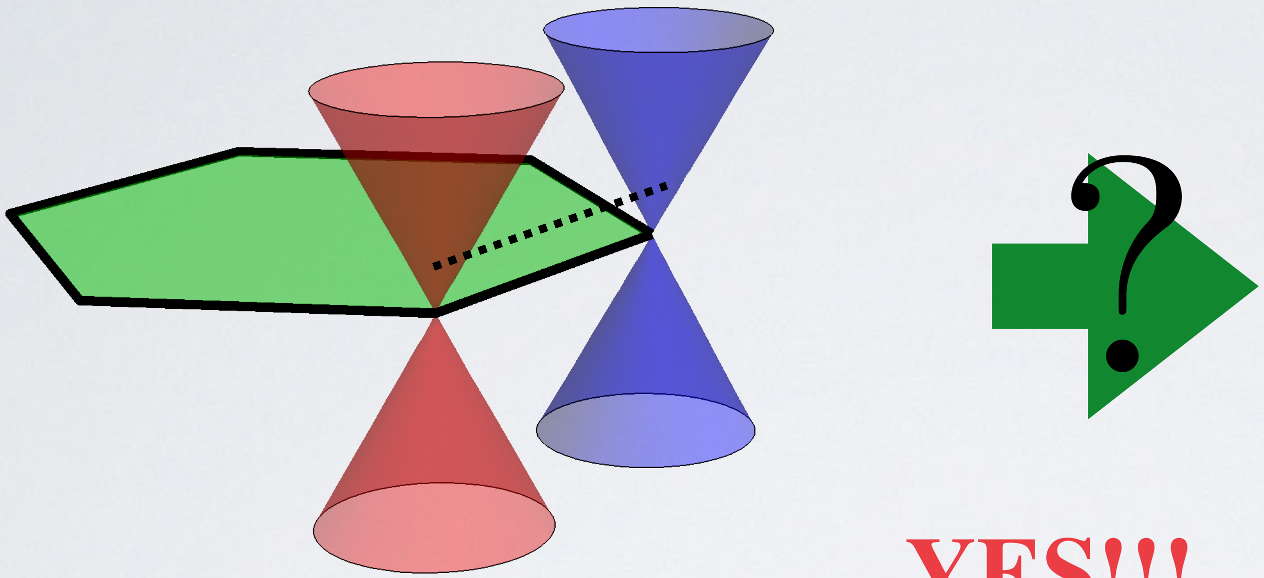
A. Vishwanath et al. PRL 122, 106405 (2019)

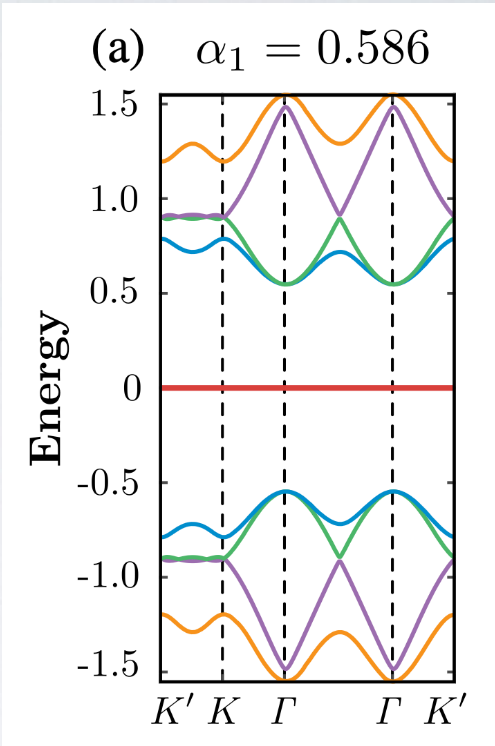
Y. Cao et al. Nature 556, 43–50 (2018)

The Dirac cones at K' and K form two identical Moiré spectra.

Question 1:

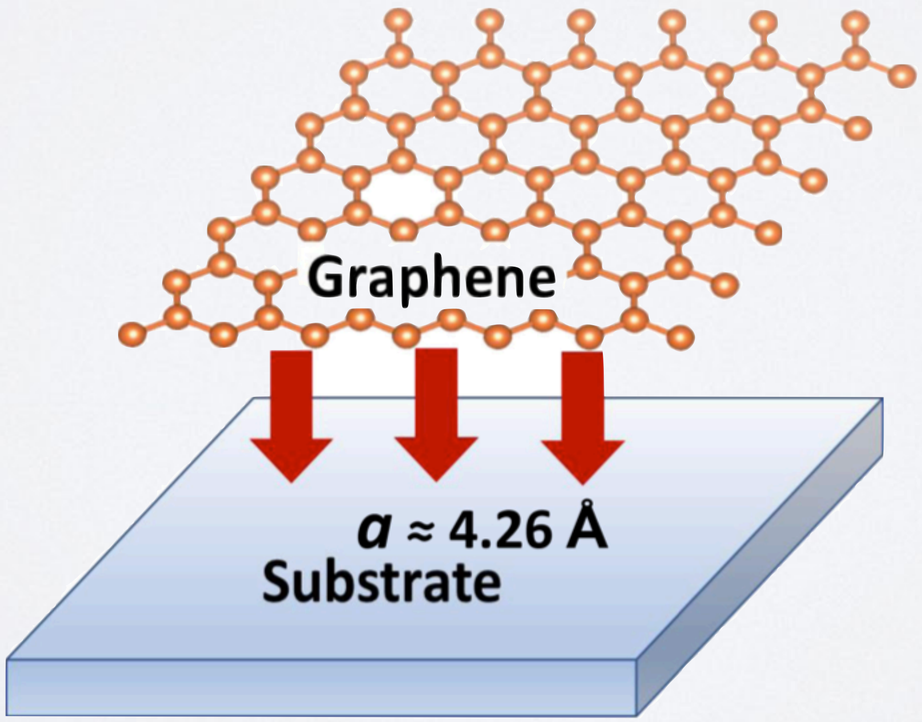
Can the two Dirac cones in monolayer graphene form flat bands?





YES!!!

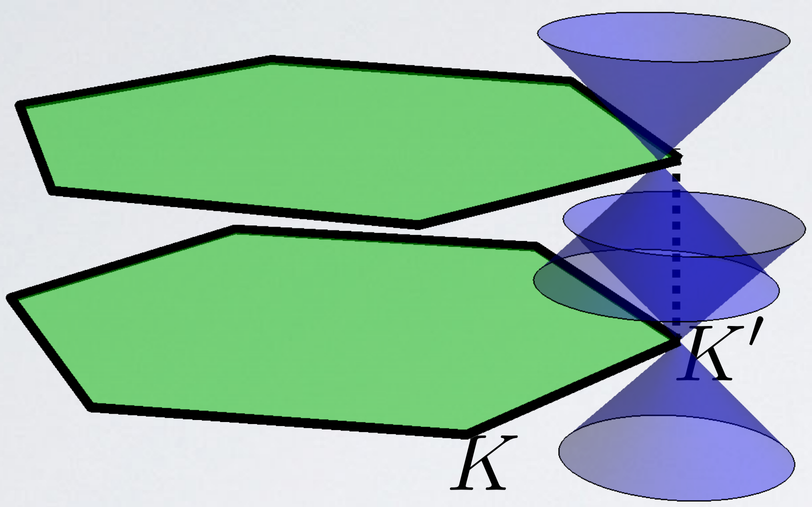
Graphene on periodic potential induced by substrate



Main problem

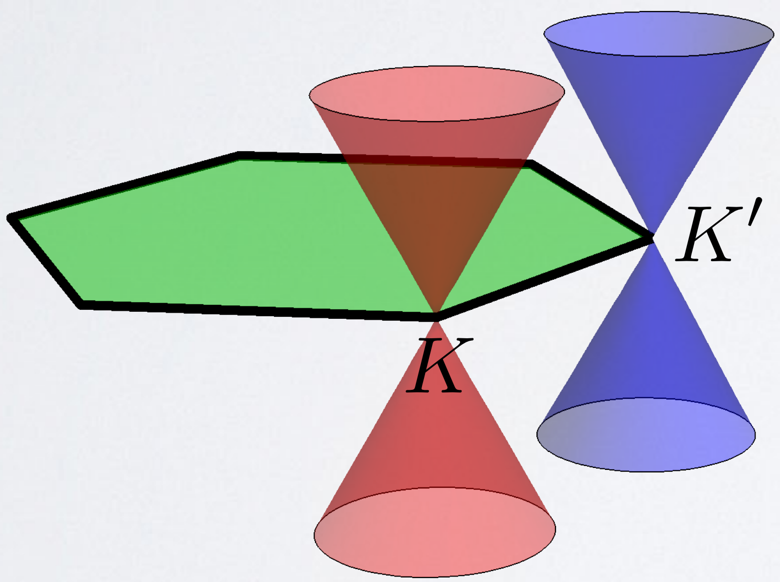
Space-time inversion symmetry or chiral symmetry quantize winding number ν

Koshino's lecture No. 1



$$v_F \Delta\mathbf{k}\cdot\boldsymbol{\sigma} = v_F(\Delta k_x \sigma_x + \Delta k_y \sigma_y) \qquad \nu = +1$$

$$v_F \Delta\mathbf{k}\cdot\boldsymbol{\sigma} = v_F(\Delta k_x \sigma_x + \Delta k_y \sigma_y) \qquad \nu = +1$$



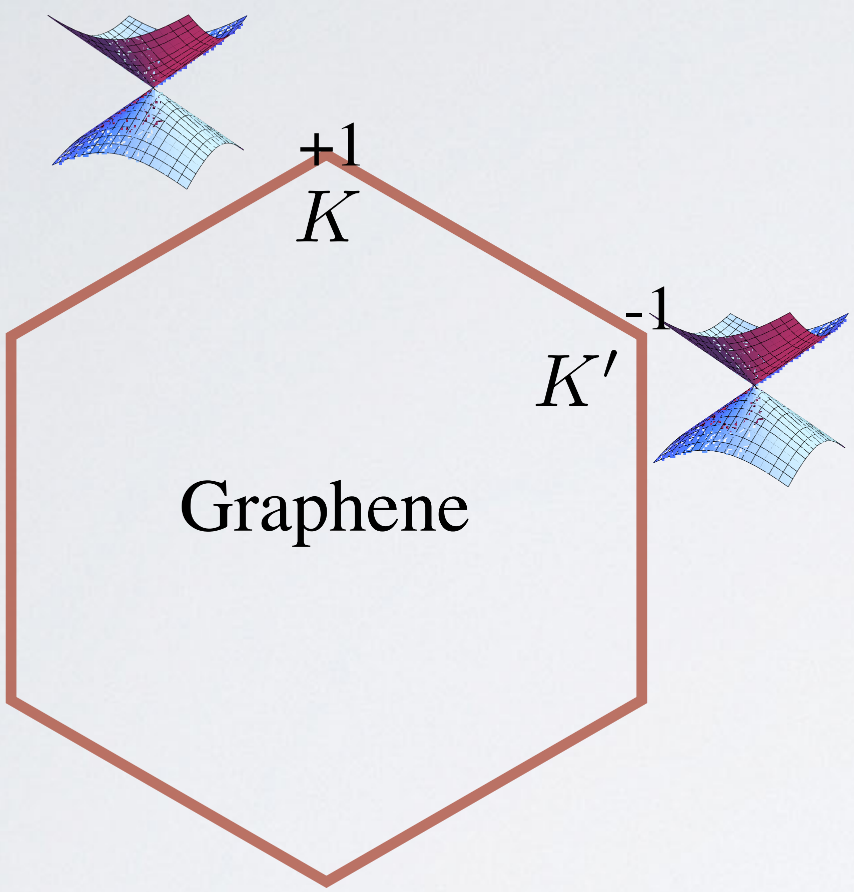
$$v_F \Delta\mathbf{k}\cdot\boldsymbol{\sigma} = v_F(\Delta k_x \sigma_x + \Delta k_y \sigma_y) \qquad \nu = +1$$

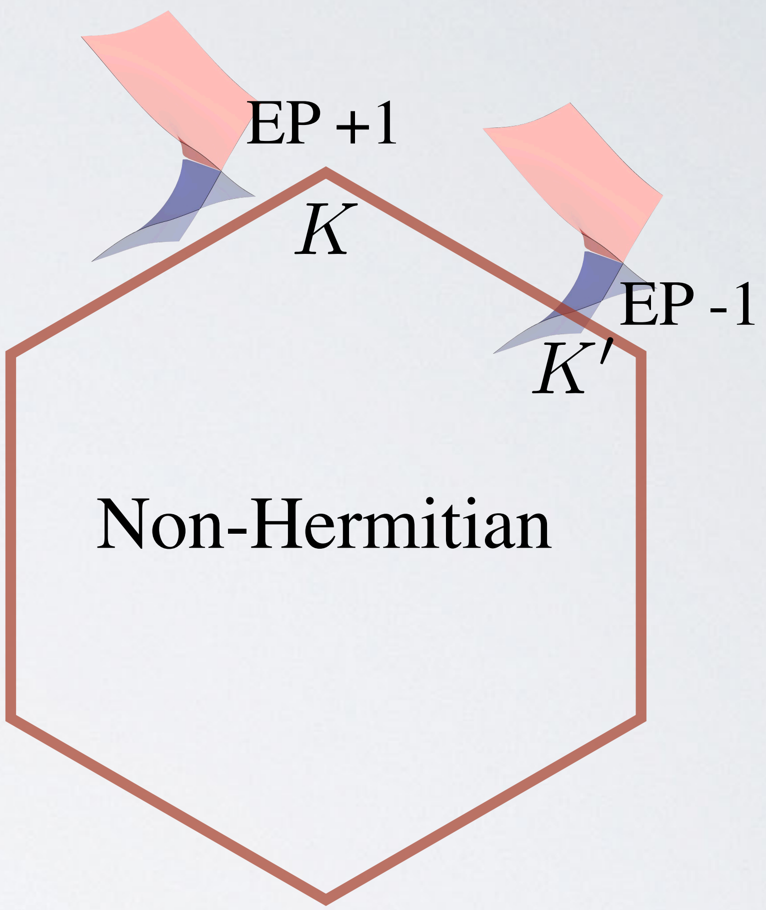
$$v_F \Delta\mathbf{k}\cdot\boldsymbol{\sigma}^* = v_F(\Delta k_x \sigma_x - \Delta k_y \sigma_y) \qquad \nu = -1$$

The different orientations can lead to flat bands?

Question 2:

In non-Hermitian physics, can two exceptional points be located at K or K' so that there is twisted physics exceptional points?





Focus: The generalized non-Hermitian 2D Nielsen-Ninomiya theorem

No. There are some constraints.

Outline

1. Monolayer graphene -> flat bands

   I. Review of twisted bilayer graphene continuum model

   II. Experiment: Monolayer graphene on SiC substrate

   III. The low-energy physics of monolayer graphene on substrate

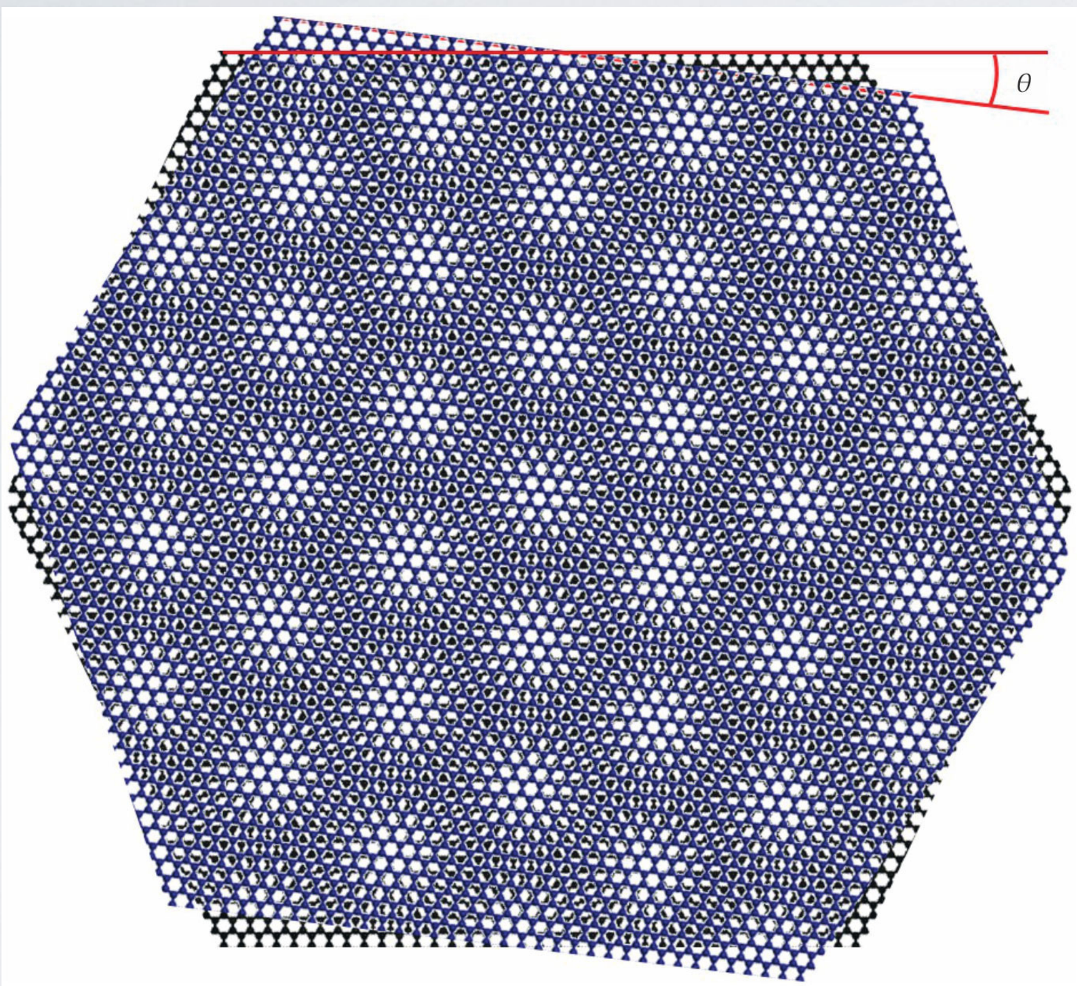
2. Exceptional points in the hexagonal Brillouin zone

