

Quantum transport in graphene

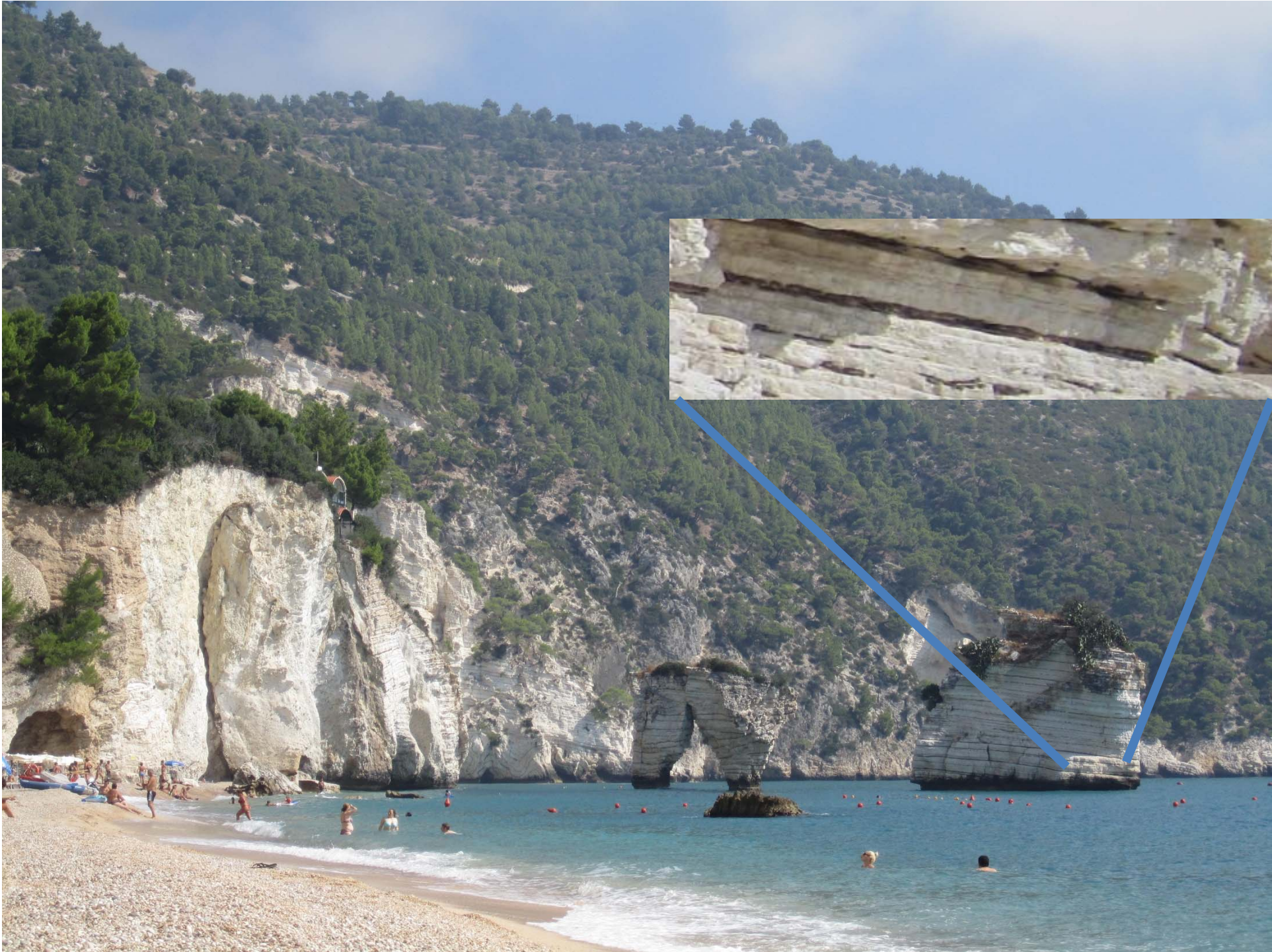
- L1 Disordered graphene (G)**
- L2 Ballistic electrons in graphene (G/hBN)**
- L3 Moiré superlattice effects in G/hBN heterostructures**