   I. The comparison of the 2D Nielsen-Ninomiya theorem between Hermitian and non-Hermitian systems

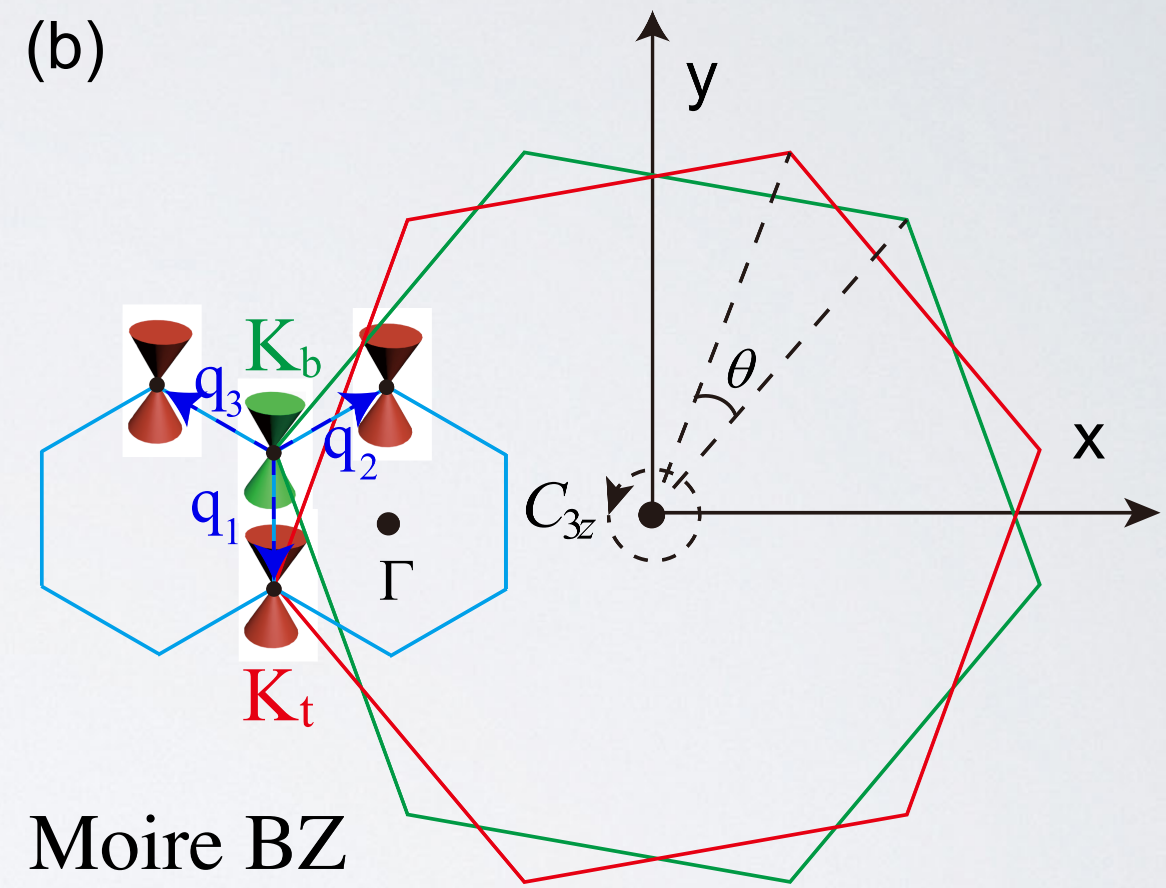
   II. The generalized Non-Hermitian Nielsen-Ninomiya theorem for the 17 wallpaper groups

Review of twisted bilayer graphene

The bilayer of the small twisted angle forms the Moire pattern in the real space



Courtesy of ICFO/Xiaobo Lu



$$|\boldsymbol{q}_i| = 2k_D \sin(\theta/2)$$

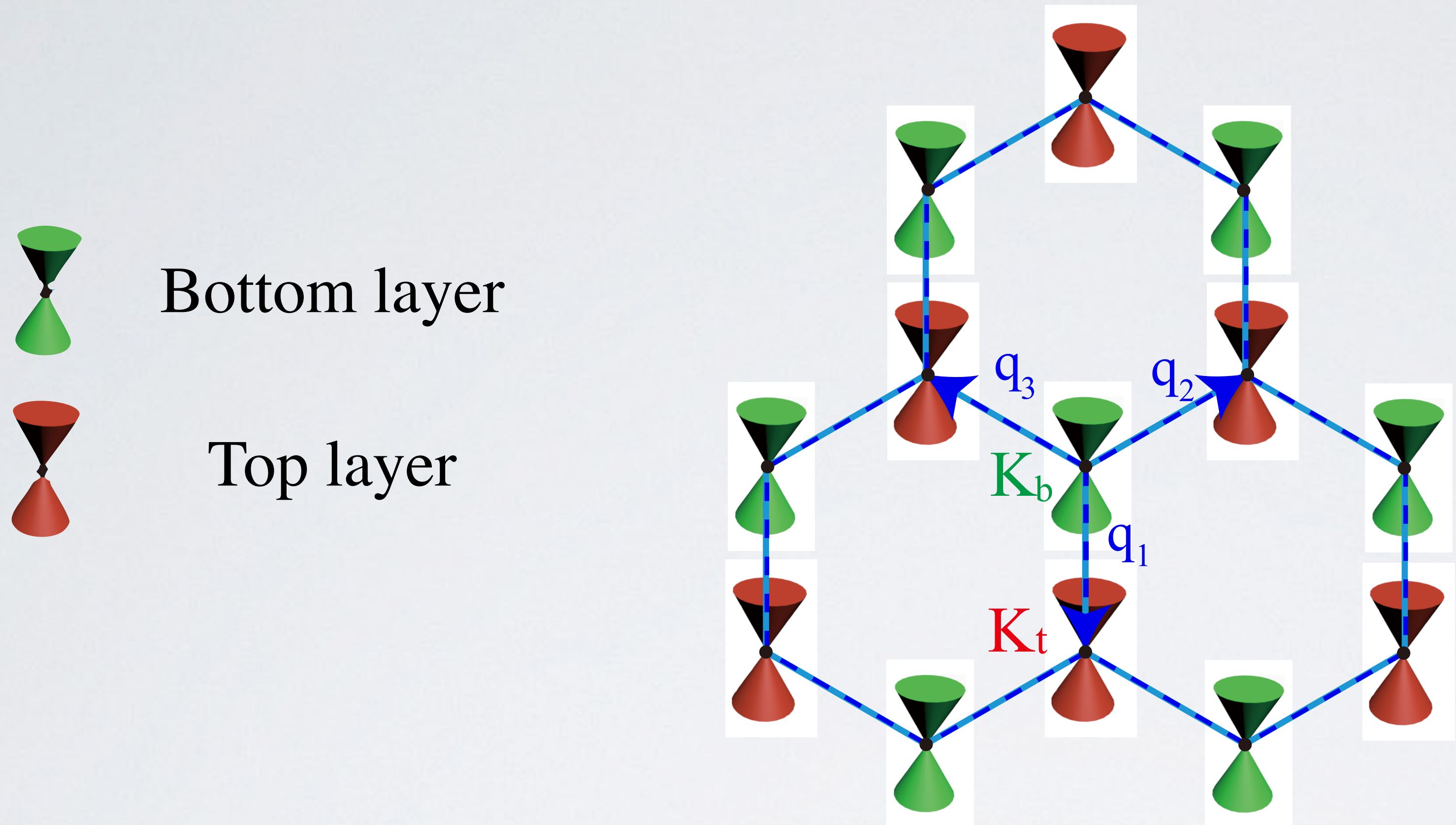
R. Bistritzer and A. H. MacDonald, Proc. Natl. Acad. Sci. 108, 12233 (2011).

The interlayer coupling, which is complicated, can be simplified in the momentum space — Continuum Model

Koshino's lectures

Continuum Model

The low-energy physics is described by momentum space hopping between the two Dirac cones in the different layers



1st nearest neighbor momentum hopping $\boldsymbol{q}_1, \boldsymbol{q}_2, \boldsymbol{q}_3$

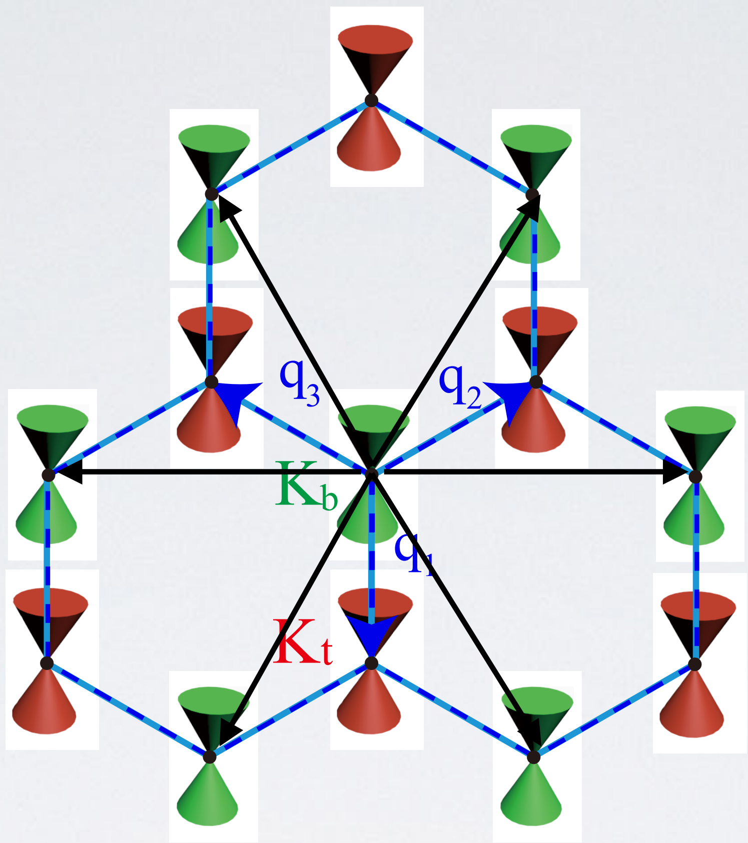
$$H_{\mathrm{TBG}}(\Delta\boldsymbol{k}) = \begin{pmatrix} H_d(\Delta\boldsymbol{k}) & wT_0 & wT_{-\psi} & wT_{\psi} \\ wT_0 & H_d(\Delta\boldsymbol{k}+\boldsymbol{q}_1) & 0 & 0 \\ wT_{-\psi} & 0 & H_d(\Delta\boldsymbol{k}+\boldsymbol{q}_2) & 0 \\ wT_{\psi} & 0 & 0 & H_d(\Delta\boldsymbol{k}+\boldsymbol{q}_3) \end{pmatrix}$$

$$H_d(\Delta\mathbf{k}) = v_F(\Delta k_x \sigma_x + \Delta k_y \sigma_y)$$

Interlayer coupling $T_\phi = \cos\phi\sigma_x + \sin\phi\sigma_y, \text{ where } \psi = 2\pi/3$ AB basis hopping

σ_0 AA basis hopping is suppressed

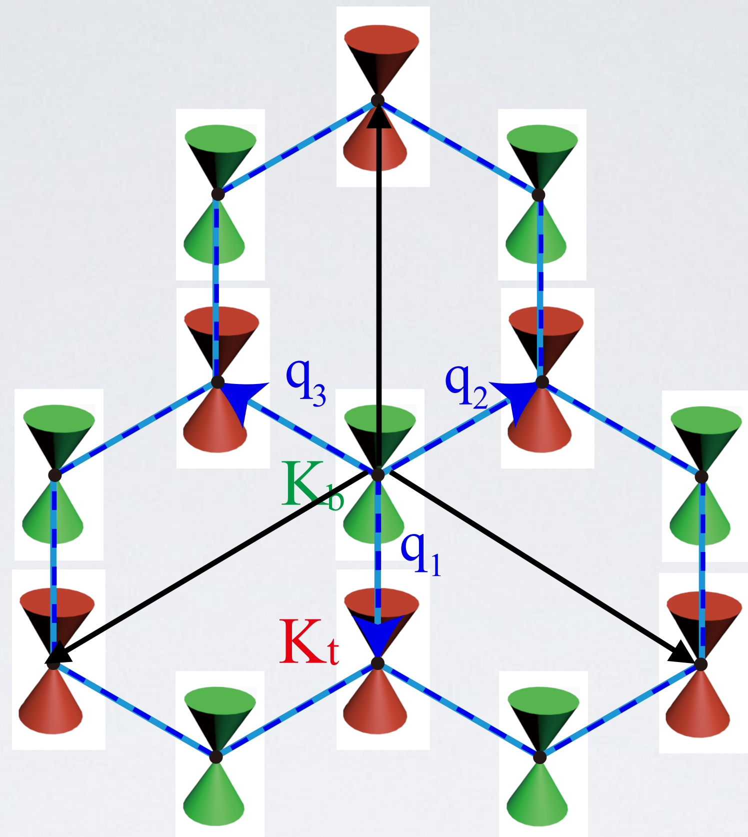
Stephen Carr, Shiang Fang, Ziyan Zhu, Efthimios Kaxiras, Phys. Rev. Research 1, 013001 (2019)



2nd nearest neighbor momentum hopping $\pm(\boldsymbol{q}_1 - \boldsymbol{q}_2),\ \pm(\boldsymbol{q}_2 - \boldsymbol{q}_3),\ \pm(\boldsymbol{q}_3 - \boldsymbol{q}_1)$

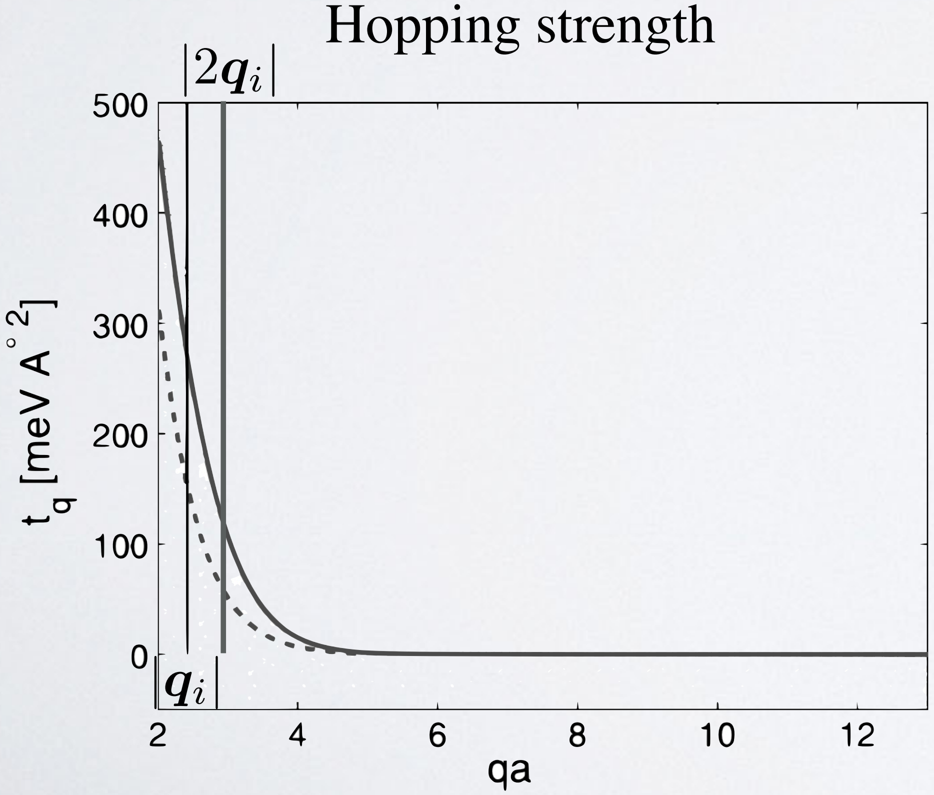
Forbidden:

Same Dirac cone in the same layer



3rd nearest neighbor momentum hopping $-2\boldsymbol{q}_1, \ -2\boldsymbol{q}_2, \ -2\boldsymbol{q}_3$

Hopping strength



Momentum distance

Hopping strength decreases as momentum distance increases

Approximation:

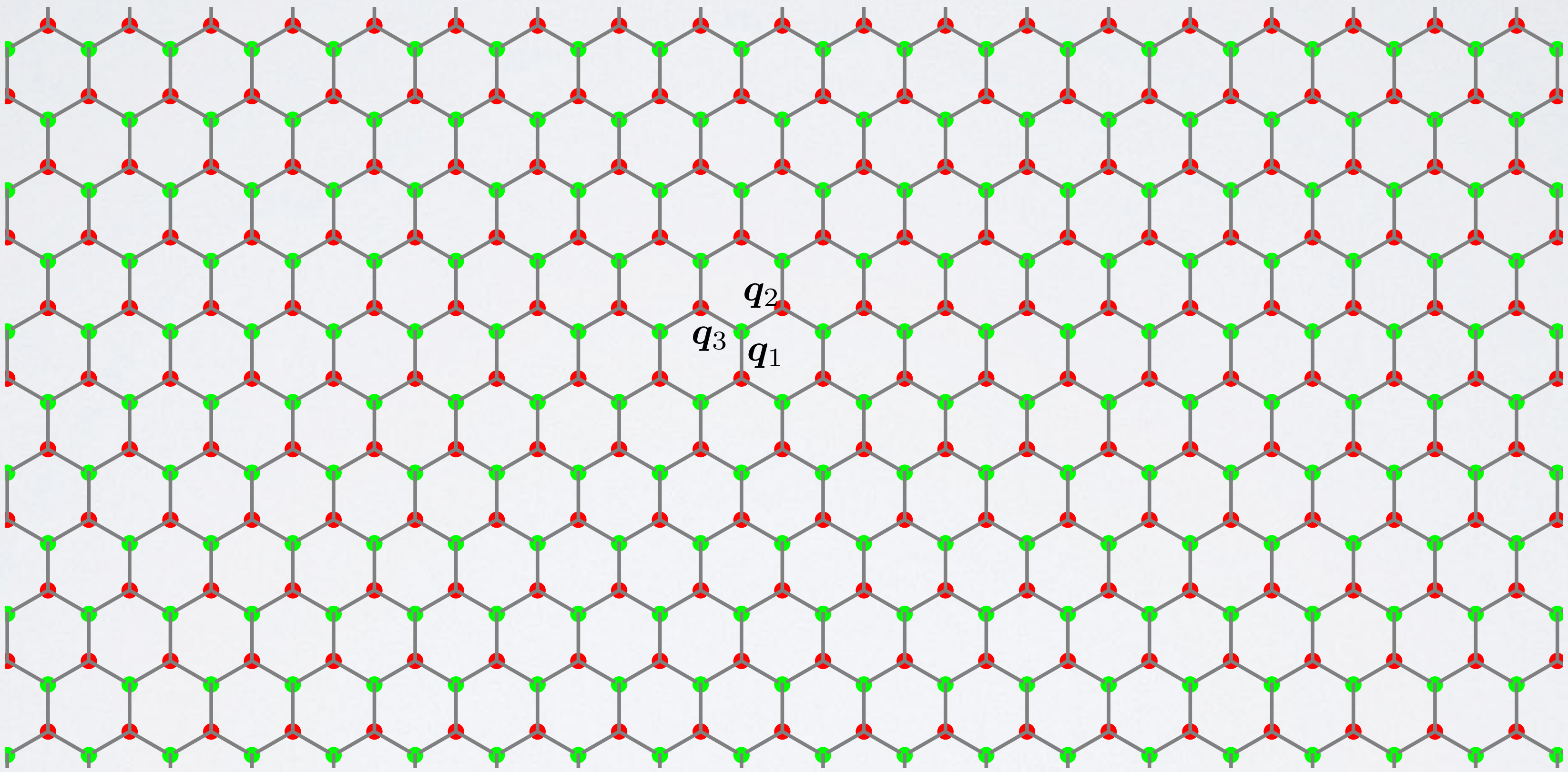
We keep the nearest momentum hopping and neglect the remaining hopping of the long distance.

R. Bistritzer and A. H. MacDonald, Proc. Natl. Acad. Sci. 108, 12233 (2011).

$$H_{\mathrm{TBG}}(\Delta \boldsymbol{k}) = \begin{pmatrix} H_d(\Delta \boldsymbol{k}) & wT_0 & wT_{-\psi} & wT_{\psi} \\ wT_0 & H_d(\Delta \boldsymbol{k} + \boldsymbol{q}_1) & 0 & 0 \\ wT_{-\psi} & 0 & H_d(\Delta \boldsymbol{k} + \boldsymbol{q}_2) & 0 \\ wT_{\psi} & 0 & 0 & H_d(\Delta \boldsymbol{k} + \boldsymbol{q}_3) \end{pmatrix}$$

$$T_\phi = \cos\phi\sigma_x + \sin\phi\sigma_y, \text{ where } \psi = 2\pi/3$$

$$H_d(\Delta \mathbf{k}) = v_F(\Delta k_x \sigma_x + \Delta k_y \sigma_y)$$



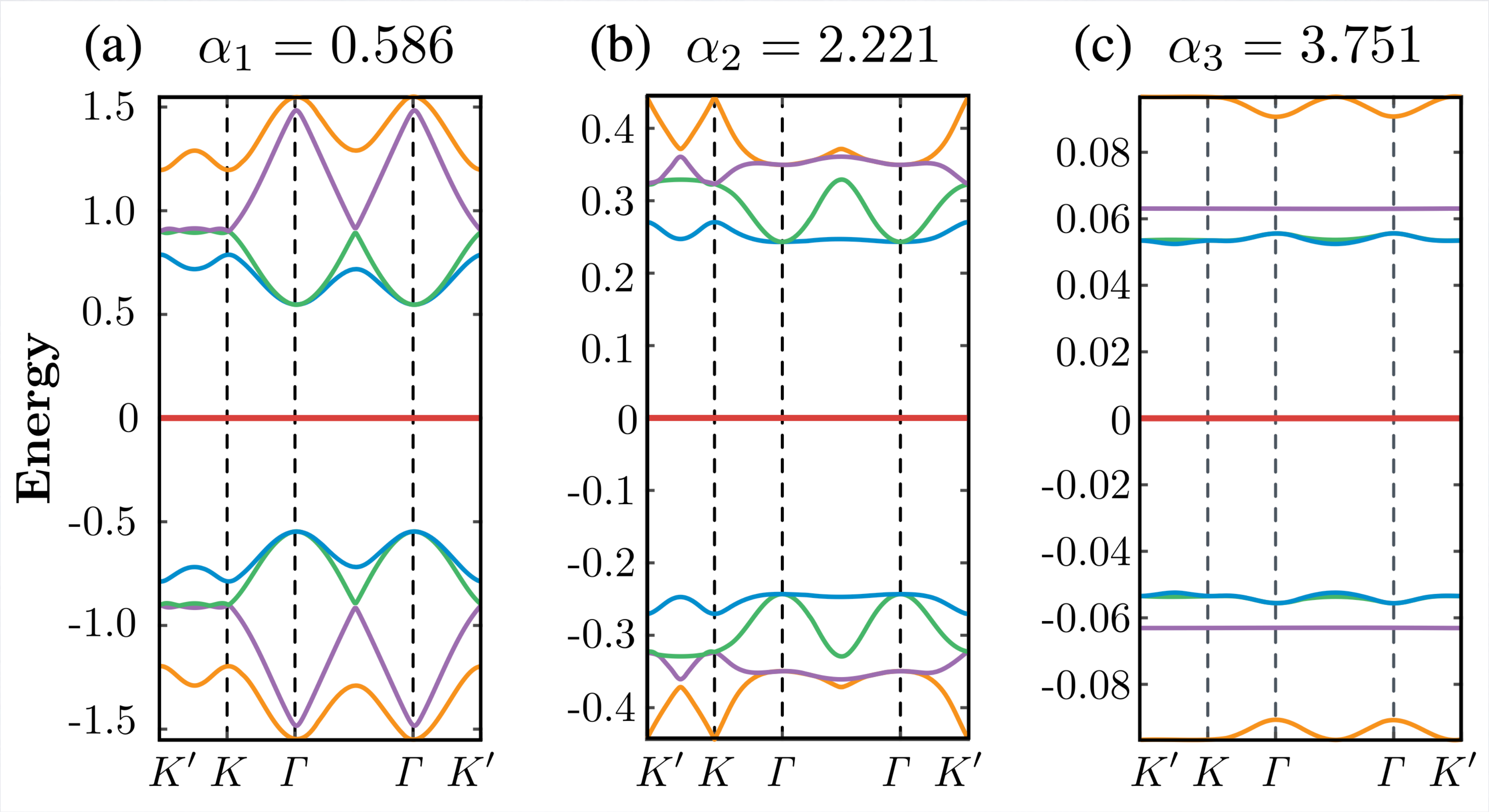
Extend to the momentum lattice and compute the energy spectrum

Parameter normalization and flat bands

$$H_{\mathrm{TBG}}(\Delta \boldsymbol{k}) = \begin{pmatrix} H_d(\Delta \boldsymbol{k}) & wT_0 & wT_{-\psi} & wT_{\psi} \\ wT_0 & H_d(\Delta \boldsymbol{k} + \boldsymbol{q}_1) & 0 & 0 \\ wT_{-\psi} & 0 & H_d(\Delta \boldsymbol{k} + \boldsymbol{q}_2) & 0 \\ wT_{\psi} & 0 & 0 & H_d(\Delta \boldsymbol{k} + \boldsymbol{q}_3) \end{pmatrix}$$

$$H_d(\Delta \mathbf{k}) = v_F(\Delta k_x \sigma_x + \Delta k_y \sigma_y)$$

$$\alpha \equiv w / v_F |\boldsymbol{q}_1|$$



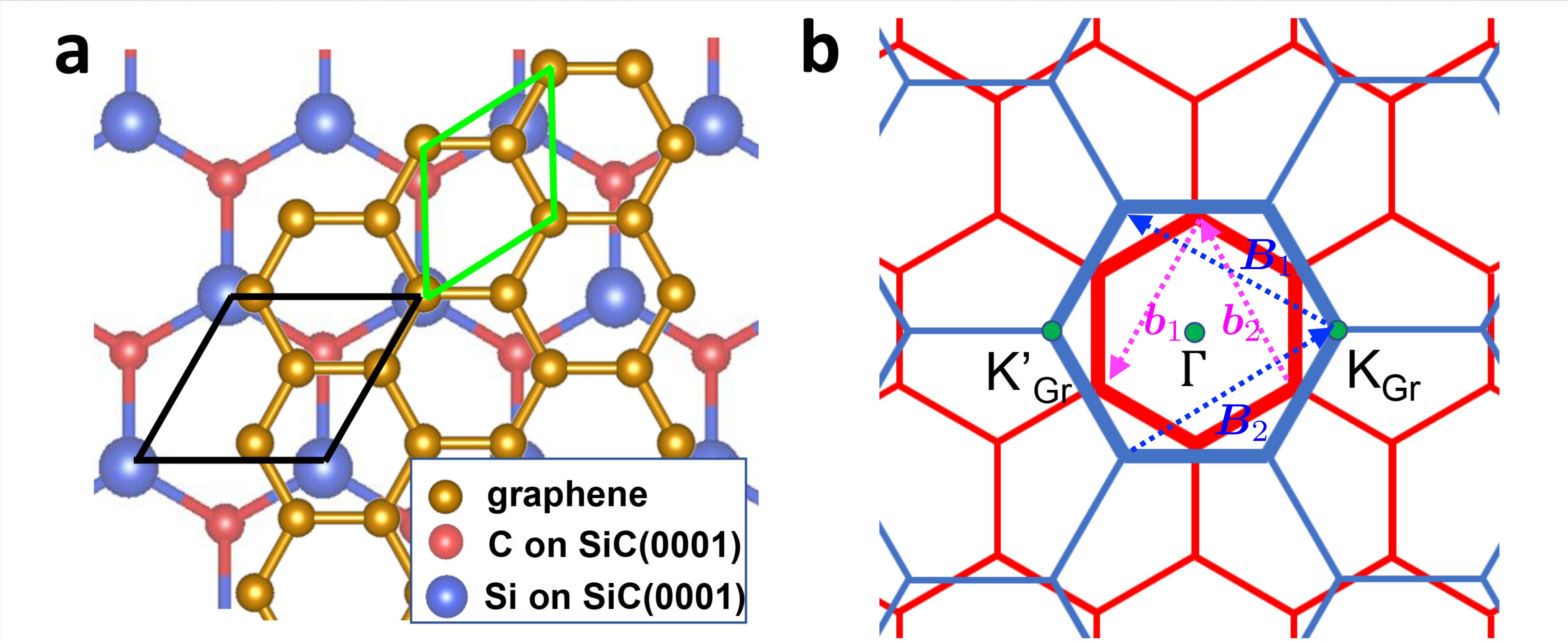
The two-fold degenerate bands are absolutely flat due to the holomorphic wave functions.

PHYSICAL REVIEW LETTERS 122, 106405 (2019)

Outline

1. Review of twisted bilayer graphene continuum model
2. **Experiment: Monolayer graphene on SiC substrate**
3. The low-energy physics of monolayer graphene on substrate

Experiment: Monolayer graphene on SiC substrate



The angle between the two sets of the reciprocal lattice vectors (Graphene: $\boldsymbol{B}_1, \boldsymbol{B}_2$, SiC: $\boldsymbol{b}_1, \boldsymbol{b}_2$) is $\pi/2$.

$$\text{Graphene lattice constant } a_{\mathrm{Gr}} = 2.46\mathring{A}$$

$$\text{SiC constant } a_{\mathrm{SiC}} = 3.07\mathring{A}$$

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University of Missouri

Congcong Le
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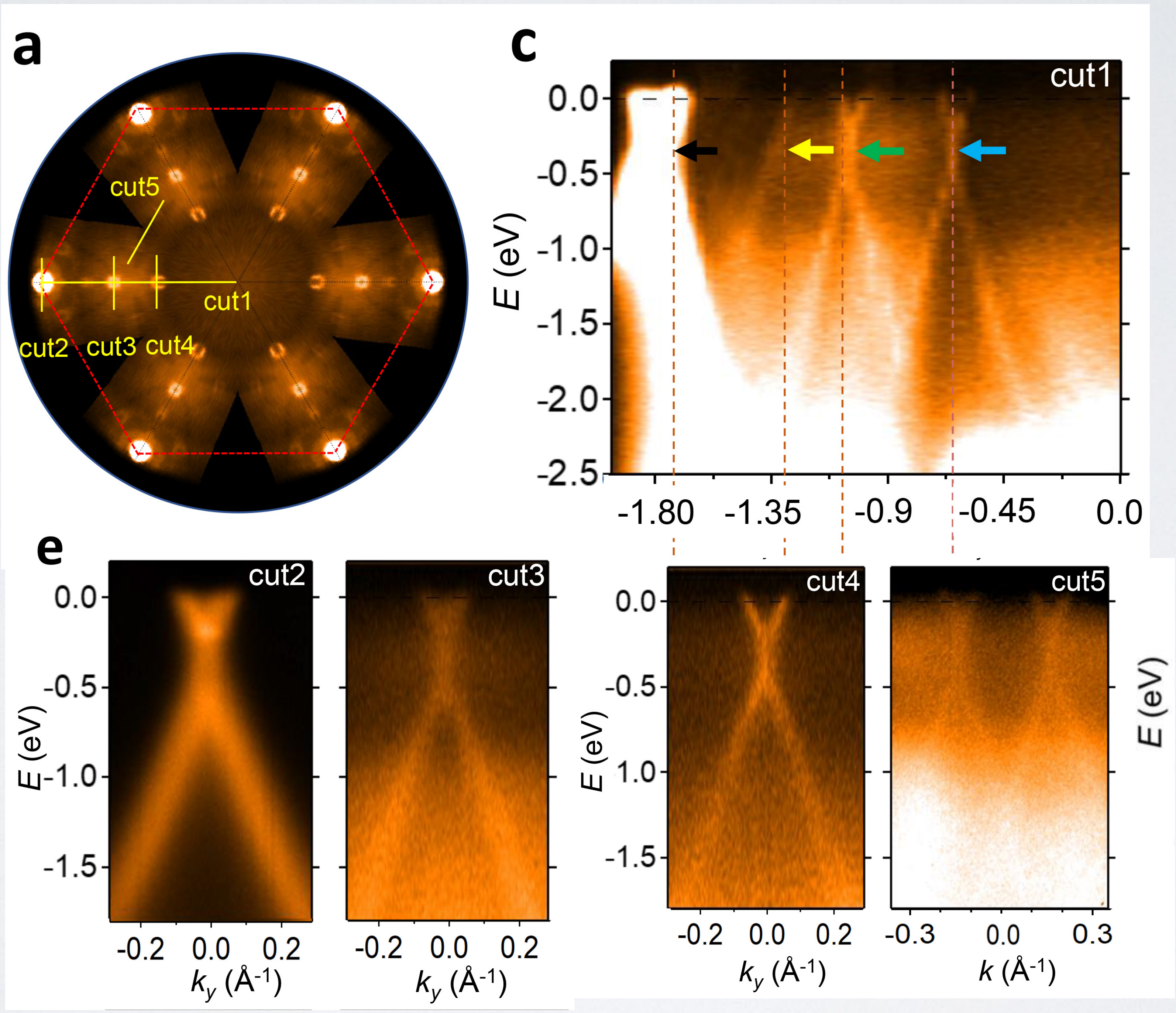
Advanced Materials 2200625 (2022)

Qiangsheng Lu, Congcong Le, Xiaoqian Zhang, Jacob Cook, Xiaoqing He, Mohammad Zarenia, Mitchel Vaninger, Paul F. Miceli, David J. Singh, Chang Liu, Hailang Qin, Tai-Chang Chiang, Ching-Kai Chiu,* Giovanni Vignale,* and Guang Bian*

ARPES measurement

Dirac Cone Cloning

Graphene Brillouin Zone



Advanced Materials 2200625 (2022)

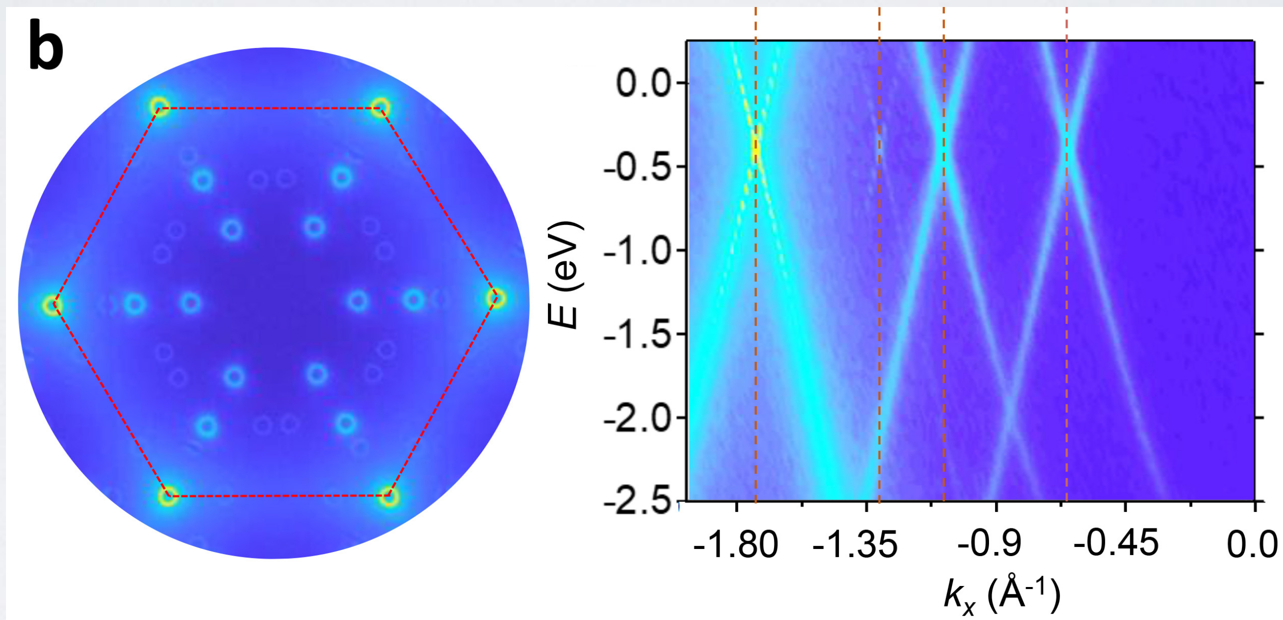
Theoretical Understanding

Simple Graphene tight-binding model (nearest neighbor hopping) with periodic potential

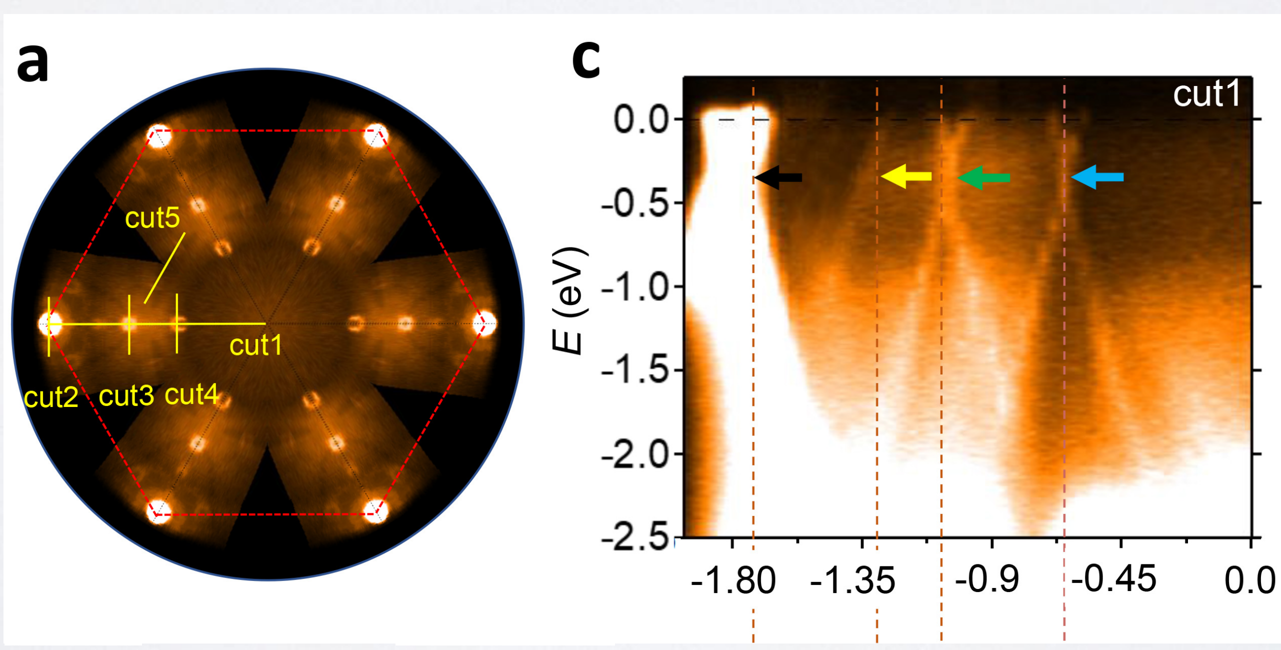
$$V(\boldsymbol{r}) = w\big(\cos(\boldsymbol{b}_1\cdot\boldsymbol{r}) + \cos(\boldsymbol{b}_2\cdot\boldsymbol{r}) + \cos(-(\boldsymbol{b}_1+\boldsymbol{b}_2)\cdot\boldsymbol{r})\big)$$