tunnelling between almost aligned graphene flakes

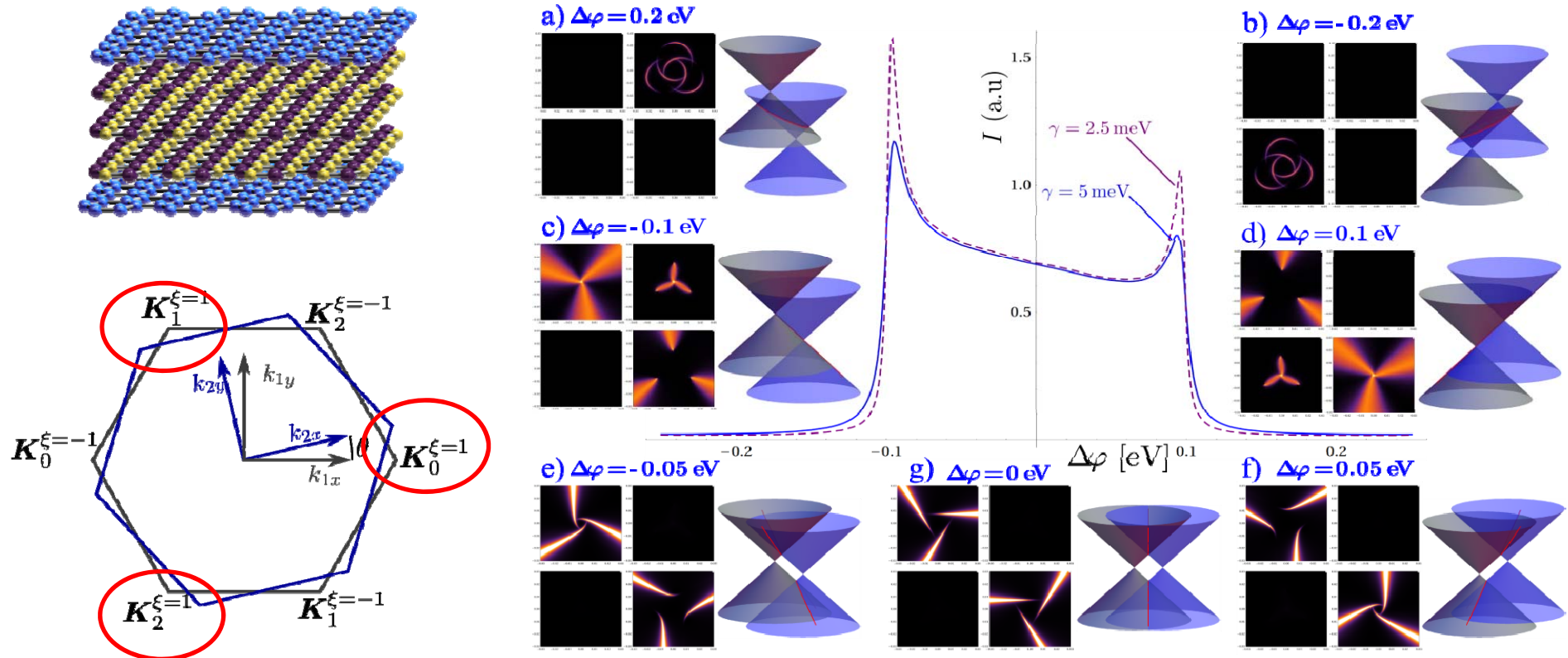
moiré superlattice in van der Waals heterostructures

moiré minibands in G/hBN

Brown-Zak magnetic minibands in G/hBN

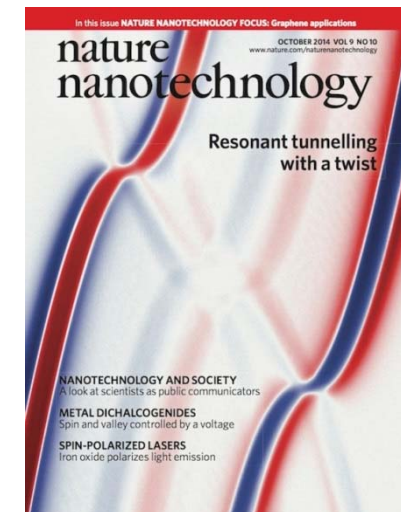
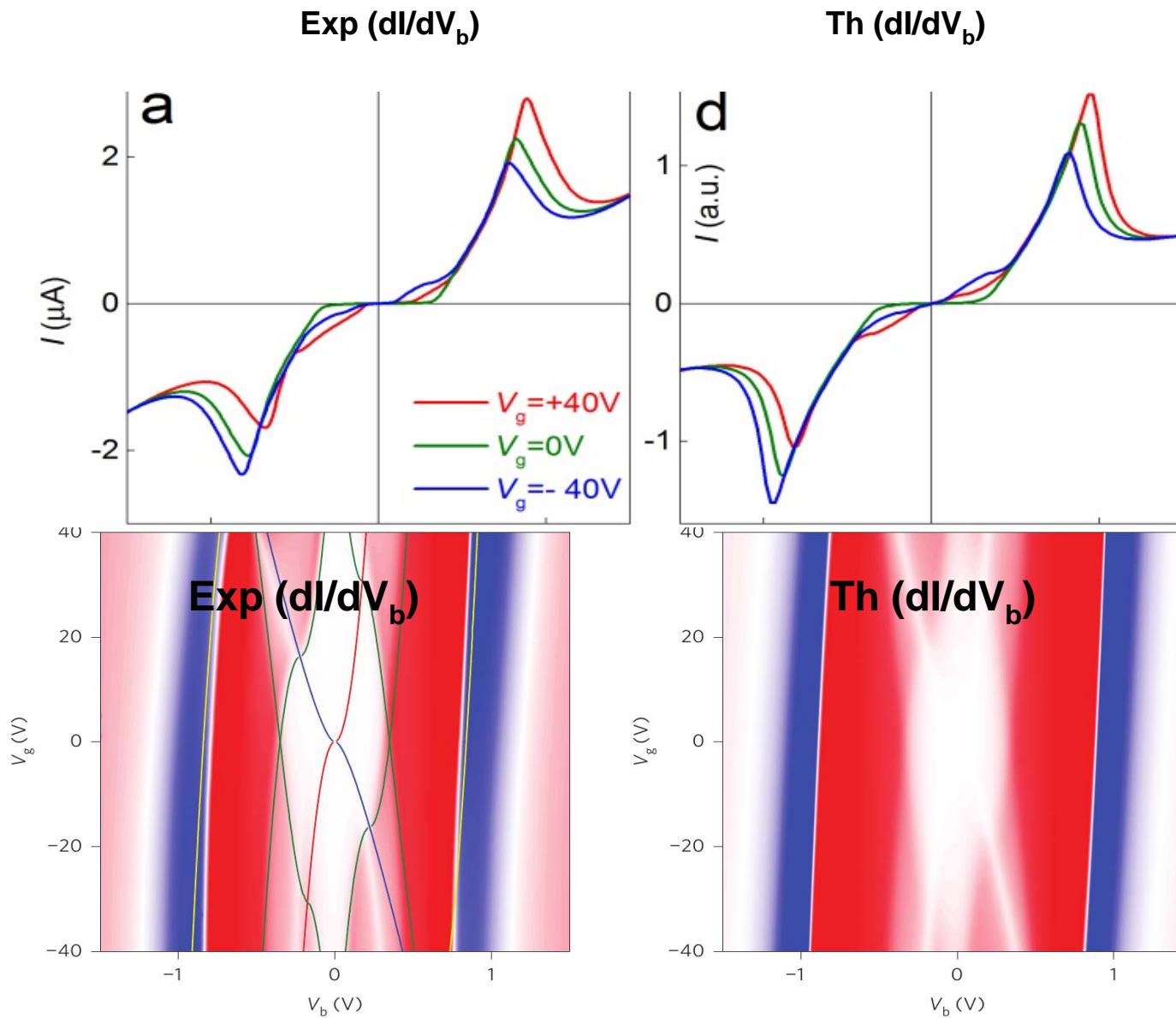


Momentum-conserving resonant tunnelling between graphene flakes in G/hBN/G structures



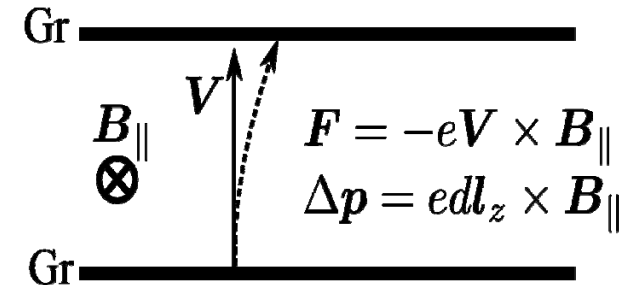
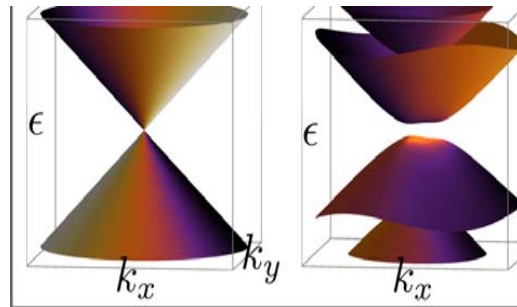
Mishchenko, Tu, Cao, Gorbachev, Wallbank, Greenaway, Morozov, Zhu, Wong, Withers, Woods, Kim, Watanabe, Taniguchi, Vdovin, Makarovskiy, Fromhold, Fal'ko, Geim, Eaves, Novoselov - Nature Nanotechnology 9, 808 (2014)