SiC: $\boldsymbol{b}_1, \boldsymbol{b}_2$

Spectra from simulation



Experiment



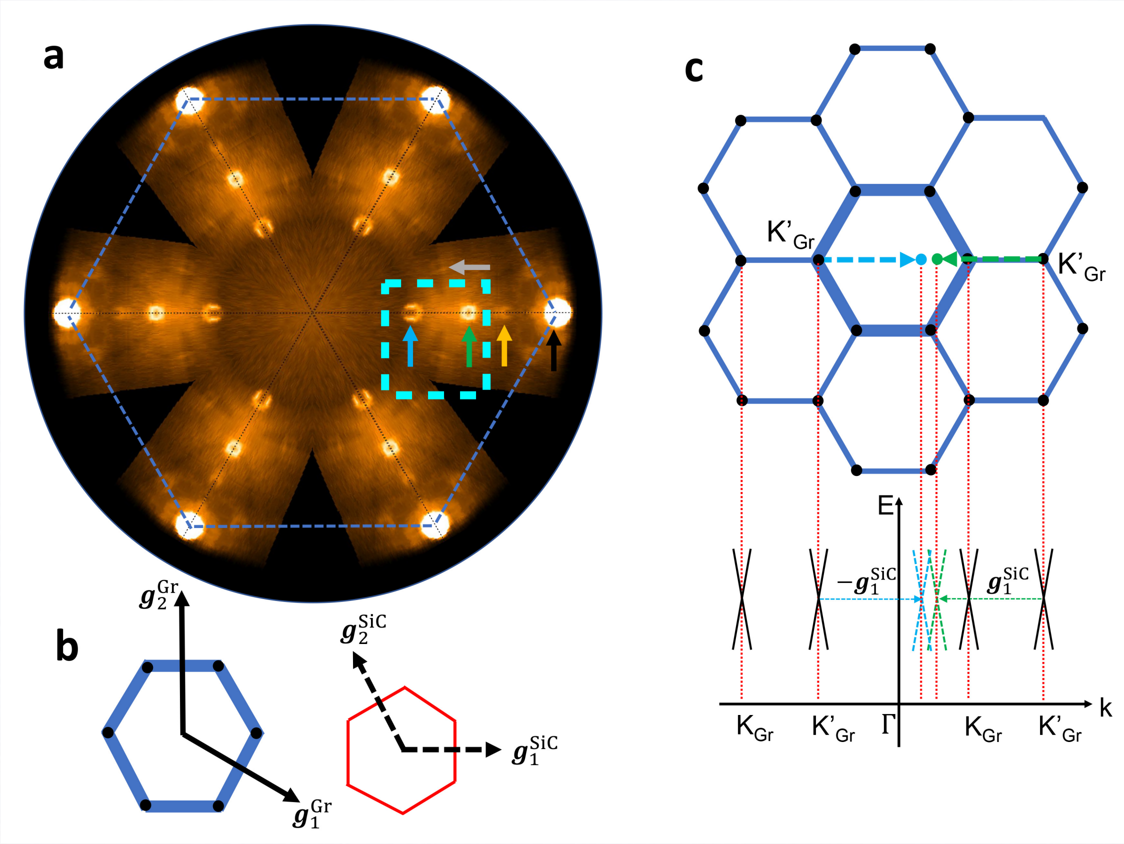
Perturbation theory

$$V(\boldsymbol{r}) = w\big(\cos(\boldsymbol{b}_1 \cdot \boldsymbol{r}) + \cos(\boldsymbol{b}_2 \cdot \boldsymbol{r}) + \cos(-(\boldsymbol{b}_1 + \boldsymbol{b}_2) \cdot \boldsymbol{r})\big)$$

$$|\Psi_{\mathbf{k}}\rangle = |\Psi^0_{\mathbf{k}}\rangle + \sum_{\boldsymbol{p}\neq\mathbf{k}} |\Psi^0_{\boldsymbol{p}}\rangle \frac{\langle\Psi^0_{\boldsymbol{p}}|V|\Psi^0_{\boldsymbol{k}}\rangle}{E^0_{\mathbf{k}} - E^0_{\boldsymbol{p}}} + \sum_{\boldsymbol{p}\neq\mathbf{k},\boldsymbol{l}\neq\mathbf{k}} |\Psi^0_{\boldsymbol{p}}\rangle \frac{\langle\Psi^0_{\boldsymbol{p}}|V|\Psi^0_{\boldsymbol{l}}\rangle\langle\Psi^0_{\boldsymbol{l}}|V|\Psi^0_{\boldsymbol{k}}\rangle}{(E^0_{\mathbf{k}} - E^0_{\boldsymbol{p}})(E^0_{\mathbf{k}} - E^0_{\boldsymbol{l}})} + \cdots$$

1st order $\boldsymbol{p} = \mathbf{k} \pm \boldsymbol{b}_1,\ \mathbf{k} \pm \boldsymbol{b}_2,\ \mathbf{k} \pm (\boldsymbol{b}_1 + \boldsymbol{b}_2)$

First clones One reciprocal vector shift



Perturbation theory

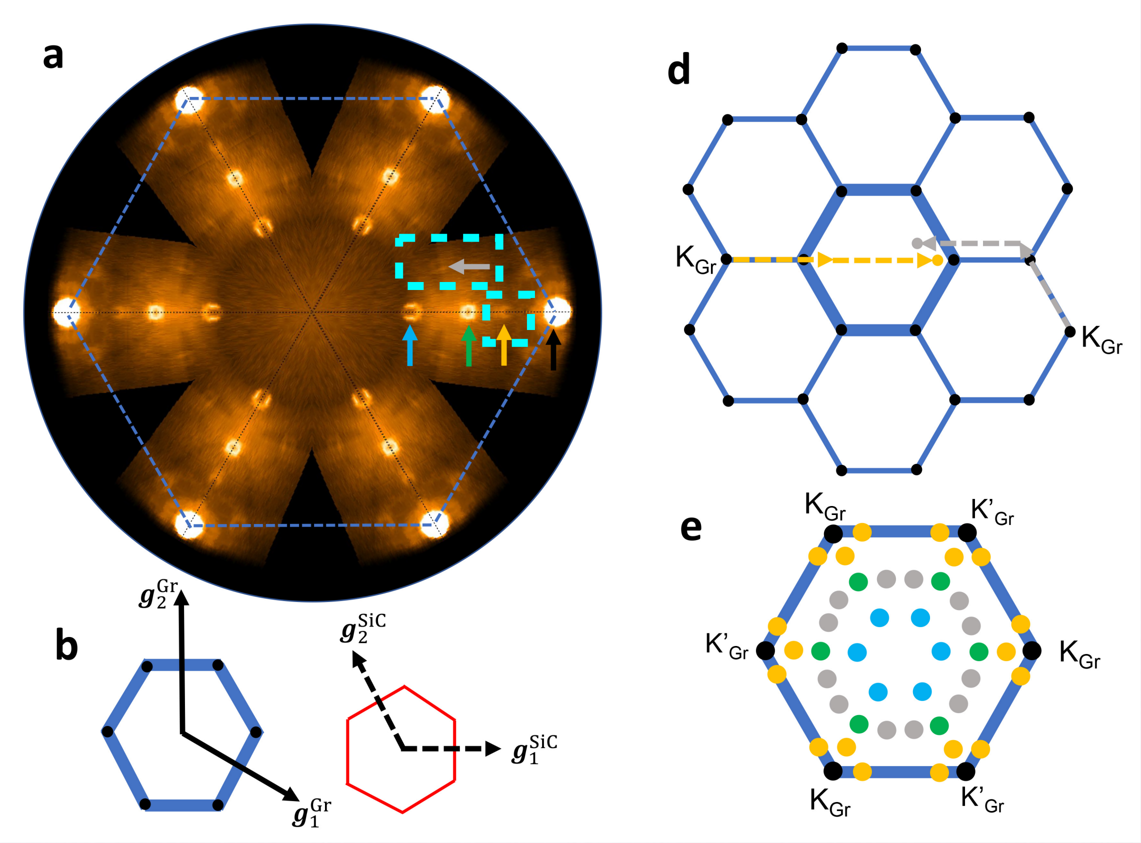
$$|\Psi_{\mathbf{k}}\rangle = |\Psi^0_{\mathbf{k}}\rangle + \sum_{\boldsymbol{p}\neq\mathbf{k}} |\Psi^0_{\boldsymbol{p}}\rangle \frac{\langle\Psi^0_{\boldsymbol{p}}|V|\Psi^0_{\boldsymbol{k}}\rangle}{E^0_{\mathbf{k}} - E^0_{\boldsymbol{p}}} + \sum_{\boldsymbol{p}\neq\mathbf{k},\boldsymbol{l}\neq\mathbf{k}} |\Psi^0_{\boldsymbol{p}}\rangle \frac{\langle\Psi^0_{\boldsymbol{p}}|V|\Psi^0_{\boldsymbol{l}}\rangle\langle\Psi^0_{\boldsymbol{l}}|V|\Psi^0_{\boldsymbol{k}}\rangle}{(E^0_{\mathbf{k}} - E^0_{\boldsymbol{p}})(E^0_{\mathbf{k}} - E^0_{\boldsymbol{l}})} + \cdots$$

2nd order

$$\boldsymbol{p} = \mathbf{k} \pm 2\boldsymbol{b}_1,\ \mathbf{k} \pm 2\boldsymbol{b}_2,\ \mathbf{k} \pm 2(\boldsymbol{b}_1 + \boldsymbol{b}_2),$$
$$\mathbf{k} \pm (\boldsymbol{b}_1 - \boldsymbol{b}_2),\ \mathbf{k} \pm (2\boldsymbol{b}_1 + \boldsymbol{b}_2),\ \mathbf{k} \pm (\boldsymbol{b}_1 + 2\boldsymbol{b}_2)$$

Second clone

Two reciprocal vector shift



Periodic potential + Graphene model can faithfully capture the low-energy physics of graphene on the substrate

Tight-binding Model

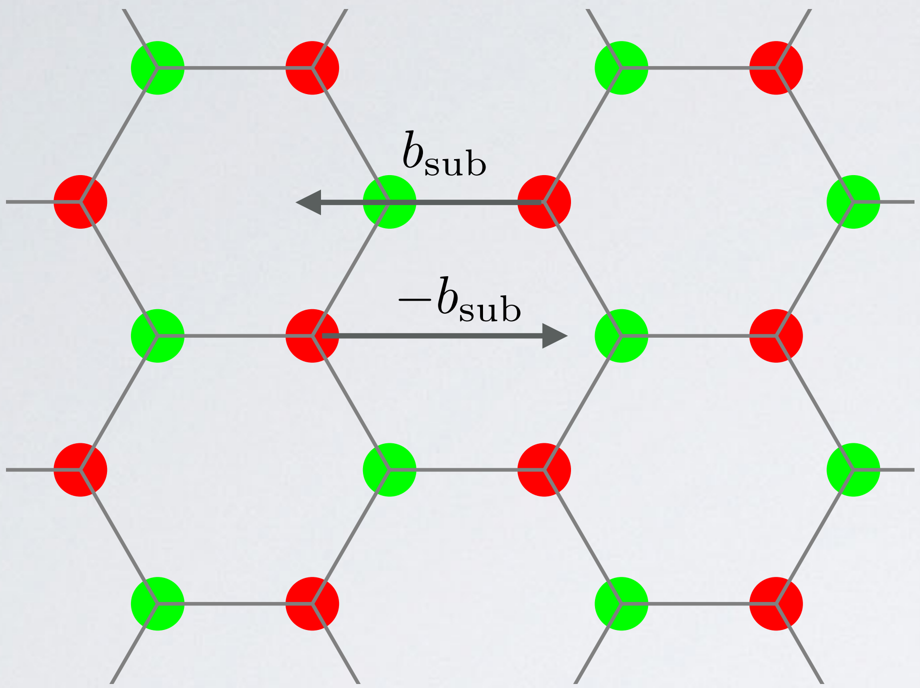
$$V(\boldsymbol{r}) = w\big(\cos(\boldsymbol{b}_1 \cdot \boldsymbol{r}) + \cos(\boldsymbol{b}_2 \cdot \boldsymbol{r}) + \cos(-(\boldsymbol{b}_1 + \boldsymbol{b}_2) \cdot \boldsymbol{r})\big)$$

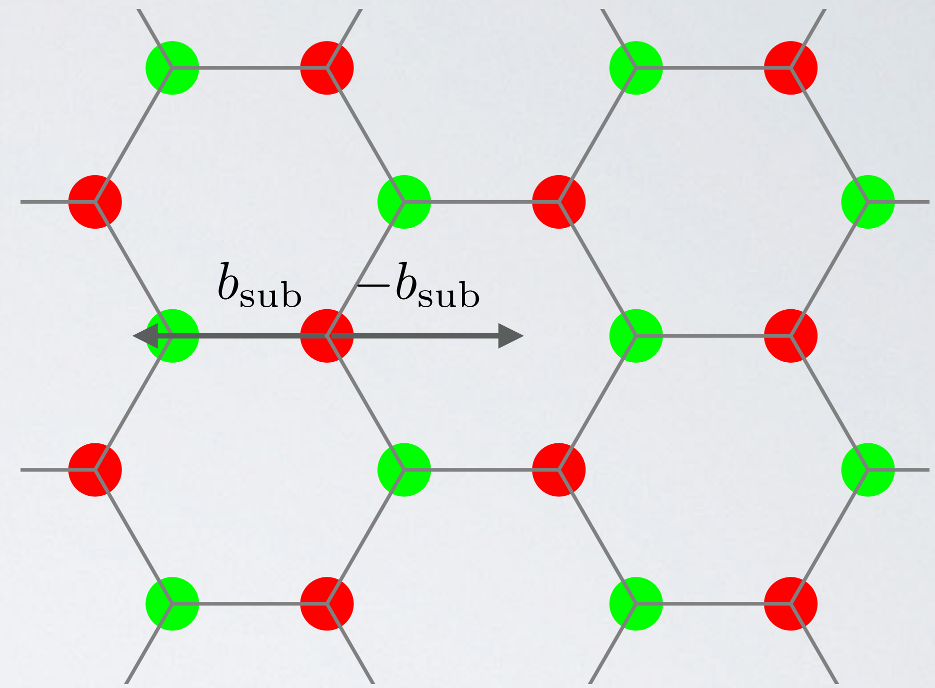
$$H_{\mathrm{Gr}}(\mathbf{k}) = \begin{pmatrix} 0 & h_{\mathbf{k}} \\ h_{\mathbf{k}}^* & 0 \end{pmatrix}$$

$$h_{\mathbf{k}} = te^{-ik_x a_{\mathrm{Gr}}/\sqrt{3}}(1 + e^{i\sqrt{3}k_x a_{\mathrm{Gr}}/2} \cos \frac{k_y a_{\mathrm{Gr}}}{2})$$

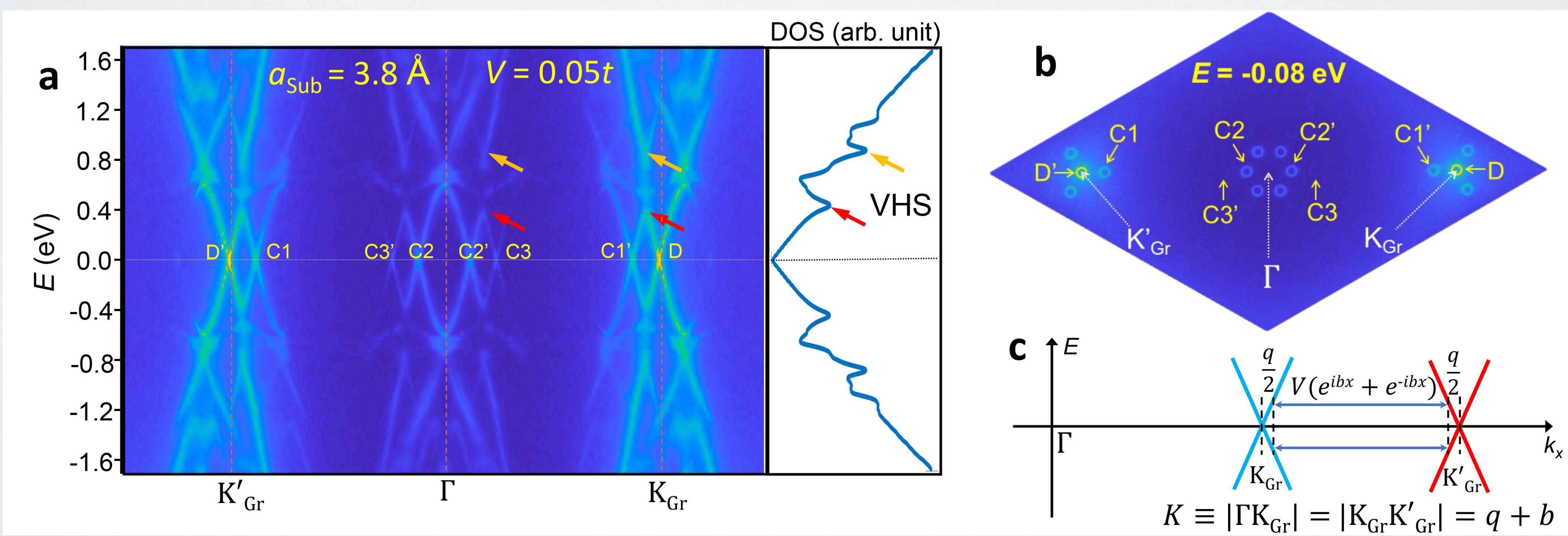
Change substrate lattice constant

SiC constant $a_{\mathrm{SiC}} = 3.07\mathring{A}$ → $a_{\mathrm{sub}} = 3.8\mathring{A}$



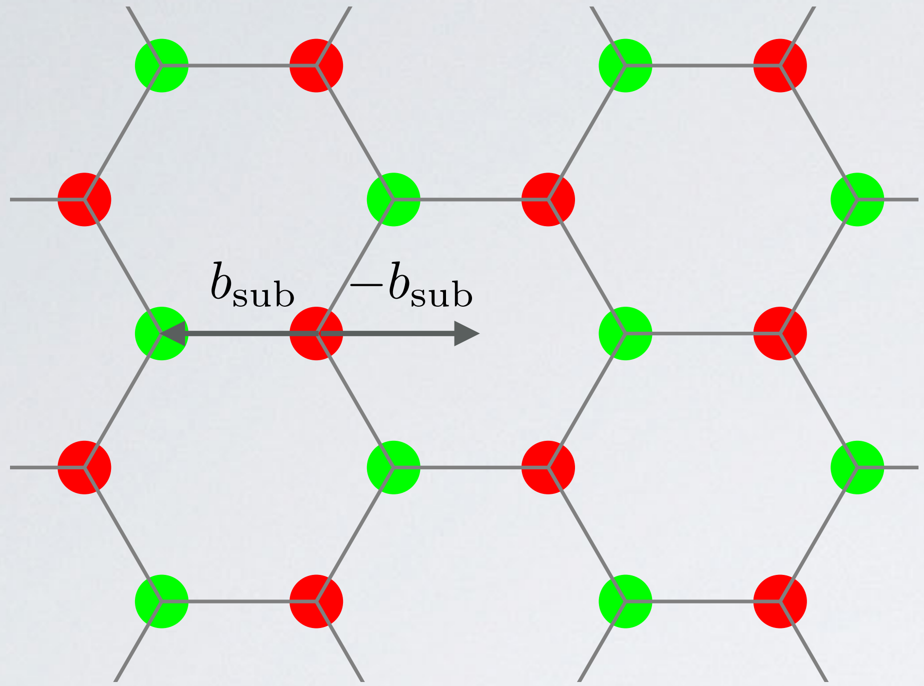


The periodic potential brings the coupling between the two Dirac cones.