Resonant tunnelling in almost aligned ballistic G/hBN/G structures



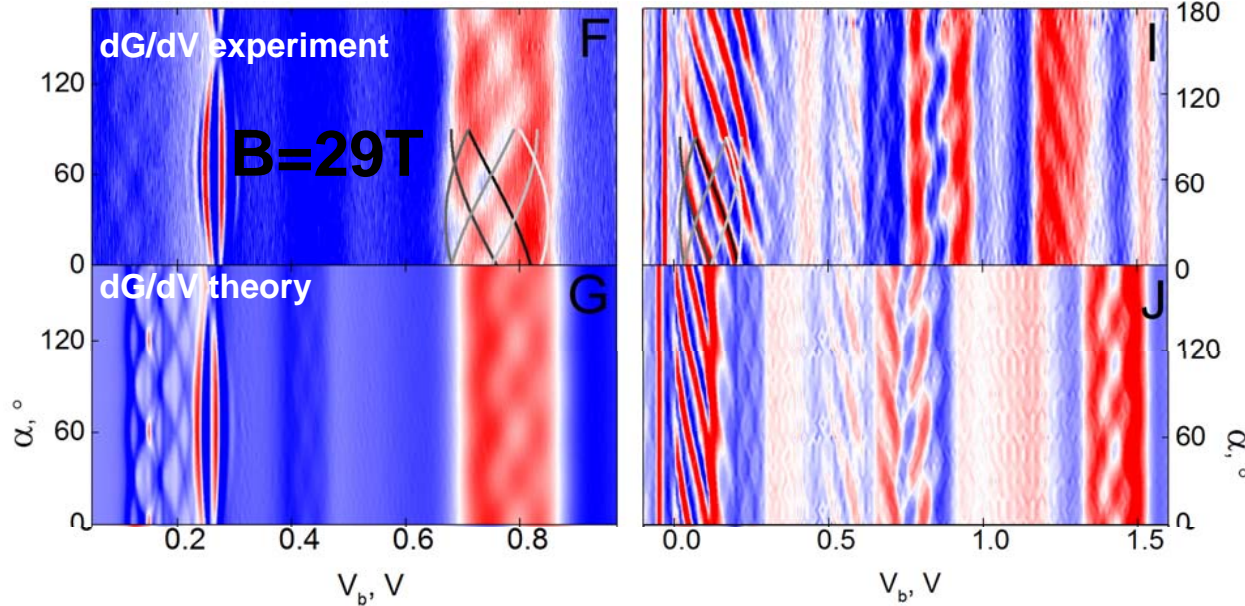
Mishchenko, Tu, Cao, Gorbachev, Wallbank, Greenaway, Morozov, Morozov, Zhu, Wong, Withers, Woods, Kim, Watanabe, Taniguchi, Vdovin, Makarovskiy, Fromhold, Fal'ko, Geim, Eaves, Novoselov - Nature Nanotechnology 9, 808 (2014)

Momentum-conserving resonant tunnelling between almost aligned graphene flakes in G/hBN/G structures



Gr-hBN-Gr

BLGr-hBN-Gr



Lorentz boost:
in-plane magnetic field
distinguishes
resonance tunneling
conditions in six
Brillouin zone corners,
probed by rotating the
in-plane magnetic field.

$$\Delta K_j \approx \theta l_z \times K_j + \Delta p$$

Wallbank, Ghazaryan, Misra, Cao, Tu, Piot, Potemski, Pezzini, Wiedmann, Zeitler, Lane, Morozov, Greenaway, Eaves, Geim, Fal'ko, Novoselov, Mishchenko - Science 353, 575 (2016)