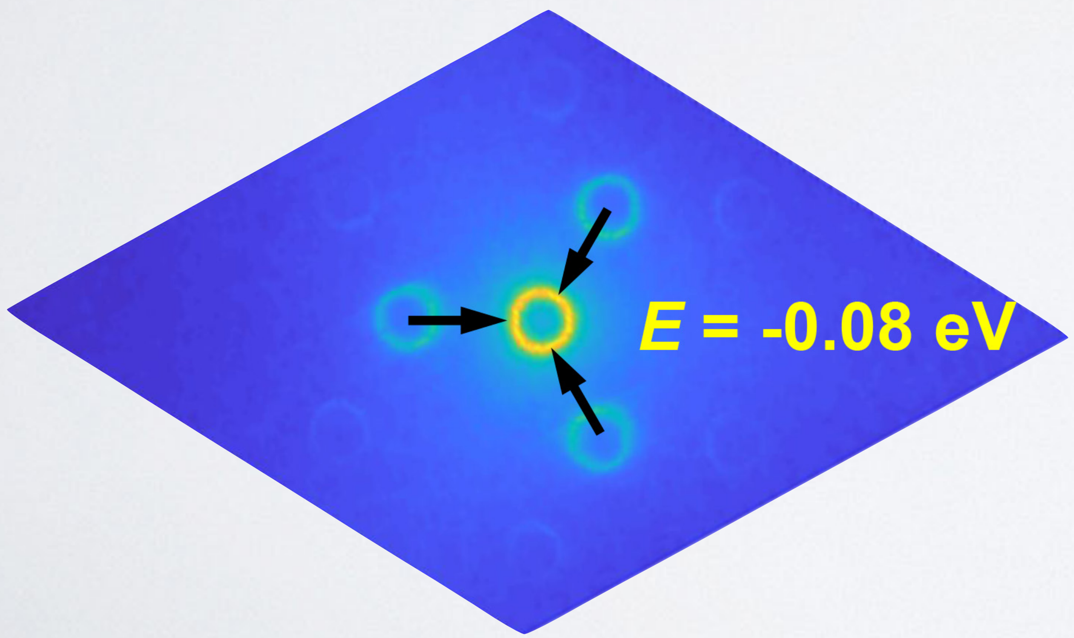


VHS: Van Hove Singularity

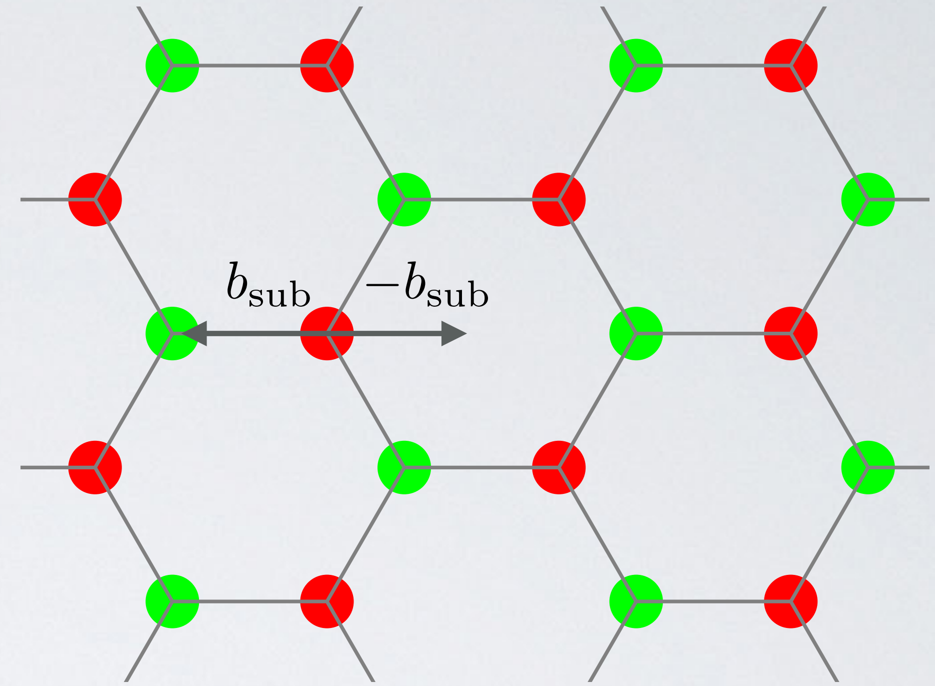
$a_{\mathrm{sub}} \to \sqrt{3}a_{\mathrm{Gr}} = 4.26\mathring{A}$



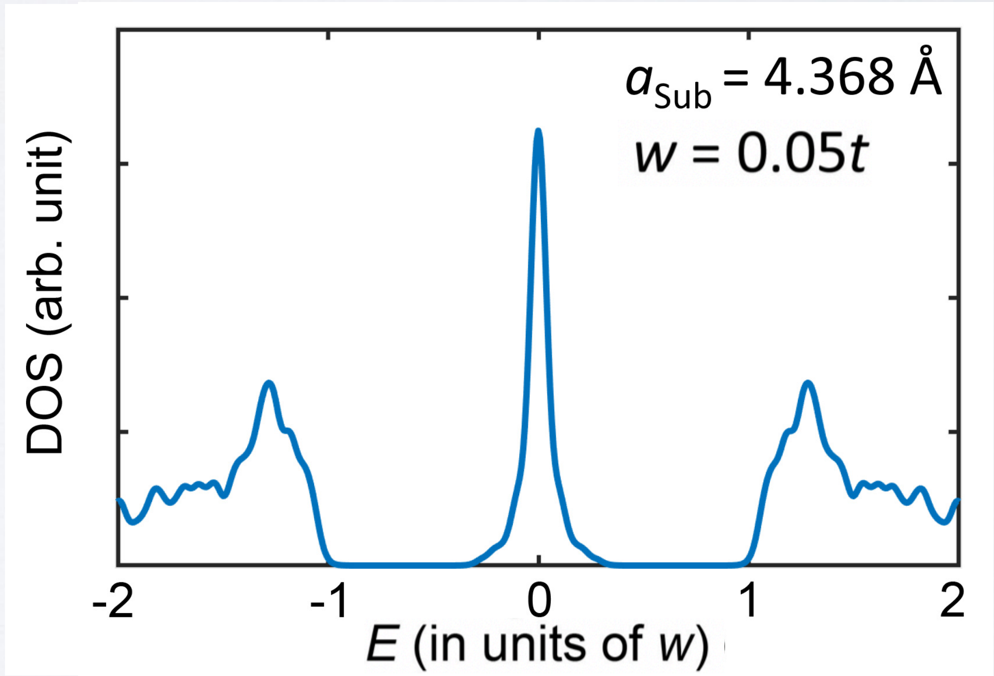
The first-ordered Dirac cones overlap the main Dirac cone



$a_{\mathrm{sub}} = 4.368\mathring{A} \approx \sqrt{3}a_{\mathrm{Gr}}$



A zero-bias peak in a gap



Hint of **flat bands** at zero energy

Outline

1. Review of twisted bilayer graphene continuum model

2. Experiment: Monolayer graphene on SiC substrate

3. **The low-energy physics of monolayer graphene on substrate**

The Continuum Model for $a_{\mathrm{sub}} \approx \sqrt{3} a_{\mathrm{Gr}}$

Periodic potential form the substrate

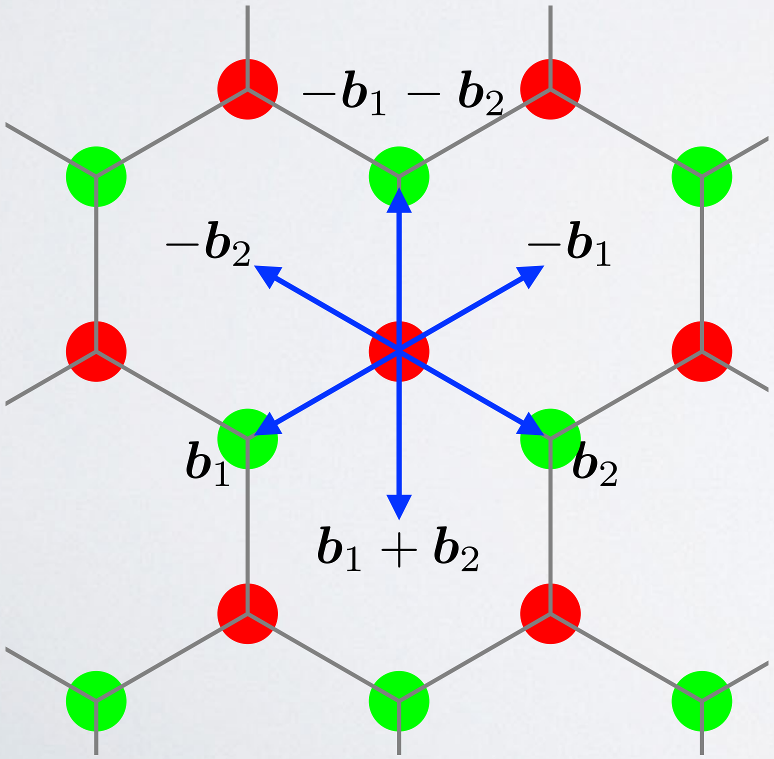
$$V(\boldsymbol{r}) = w\Big(\cos(\boldsymbol{b}_1 \cdot \boldsymbol{r}) + \cos(\boldsymbol{b}_2 \cdot \boldsymbol{r}) + \cos(-(\boldsymbol{b}_1 + \boldsymbol{b}_2) \cdot \boldsymbol{r})\Big)$$

Six momentum hopping terms

$$\hat{V} = \sum_{\boldsymbol{r}} c^{\dagger}_{\boldsymbol{r}} V(\boldsymbol{r}) c_{\boldsymbol{r}}$$

$$\propto w \sum_{\mathbf{k}} \big[c^{\dagger}_{\mathbf{k}+\boldsymbol{b}_1} \sigma_0 c_{\mathbf{k}} + c^{\dagger}_{\mathbf{k}+\boldsymbol{b}_2} \sigma_0 c_{\mathbf{k}} + c^{\dagger}_{\mathbf{k}-\boldsymbol{b}_1-\boldsymbol{b}_2} \sigma_0 c_{\mathbf{k}} \qquad (1)$$

$$+ c^{\dagger}_{\mathbf{k}-\boldsymbol{b}_1} \sigma_0 c_{\mathbf{k}} + c^{\dagger}_{\mathbf{k}-\boldsymbol{b}_2} \sigma_0 c_{\mathbf{k}} + c^{\dagger}_{\mathbf{k}+\boldsymbol{b}_1+\boldsymbol{b}_2} \sigma_0 c_{\mathbf{k}} \big] \qquad (2)$$



(1)

Momentum hoppings between the two Dirac cones

(2)

The Dirac cone couples to the high energy bands

Approximation: keep (1), neglect (2)

The Continuum Model

$$H_{\rm MG}(\Delta \boldsymbol{k}) = \begin{pmatrix} H_d(\Delta \boldsymbol{k}) & w\sigma_0 & w\sigma_0 & w\sigma_0 \\ w\sigma_0 & H_D^*(0, \Delta \boldsymbol{k} + \boldsymbol{q}_1) & 0 & 0 \\ w\sigma_0 & 0 & H_D^*(\psi, \Delta \boldsymbol{k} + \boldsymbol{q}_2) & 0 \\ w\sigma_0 & 0 & 0 & H_D^*(-\psi, \Delta \boldsymbol{k} + \boldsymbol{q}_3) \end{pmatrix}$$

Off-diagonal: $w \sum_{\mathbf{k}} \left[c^\dagger_{\mathbf{k}+\boldsymbol{b}_1} \sigma_0 c_{\mathbf{k}} + c^\dagger_{\mathbf{k}+\boldsymbol{b}_2} \sigma_0 c_{\mathbf{k}} + c^\dagger_{\mathbf{k}-\boldsymbol{b}_1-\boldsymbol{b}_2} \sigma_0 c_{\mathbf{k}} \right]$

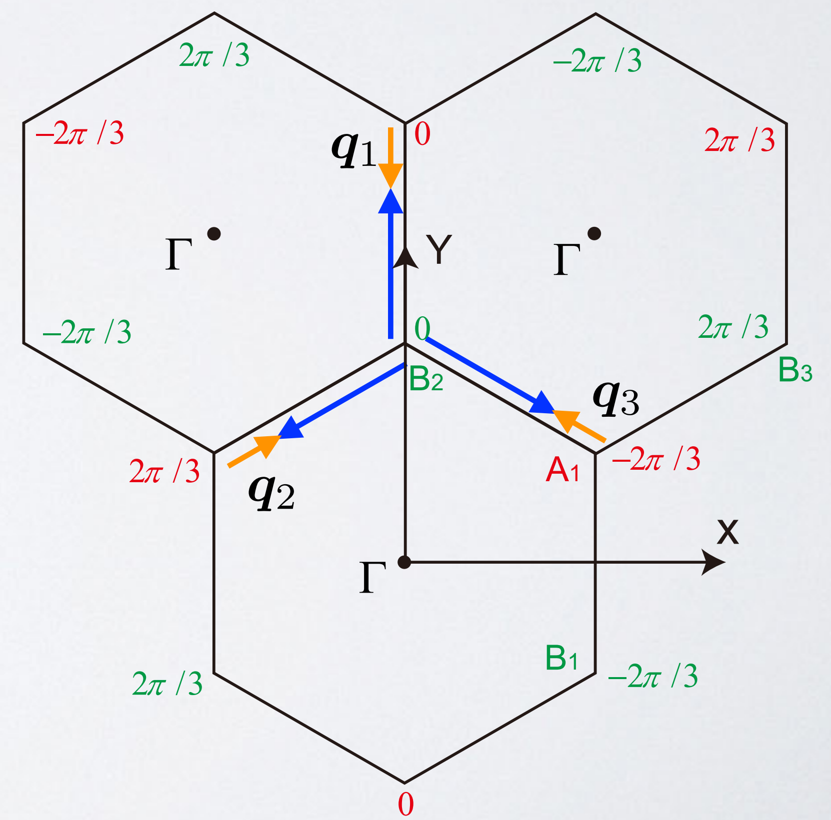
Diagonal: Dirac cones with adjustment

$$\boldsymbol{q}_i = \boldsymbol{b}_i^{\overline{KK'}} - \boldsymbol{b}_i^{\rm sub}$$

Momentum shifts $\boldsymbol{q}_1, \; \boldsymbol{q}_2, \; \boldsymbol{q}_3$

Form Moire BZ

Phase shifts



$$H_d(\Delta \mathbf{k}) = v_F(\Delta k_x \sigma_x + \Delta k_y \sigma_y)$$

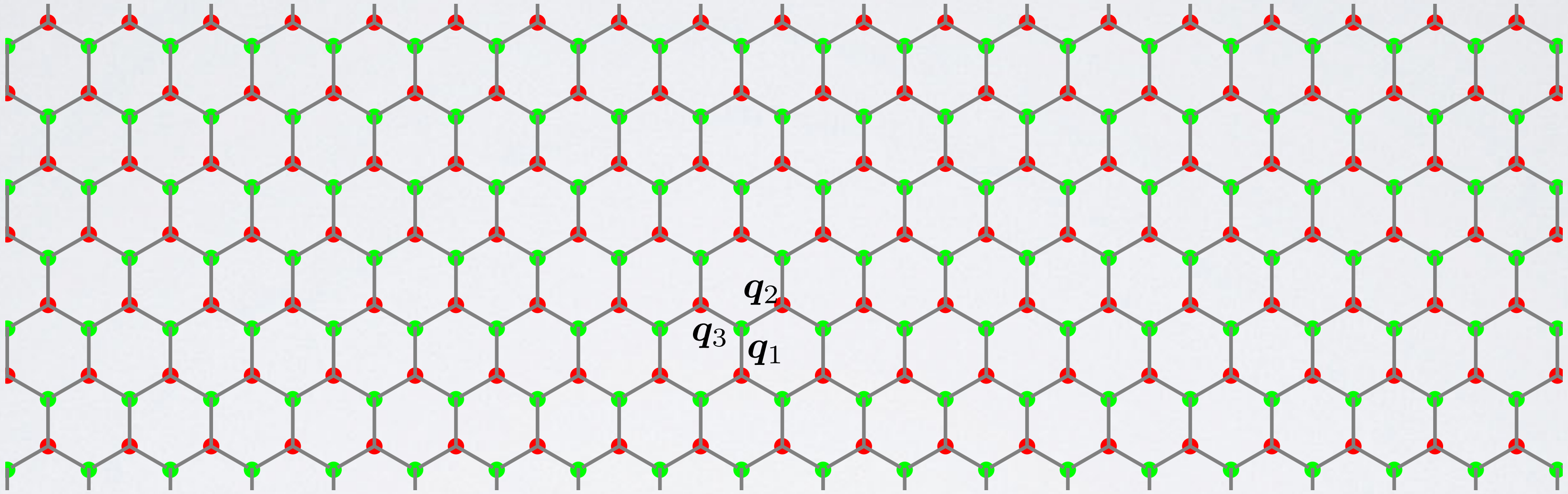
$$H_D^*(\phi, \Delta \mathbf{k}) = R_\phi v_F(\Delta k_x \sigma_x - \Delta k_y \sigma_y) R_\phi^{-1}$$

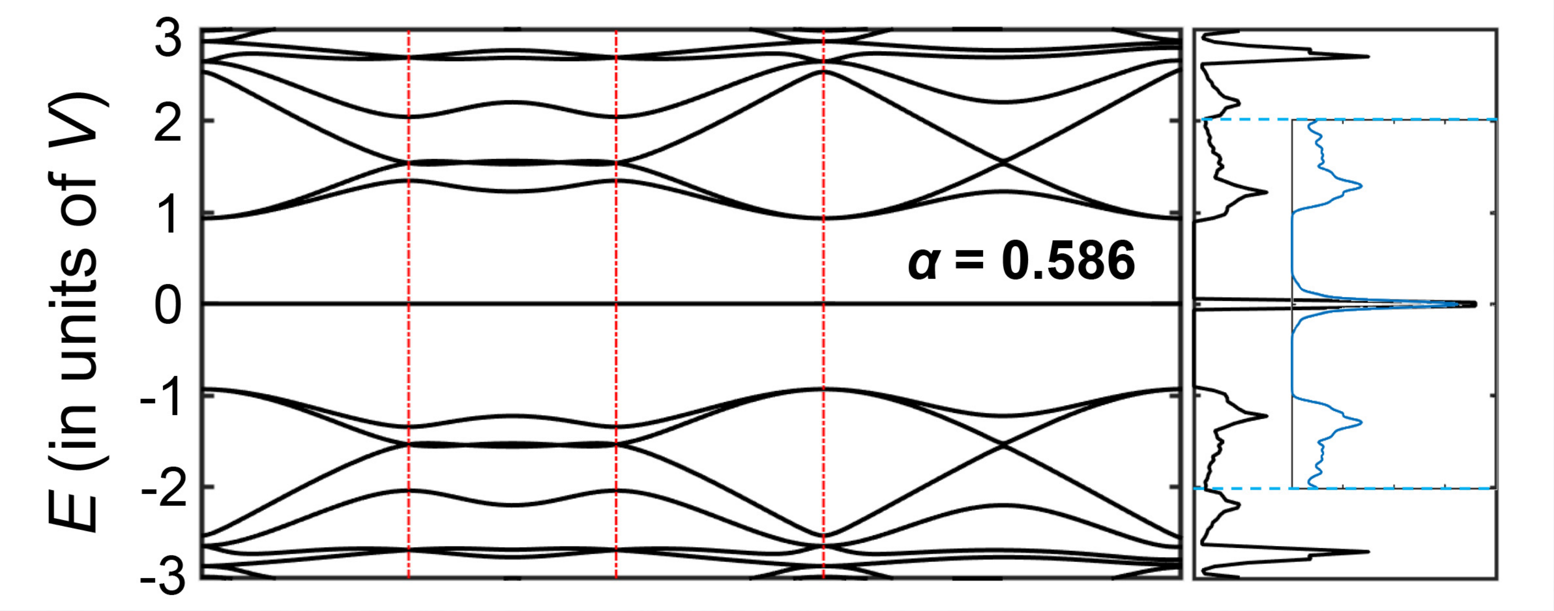
$$R_\phi = \cos\phi/2\sigma_0 - i \sin\phi/2\sigma_z$$

The Tight-binding model and the continuum model are in agreement

$$H_{\mathrm{MG}}(\Delta\boldsymbol{k}) = \begin{pmatrix} H_d(\Delta\boldsymbol{k}) & w\sigma_0 & w\sigma_0 & w\sigma_0 \\ w\sigma_0 & H_D^*(0, \Delta\boldsymbol{k}+\boldsymbol{q}_1) & 0 & 0 \\ w\sigma_0 & 0 & H_D^*(\psi, \Delta\boldsymbol{k}+\boldsymbol{q}_2) & 0 \\ w\sigma_0 & 0 & 0 & H_D^*(-\psi, \Delta\boldsymbol{k}+\boldsymbol{q}_3) \end{pmatrix}$$

$$\alpha \equiv w/v_F|\boldsymbol{q}_1|$$





The approximation is good

The low-energy physics in Twisted Bilayer Graphene is equivalent to monolayer graphene on the substrate

$$H_{\mathrm{TBG}}(\Delta\boldsymbol{k}) = \begin{pmatrix} H_d(\Delta\boldsymbol{k}) & wT_0 & wT_{-\psi} & wT_{\psi} \\ wT_0 & H_d(\Delta\boldsymbol{k}+\boldsymbol{q}_1) & 0 & 0 \\ wT_{-\psi} & 0 & H_d(\Delta\boldsymbol{k}+\boldsymbol{q}_2) & 0 \\ wT_{\psi} & 0 & 0 & H_d(\Delta\boldsymbol{k}+\boldsymbol{q}_3) \end{pmatrix}$$

$$T_\phi = \cos\phi\sigma_x + \sin\phi\sigma_y, \text{ where } \psi = 2\pi/3$$

$$H_d(\Delta\mathbf{k}) = v_F(\Delta k_x\sigma_x + \Delta k_y\sigma_y)$$

$$H_{\mathrm{MG}}(\Delta\boldsymbol{k}) = \begin{pmatrix} H_d(\Delta\boldsymbol{k}) & w\sigma_0 & w\sigma_0 & w\sigma_0 \\ w\sigma_0 & H_D^*(0,\Delta\boldsymbol{k}+\boldsymbol{q}_1) & 0 & 0 \\ w\sigma_0 & 0 & H_D^*(\psi,\Delta\boldsymbol{k}+\boldsymbol{q}_2) & 0 \\ w\sigma_0 & 0 & 0 & H_D^*(-\psi,\Delta\boldsymbol{k}+\boldsymbol{q}_3) \end{pmatrix}$$

$$H_D^*(\phi,\Delta\mathbf{k}) = R_\phi v_F(\Delta k_x\sigma_x - \Delta k_y\sigma_y)R_\phi^{-1}$$

Unitary Transformation

$$H_{\mathrm{TBG}}(\Delta\boldsymbol{k}) = U H_{\mathrm{MG}} U^\dagger$$

$$\text{where } U = \mathrm{diag}(\sigma_0, T_0, T_{-\psi}, T_\psi)$$

Comparison

	Twisted Bilayer Graphene	Monolayer Graphene on substrate
Coupling	Interlayer coupling	Periodic potential
Size of Moire BZ	Twisted Angle (Magic Angle)	Substrate lattice constant (Magic lattice constant)
Coupled Dirac cones	Two identical Dirac cones	Two Dirac cones with opposite orientations
Approximation	Neglect longer momentum hopping	Neglect hopping between a Dirac cone and high energy bands

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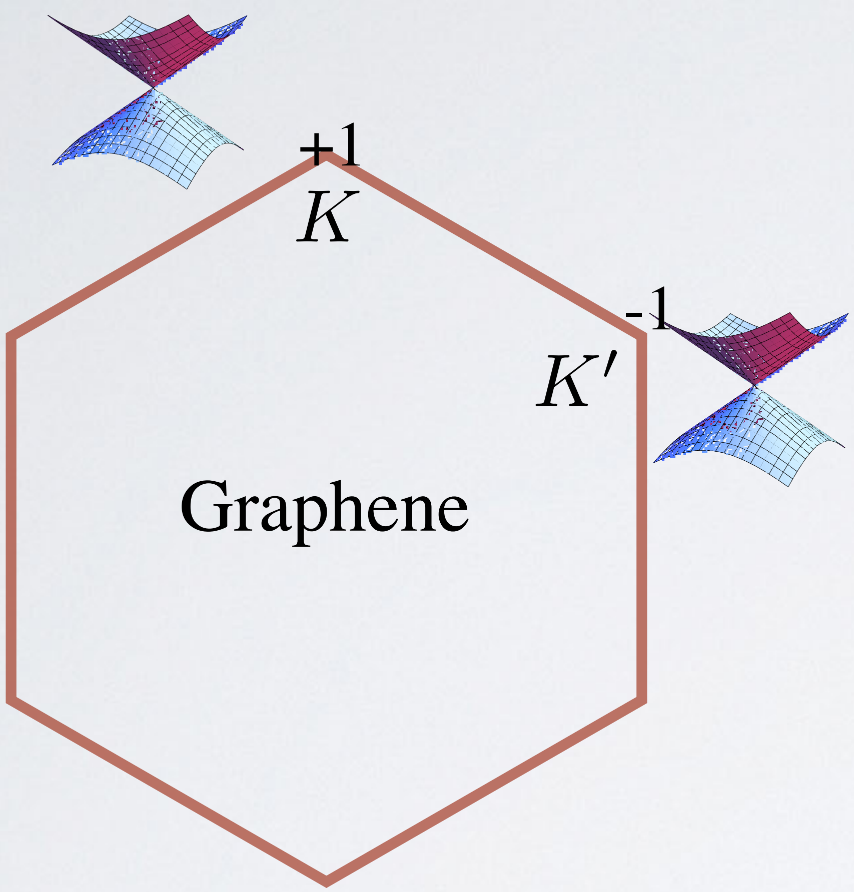
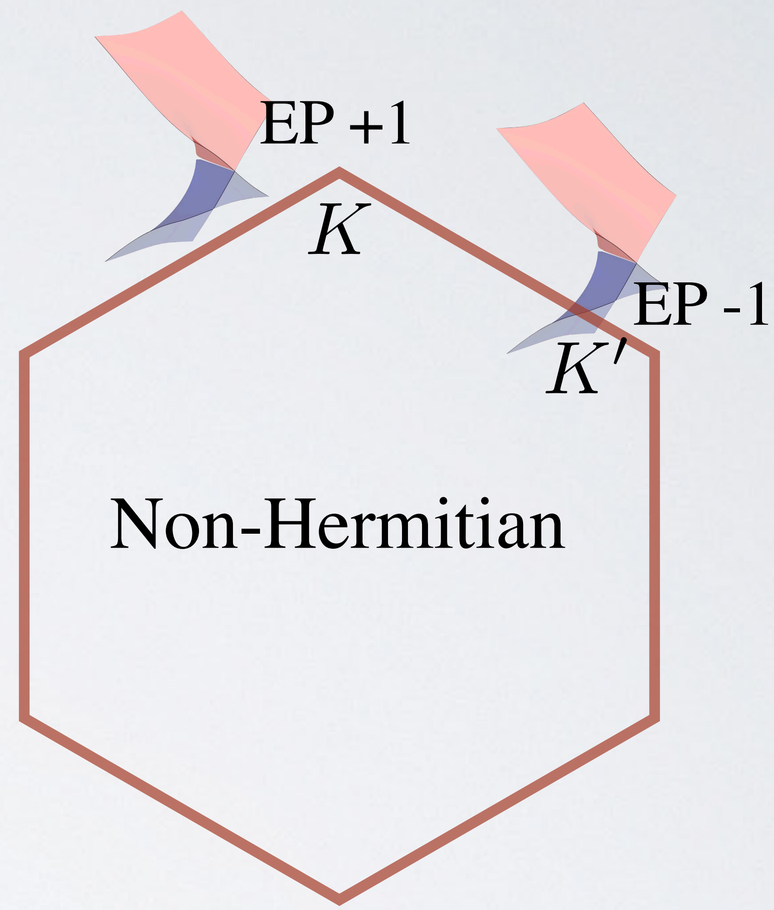
Question 2:

In non-Hermitian physics, can two exceptional points be located at K or K' so that there is twisted physics exceptional points?





Focus: The generalized non-Hermitian 2D Nielsen-Ninomiya theorem

Nielsen-Ninomiya Theorem for non-Hermitian exceptional points

In 2D non-Hermitian lattices

Integer discriminant numbers quantizes **exceptional points**

$$\nu(\mathbf{k}_d^l) = \frac{i}{2\pi} \oint_{\Gamma(\mathbf{k}_d^l)} d\boldsymbol{k} \cdot \nabla_{\boldsymbol{k}} \ln \mathrm{Disc}_E[\mathcal{H}](\mathbf{k})$$

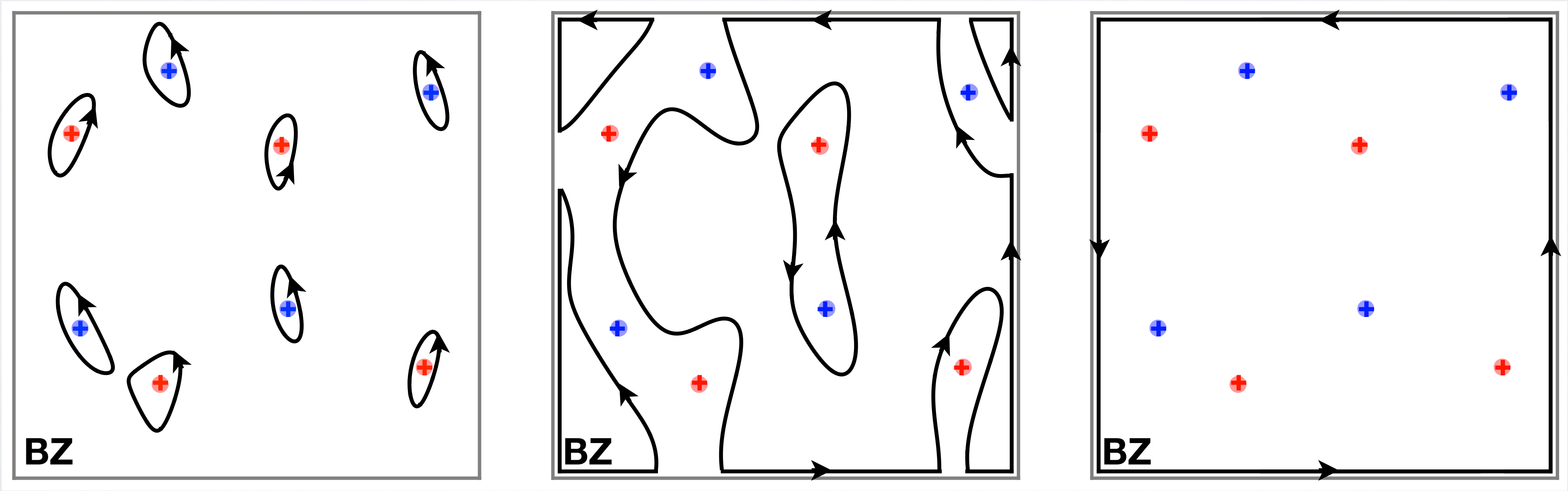
$$\mathrm{Disc}_E[\mathcal{H}](\boldsymbol{k}) = \prod_{i<j} [E_i(\boldsymbol{k}) - E_j(\boldsymbol{k})]^2$$

L. Fu et al, PRL 120, 146402 (2018)
M. Sato et al, PRL 123, 066405 (2019)

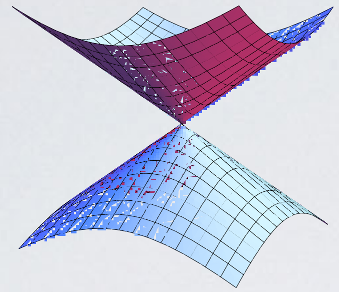
Yes, the Nielsen-Ninomiya theorem still holds

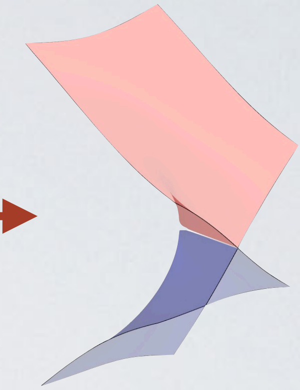
$$\sum_{\mathbf{k}_d^j \in \mathrm{BZ}} \nu(\mathbf{k}_d^j) = \frac{i}{2\pi} \oint_{\partial \mathrm{BZ}} d\boldsymbol{k} \cdot \nabla_{\boldsymbol{k}} \ln \mathrm{Disc}_E[\mathcal{H}](\mathbf{k}) = 0$$

Charge neutralization



Z Yang, AP Schnyder, J Hu, CK Chiu, Physical Review Letters 126 (8), 086401 (2021)





$$\begin{pmatrix} E & a \\ 0 & E \end{pmatrix}$$

	Hermitian Dirac node	Non-Hermitian exceptional point (EP)
Symmetry	Chiral symmetry $S = \sigma_z$ $\mathcal{H} = \begin{pmatrix} 0 & h \\ h & 0 \end{pmatrix}$	X
Topological invariant	Winding number w	Discriminant number ν
Doubling theorem	Yes Node $\# \geq 2$	Yes Node $\# \geq 2$
Difference	Nodes at zero energy	EPs for all energy levels $\mathrm{Disc}_E[\mathcal{H}](\boldsymbol{k}) = \prod_{i<j} [E_i(\boldsymbol{k}) - E_j(\boldsymbol{k})]^2$

$$\sum_{\mathbf{k}_n^j \in \mathrm{BZ}} \nu\left(\boldsymbol{k}_n^j\right) = \sum_{\mathbf{k}_n^j \in \mathrm{BZ}} \frac{i}{2\pi} \oint_{\Gamma(\mathbf{k}_n^j)} d\boldsymbol{k} \cdot \nabla_{\boldsymbol{k}} \ln \det[h(\boldsymbol{k})] = 0$$

$$\sum_{\mathbf{k}_d^j \in \mathrm{BZ}} \nu(\mathbf{k}_d^j) = \frac{i}{2\pi} \oint_{\partial \mathrm{BZ}} d\boldsymbol{k} \cdot \nabla_{\boldsymbol{k}} \ln \mathrm{Disc}_E[\mathcal{H}](\mathbf{k}) = 0$$

Z Yang, AP Schnyder, J Hu, CK Chiu, Physical Review Letters 126 (8), 086401 (2021)

If crystalline symmetries are preserved, is the minimal number of the nodes greater than 2?

17 2D wallpaper groups

Crystalline symmetry constraints

The generalized Nielsen-Ninomiya Theorem for the 17 wallpaper groups

Zero-energy (Dirac) nodes protected by chiral symmetry

Number= $\sum_{\mathbf{k}_i \in \mathrm{BZ}} |w(\mathbf{k}_i)| \sim$ number of Dirac nodes

The minimal number of the topological nodes

WG	Generators	AIII	BDI/CII T^+	DIII/CI T^-
#1		2	$\tilde{2}$	4
#2	C_2^+	4 or 4(Γ, M, X, Y)	0	4
	C_2^-	$\tilde{2}$	$\tilde{2}$	0
#3,4,5	M_x^+	$\tilde{2}$	$\tilde{2}^{\circ}$MLs or $\tilde{4}$	$\tilde{4}$
	M_x^-	2 MLs including (Γ, M, X, Y) or 4	$\tilde{2}$ MLs or $\tilde{4}$	$4^{\bullet}$MLs or 8
#6,7	C_2^+ and M_x^+	$\tilde{4}$	0	$\tilde{4}$
8,9	C_2^+ and M_x^-	4 MLs or 4(Γ, M, X, Y) or 8	0	4 MLs or 8
	C_2^- and $M_x^\pm$	$\tilde{2}$ MLs or $\tilde{4}$	$\tilde{2}$ MLs or $\tilde{4}$	0
#10	C_4^+	4(Γ, M, X, Y) or 8	0	8
	C_4^-	$\tilde{4}$	0	$\tilde{4}$
#11,12	C_4^+ and M_x^+	$\tilde{8}$	0	$\tilde{8}$
	C_4^+ and M_x^-	4(Γ, M, X, Y) or 8 MLs or 16	0	8 MLs or 16
	C_4^- and $M_x^\pm$	$\tilde{4}$ MLs or $\tilde{8}$	0	$\tilde{4}$ MLs or $\tilde{8}$
#13	C_3^+	2(K, K$'$) or 4^*(K, K$'$, Γ) or 6(K, K$'$, Γ, $\mathrm{M}_{1/2/3}$) or 6^*(Γ, $\mathrm{M}_{1/2/3}$) or 6	$\tilde{2}$(K, K$'$) or $\tilde{6}$	12
	C_3^-	0	0	0
#14	C_3^+ and M_y^+	$\tilde{2}$(K, K$'$) or $\tilde{6}$	$\tilde{2}$(K, K$'$) or $\tilde{6}^{\circ}$MLs or $\tilde{12}$	$\tilde{12}$
	C_3^+ and M_y^-	4^*(K, K$'$, Γ) or 6 MLS or 6(K, K$'$, Γ, $\mathrm{M}_{1/2/3}$) or 6^*(Γ, $\mathrm{M}_{1/2/3}$) or 12	$\tilde{6}$ MLs or $\tilde{12}$	$12^{\bullet}$MLs or 24
	C_3^- and $M_y^\pm$	0	0	0
#15	C_3^+ and M_x^+	$\tilde{6}$	$\tilde{6}^{\circ}$MLs or $\tilde{12}$	$\tilde{12}$
	C_3^+ and M_x^-	2(K, K$'$), 4^*(K, K$'$, Γ), 6 MLs, 6(K, K$'$, Γ, $\mathrm{M}_{1/2/3}$), 6^*(Γ, $\mathrm{M}_{1/2/3}$), or 12	$\tilde{2}$(K, K$'$) or $\tilde{6}$ MLs or $\tilde{12}$	$12^{\bullet}$MLs or 24
	C_3^- and $M_x^\pm$	0	0	0
#16	C_6^+	4^*(K, K$'$, Γ) or 6(K, K$'$, Γ, $\mathrm{M}_{1/2/3}$) or 6^*(Γ, $\mathrm{M}_{1/2/3}$) or 12	0	12
	C_6^-	$\tilde{2}$(K, K$'$) or $\tilde{6}$	$\tilde{2}$(K, K$'$) or $\tilde{6}$	0
#17	C_6^+ and M_x^+	$\tilde{12}$	0	$\tilde{12}$
	C_6^+ and M_x^-	4^*(K, K$'$, Γ) or 6(K, K$'$, Γ, $\mathrm{M}_{1/2/3}$) or 6^*(Γ, $\mathrm{M}_{1/2/3}$) or 12 MLs or 24	0	12 MLs or 24
	C_6^- and M_x^+	$\tilde{6}$ MLs or $\tilde{12}$	$\tilde{6}$ MLs or $\tilde{12}$	0
	C_6^- and M_x^-	$\tilde{2}$(K, K$'$) or $\tilde{6}$ MLs or $\tilde{12}$	$\tilde{2}$(K, K$'$) or $\tilde{6}$ MLs or $\tilde{12}$	0

$\{C_6^-, S\} = 0,\ \{M_x^-, S\} = 0$ Graphene

C Le, Z Yang, F Cui, AP Schnyder, CK Chiu, PRB **106**, 045126 (2022)

What about exceptional points in non-Hermitian systems?

Hermitian

$$\sum_{\mathbf{k}_n^j \in \mathrm{BZ}} \nu\left(\boldsymbol{k}_n^j\right) = \sum_{\mathbf{k}_n^j \in \mathrm{BZ}} \frac{i}{2\pi} \oint_{\Gamma(\mathbf{k}_n^j)} d\boldsymbol{k} \cdot \nabla_{\boldsymbol{k}} \ln \det[h(\boldsymbol{k})] = 0$$

non-Hermitian

$$\sum_{\mathbf{k}_d^j \in \mathrm{BZ}} \nu(\mathbf{k}_d^j) = \frac{i}{2\pi} \oint_{\partial \mathrm{BZ}} d\boldsymbol{k} \cdot \nabla_{\boldsymbol{k}} \ln \mathrm{Disc}_E[\mathcal{H}](\mathbf{k}) = 0$$

They share the similar mathematical structure

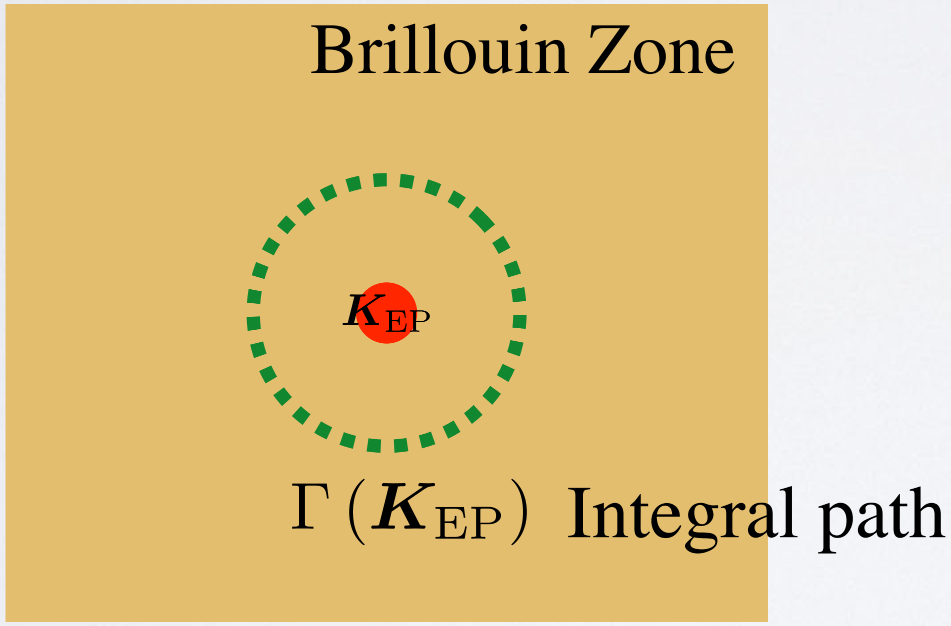
But the discriminant number of an EP has an additional constraint.

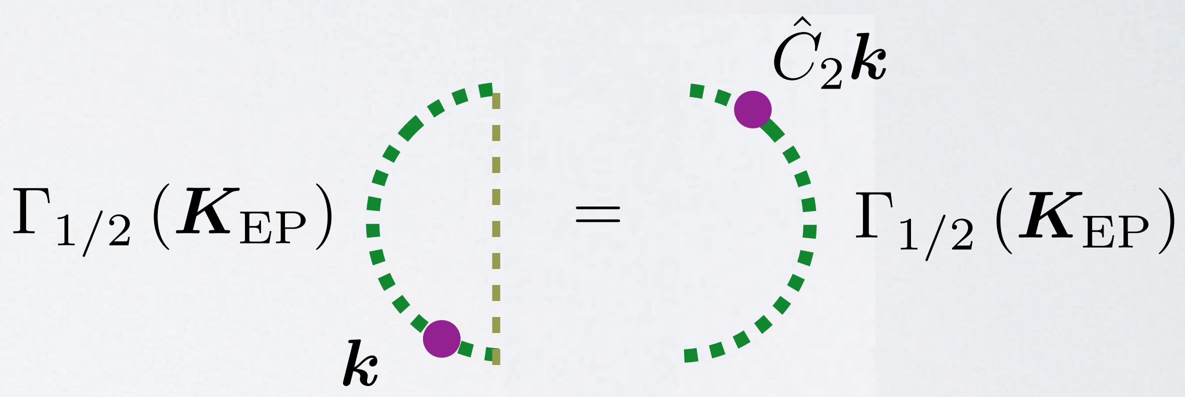
EP at a C_2 rotation center

$$\nu_{\mathrm{disc}}(\boldsymbol{K}_{\mathrm{EP}}) = \frac{i}{2\pi}\int_{\Gamma_{1/2}(\boldsymbol{K}_{\mathrm{EP}})}\Big[d\ln\big(\mathrm{Disc}_E[\mathcal{H}_{\mathrm{nH}}](\boldsymbol{k})\big) + d\ln\big(\mathrm{Disc}_E[\mathcal{H}_{\mathrm{nH}}](\hat{C}_2\boldsymbol{k})\big)\Big]$$
$$= 2\times\frac{i}{2\pi}\oint_{\Gamma_{1/2}(\boldsymbol{K}_{\mathrm{EP}})} d\Big(\ln\big(\mathrm{Disc}_E[\mathcal{H}_{\mathrm{nH}}](\boldsymbol{k})\big)\Big)$$
$$= 2j$$

C_2 rotation symmetry

$$\ln\big(\mathrm{Disc}_E[\mathcal{H}_{\mathrm{nH}}](\boldsymbol{k})\big) = \ln\big(\mathrm{Disc}_E[\mathcal{H}_{\mathrm{nH}}](\hat{C}_2\boldsymbol{k})\big)$$





C_n rotation center

$$\nu_{\mathrm{disc}}(\boldsymbol{K}_{\mathrm{EP}}) = nj$$

For chiral symmetry

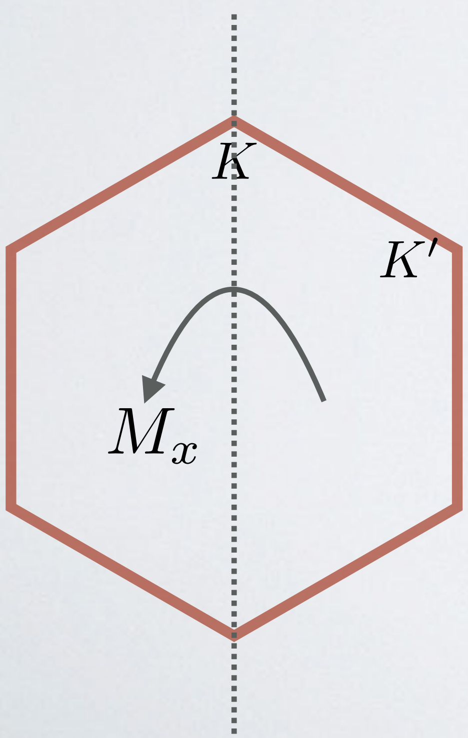
$$\ln\det[h(\boldsymbol{k})] \neq \ln\det[h(\hat{C}_2\boldsymbol{k})]$$
$$\nu \neq nj$$

The generalized non-Hermitian Nielsen-Ninomiya Theorem

Hermitian nodes with $[C_n^+, S] = 0, \; [M_x^+, S] = 0$

The minimal number of exceptional points

WG	Generators	Rotation centers	ν_{abs}
#1		No centers	2
#2	C_2	$(\Gamma, X, Y, M) : 2\mathbb{Z}$	4 $(G,\ \Gamma,\ X,\ Y,$ or $M)$
#3,4,5	M_x	$\times$	$\tilde{2}$
#6,7,8,9	C_2 and M_x	$\times$	$\tilde{4}$
#10	C_4	$(\Gamma, M) : 4\mathbb{Z}$ & $(X, Y) : 2\mathbb{Z}$	8 $(G,\ \Gamma,\ X,\ Y,$ or $M)$
#11,12	C_4 and M_x	$\times$	$\tilde{8}$
#13	C_3	$(\Gamma, K, K') : 3\mathbb{Z}$	6 $(G,\ \Gamma,\ K,\ K',$ or $M_{1/2/3})$
#14	C_3 and M_y	$(K, K') : 3\mathbb{Z}$	$\tilde{6}$ or $\tilde{6}(K, K')$
#15	C_3 and M_x	$\times$	$\tilde{6}$
#16	C_6	$(\Gamma) : 6\mathbb{Z}$ & $(K, K') : 3\mathbb{Z}$ & $(M_{1/2/3}) : 2\mathbb{Z}$	12 $(G,\ \Gamma,\ K,\ K',$ or $M_{1/2/3})$
#17	C_6 and M_x	$\times$	$\tilde{12}$



C_n rotation constraint: $\nu_{\mathrm{disc}}(\boldsymbol{K}_{\mathrm{EP}}) = nj$

Minimal EP #: $\nu_{\mathrm{abs}} = \sum_{\mathbf{k}_i \in \mathrm{BZ}} |\nu_{\mathrm{disc}}(\mathbf{k}_i)|$

M_x reflection symmetry destroys exceptional points at K and K'

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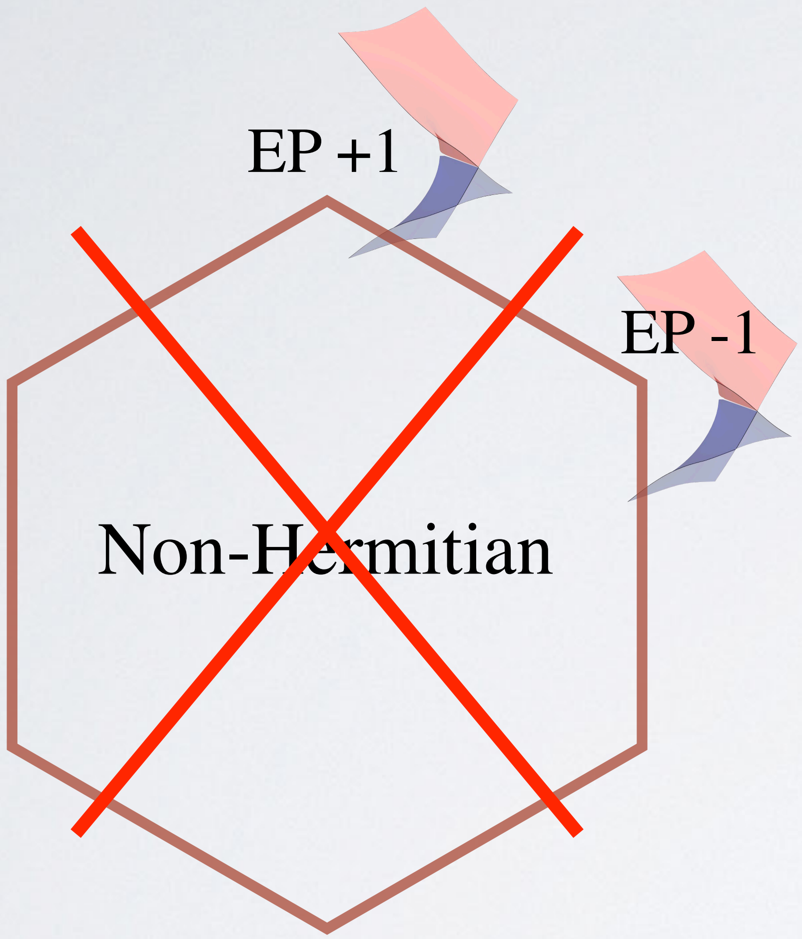
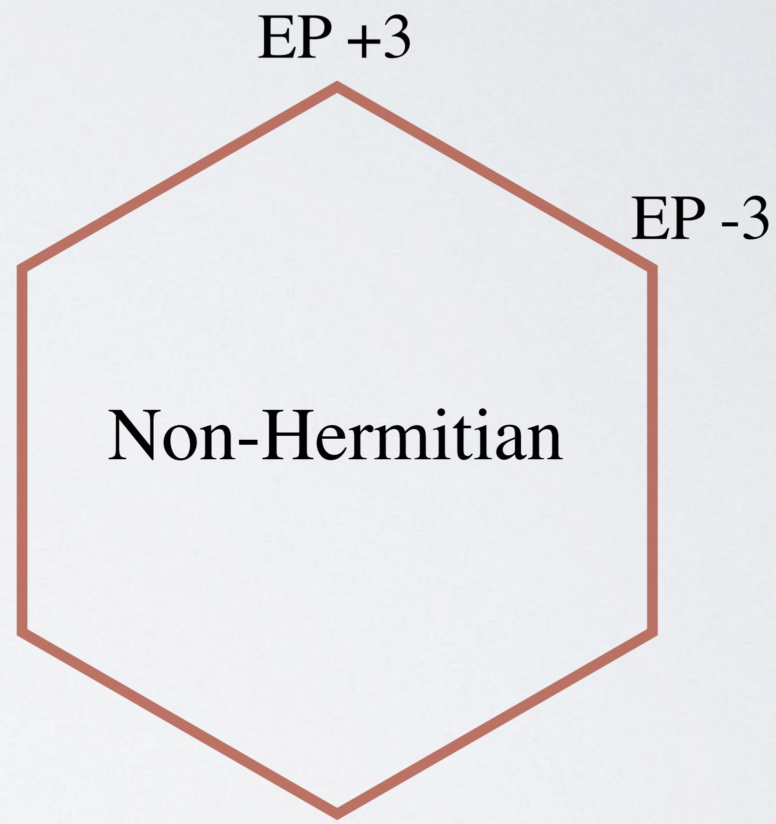
K and K' are C_3 rotation centers

$$\nu_{\mathrm{disc}}(\boldsymbol{K}_{\mathrm{EP}}) = 3j$$





No M_x reflection symmetry

Non-Hermitian EP system: no analogous twisted bilayer graphene

The extension of the non-Hermitian Nielsen-Ninomiya Theorem

Magnetic Wallpaper Group

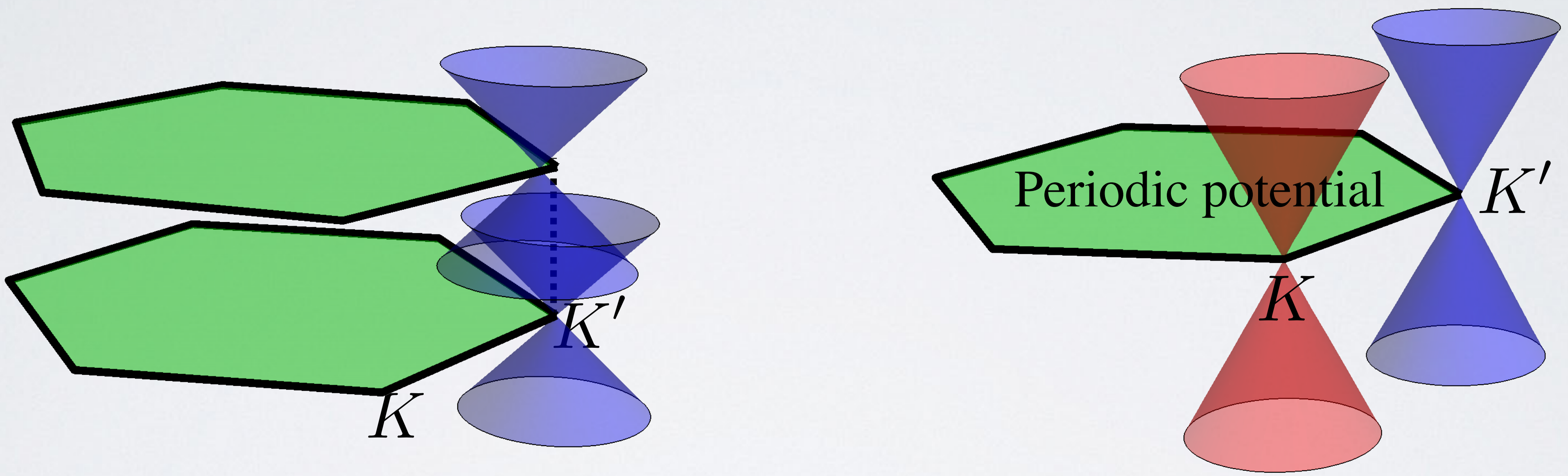
Conjugation crystalline symmetries $\bar{g}$

$\bar{C}_n = C_n\mathcal{K}$ $\bar{M}_i = M_i\mathcal{K}$ $\mathcal{K}$ Complex conjugation

WG	Generators	Rotation centers	ν_{abs}
#1		No centers	2
#2	C_2	$(\Gamma, X, Y, M) : 2\mathbb{Z}$	$4\ (G, \Gamma,\ X,\ Y, \text{ or } M)$
	$\bar{C}_2$	$\times$	$\tilde{2}$
#3,4,5	M_x	$\times$	$\tilde{2}$
	$\bar{M}_x$	No centers	$2\ (\text{MLs}, \Gamma,\ X,\ Y, \text{ or } M) \text{ or } 4$
#6,7,8,9	C_2 and M_x	$\times$	$\tilde{4}$
	C_2 and $\bar{M}_x$	$(\Gamma, X, Y, M) : 2\mathbb{Z}$	$4\ (\text{MLs}, \Gamma,\ X,\ Y, \text{ or } M) \text{ or } 8$
	$\bar{C}_2$ and $M_x/\bar{M}_x$	$\times$	$\tilde{2}$ MLs or $\tilde{4}$
#10	C_4	$(\Gamma, M) : 4\mathbb{Z}\ \&\ (X, Y) : 2\mathbb{Z}$	$8\ (G,\ \Gamma,\ X,\ Y, \text{ or } M)$
	$\bar{C}_4$	$\times$	$\tilde{4}$
#11,12	C_4 and M_x	$\times$	$\tilde{8}$
	C_4 and $\bar{M}_x$	$(\Gamma, M) : 4\mathbb{Z}\ \&\ (X, Y) : 2\mathbb{Z}$	$8\ (\text{MLs}, \Gamma,\ X,\ Y, \text{ or } M) \text{ or } 16$
	$\bar{C}_4$ and $M_x/\bar{M}_x$	$\times$	$\tilde{4}$ MLs or $\tilde{8}$
#13	C_3	$(\Gamma, K, K') : 3\mathbb{Z}$	$6\ (G,\ \Gamma,\ K,\ K', \text{ or } M_{1/2/3})$
	$\bar{C}_3$	$\times$	0
#14	C_3 and M_y	$(K, K') : 3\mathbb{Z}$	$\tilde{6}$ or $\tilde{6}(K, K')$
	C_3 and $\bar{M}_y$	$(\Gamma, K, K') : 3\mathbb{Z}$	$6\ (\text{MLs},\ \Gamma, \text{ or } M_{1/2/3}) \text{ or } 12\ (G,\ K, \text{ or } K')$
	$\bar{C}_3$ and $M_y/\bar{M}_y$	$\times$	0
#15	C_3 and M_x	$\times$	$\tilde{6}$
	C_3 and $\bar{M}_x$	$(\Gamma, K, K') : 3\mathbb{Z}$	$6\ (\text{MLs},\ \Gamma,\ K,\ K', \text{ or } M_{1/2/3}) \text{ or } 12$
	$\bar{C}_3$ and $M_x/\bar{M}_x$	$\times$	0
#16	C_6	$(\Gamma) : 6\mathbb{Z}\ \&\ (K, K') : 3\mathbb{Z}\ \&\ (M_{1/2/3}) : 2\mathbb{Z}$	$12\ (G,\ \Gamma,\ K,\ K', \text{ or } M_{1/2/3})$
	$\bar{C}_6$	$(K, K') : 3\mathbb{Z}$	$\tilde{6}$ or $\tilde{6}(K, K')$
#17	C_6 and M_x	$\times$	$\tilde{12}$
	C_6 and $\bar{M}_x$	$(\Gamma) : 6\mathbb{Z}\ \&\ (K, K') : 3\mathbb{Z}\ \&\ (M_{1/2/3}) : 2\mathbb{Z}$	$12\ (\text{MLs},\ \Gamma,\ K,\ K', \text{ or } M_{1/2/3}) \text{ or } 24$
	$\bar{C}_6$ and M_x	$\times$	$\tilde{6}$ MLs or $\tilde{12}$
	$\bar{C}_6$ and $\bar{M}_x$	$(K, K') : 3\mathbb{Z}$	$\tilde{6}$ MLs or $\tilde{6}(K, K')$ or $\tilde{12}$

Summary

- Twisted bilayer graphene and monolayer graphene with specific periodic potential approximately share the identical low energy physics, which can host flat bands.



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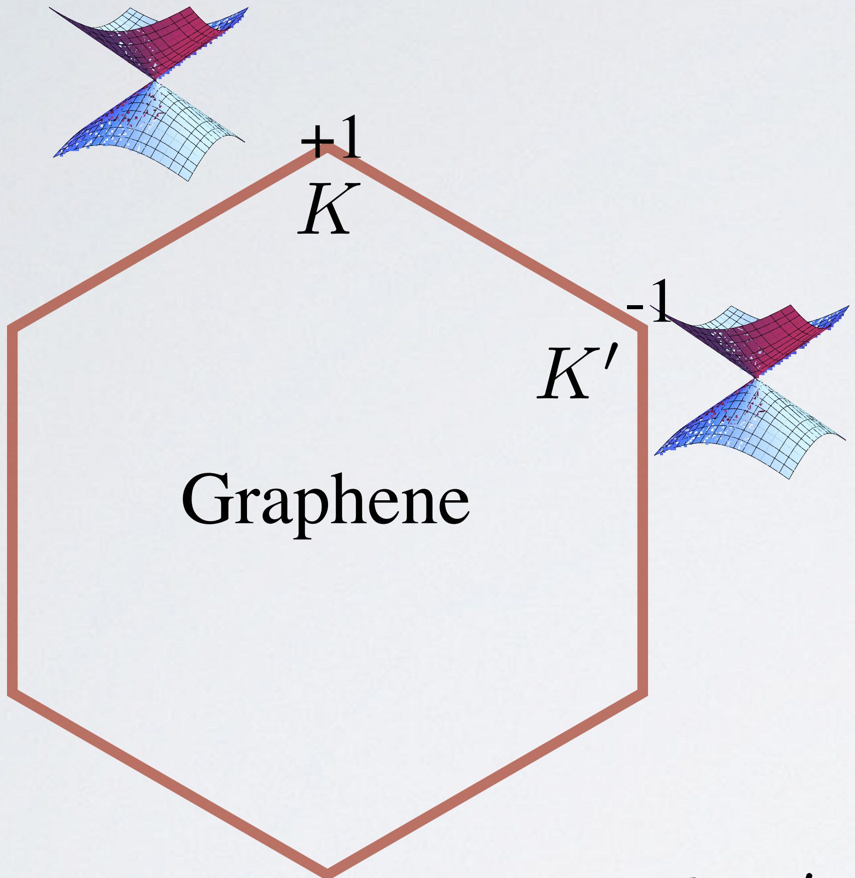
- Having exceptional points at K and K' is difficult. The discriminate number must be a multiple of 3 and the reflection symmetry along $\overline{K\Gamma}$ must be broken.

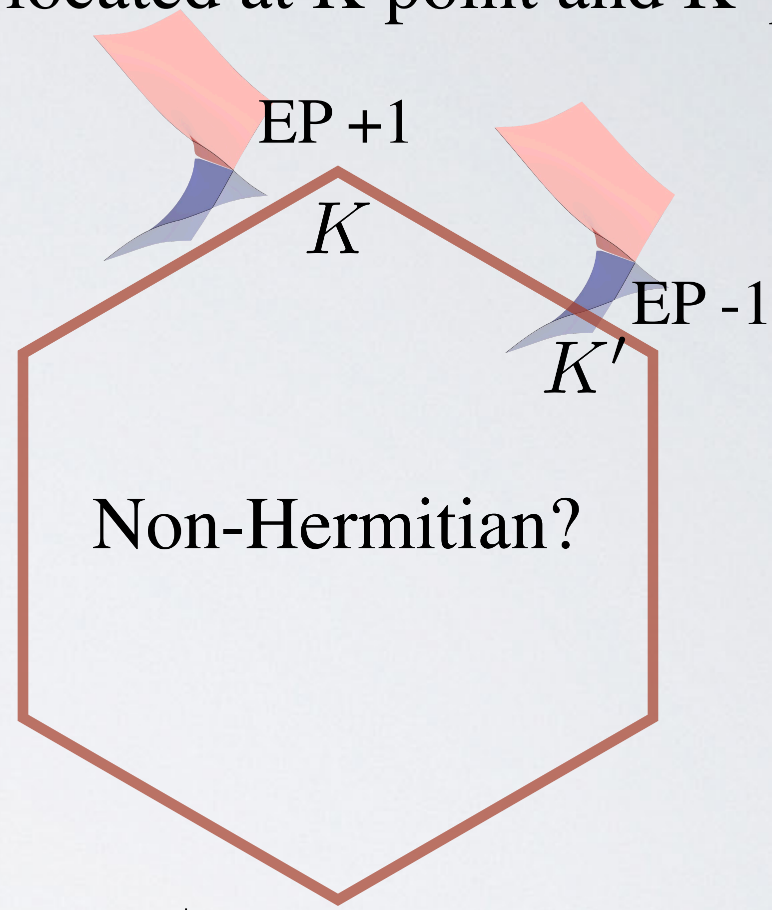
PRB **106**, 045126 (2022)

Thank you !

Questions

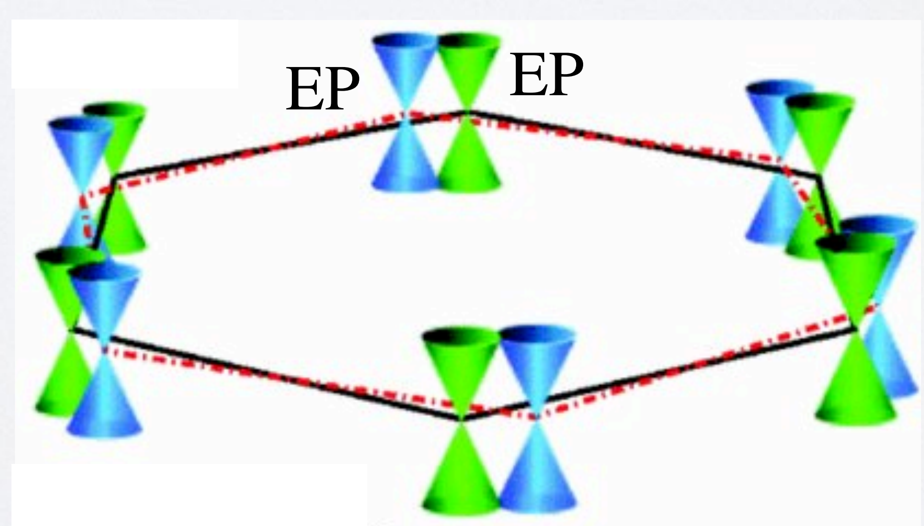
Is it possible to have exceptional points separately located at K point and K' point?



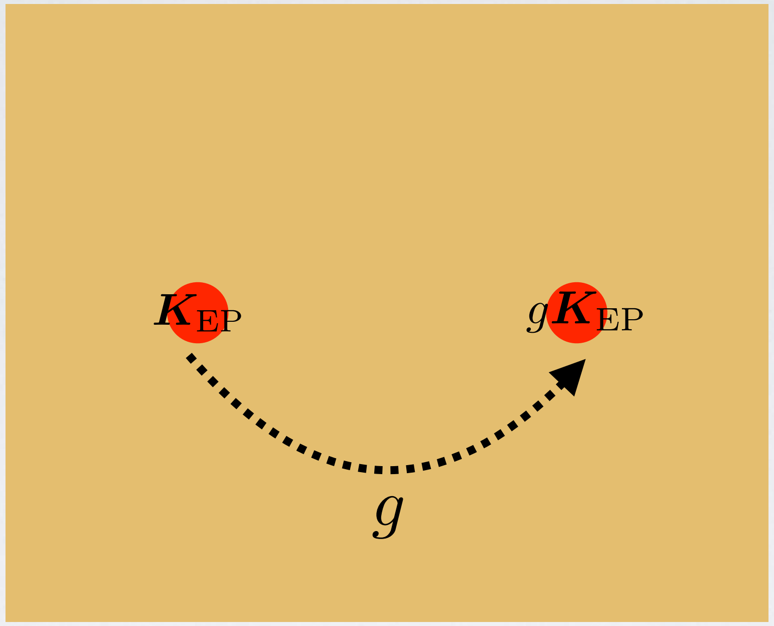


K and K' are C_3 rotation centers

If so, it can lead to twisted non-Hermitian bilayer.



$$\nu_{\mathrm{disc}}(\hat{C}_n \boldsymbol{K}_{\mathrm{EP}}) = \nu_{\mathrm{disc}}(\boldsymbol{K}_{\mathrm{EP}}), \nu_{\mathrm{disc}}(\hat{M} \boldsymbol{K}_{\mathrm{EP}}) = -\nu_{\mathrm{disc}}(\boldsymbol{K}_{\mathrm{EP}})$$



The generalized Nielsen-Ninomiya Theorem

WG	Generators	Rotation centers	ν_{abs}
#1		No centers	2
#2	C_2	$(\Gamma, X, Y, M) : 2\mathbb{Z}$	4 (G, Γ, X, Y, or M)
#3,4,5	M_x	×	$\tilde{2}$
#6,7,8,9	C_2 and M_x	×	$\tilde{4}$
#10	C_4	$(\Gamma, M) : 4\mathbb{Z}$ & $(X, Y) : 2\mathbb{Z}$	8 (G, Γ, X, Y, or M)
#11,12	C_4 and M_x	×	$\tilde{8}$
#13	C_3	$(\Gamma, K, K') : 3\mathbb{Z}$	6 (G, Γ, K, K', or $M_{1/2/3}$)
#14	C_3 and M_y	$(K, K') : 3\mathbb{Z}$	$\tilde{6}$ or $\tilde{6}(K, K')$
#15	C_3 and M_x	×	$\tilde{6}$
#16	C_6	$(\Gamma) : 6\mathbb{Z}$ & $(K, K') : 3\mathbb{Z}$ & $(M_{1/2/3}) : 2\mathbb{Z}$	12 (G, Γ, K, K', or $M_{1/2/3}$)
#17	C_6 and M_x	×	$\tilde{12}$

The generalized Nielsen-Ninomiya Theorem

WG	Generators	Rotation centers	ν_{abs}
#1		No centers	2
#2	C_2	$(\Gamma, X, Y, M) : 2\mathbb{Z}$	4 $(G,\ \Gamma,\ X,\ Y,$ or $M)$
#3,4,5	M_x	×	$\tilde{2}$
#6,7,8,9	C_2 and M_x	×	$\tilde{4}$
#10	C_4	$(\Gamma, M) : 4\mathbb{Z}$ & $(X, Y) : 2\mathbb{Z}$	8 $(G,\ \Gamma,\ X,\ Y,$ or $M)$
#11,12	C_4 and M_x	×	$\tilde{8}$
#13	C_3	$(\Gamma, K, K') : 3\mathbb{Z}$	6 $(G,\ \Gamma,\ K,\ K',$ or $M_{1/2/3})$
#14	C_3 and M_y	$(K, K') : 3\mathbb{Z}$	$\tilde{6}$ or $\tilde{6}(K, K')$
#15	C_3 and M_x	×	$\tilde{6}$
#16	C_6	$(\Gamma) : 6\mathbb{Z}$ & $(K, K') : 3\mathbb{Z}$ & $(M_{1/2/3}) : 2\mathbb{Z}$	12 $(G,\ \Gamma,\ K,\ K',$ or $M_{1/2/3})$
#17	C_6 and M_x	×	$\tilde{12}$

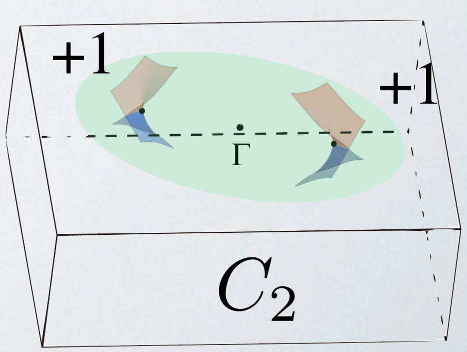
The simple rule for a wallpaper group with C_n rotation generator:

$$\nu_{\mathrm{abs}} = 2n$$

$$C_n \text{ rotation symmetry connects } n \text{ EPs with } \nu_{\mathrm{disc}} = +1$$
$$\text{connects } n \text{ EPs with } \nu_{\mathrm{disc}} = -1$$

Application: A surface of a 3D non-Hermitian topological insulator can violate the Nielsen-Ninomiya theorem. Without breaking C_n rotation symmetry, the anomalous surface has n EPs.

3D topological invariant $\nu_{3D} = nl$



Summary

1. When crystalline symmetries are preserved, the minimal number ν_{abs} of exceptional points is more than **two.**

2. At the C_n rotation center, the charge of the EP is limited to

$$\nu_{\mathrm{disc}}(\boldsymbol{K}_{\mathrm{EP}}) = nj$$

3. The simple rule for a wallpaper group with C_n rotation generator:

$$\nu_{\mathrm{abs}} = 2n$$

4. Application: C_n rotation symmetry leads to that the topological invariant of the non-Hermitian 3D topological bulk must be a multiple of n.

$$\nu_{3D} = nl$$

C Le, Z Yang, F Cui, AP Schnyder, CK Chiu, PRB 105, 045126 (2022)