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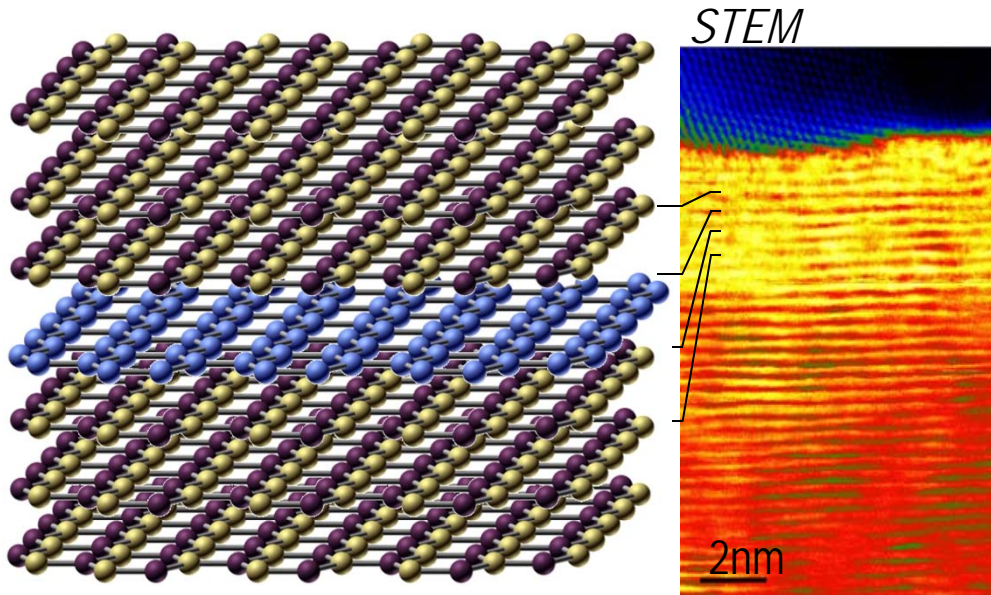
moiré superlattice in van der Waals heterostructures

moiré minibands in G/hBN

Brown-Zak magnetic minibands in G/hBN

Graphene: gapless semiconductor
with Dirac electrons

$$\hat{H} = v\vec{\sigma} \cdot \vec{p}$$

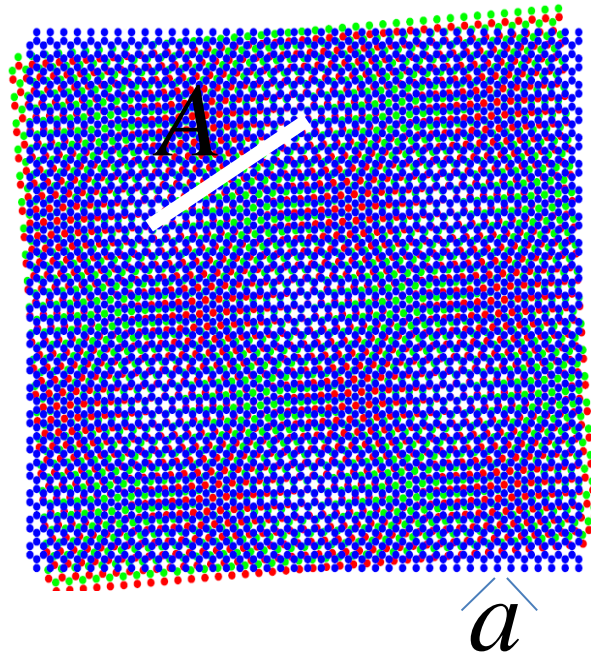


hBN ('white graphene')
 sp^2 – bonded insulator with
a large band gap, $\Delta > 5\text{eV}$

$$\hat{H} = \Delta\sigma_z + v'\vec{\sigma} \cdot \vec{p}$$

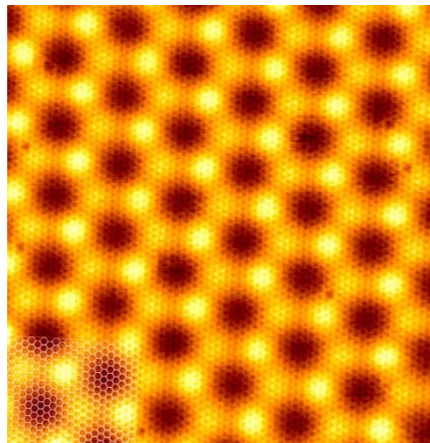
- Hexagonal boron nitride (hBN) is an ideal atomically flat substrate and insulating environment for graphene
- Almost aligned graphene – hBN heterostructures feature moiré superlattices generating moiré minibands for Dirac electrons in graphene and Zak-Brown magnetic minibands ('Hofstadter butterfly'), observable at high temperatures

Moiré pattern

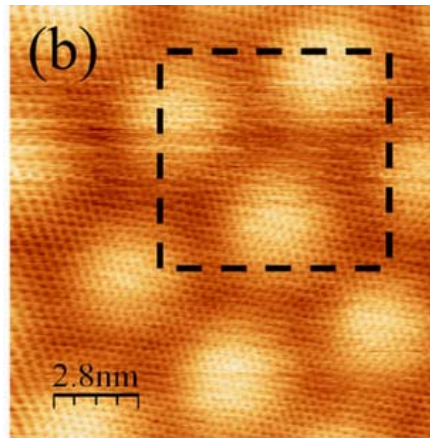


$$A \approx \frac{a}{\sqrt{\delta^2 + \theta^2}}$$

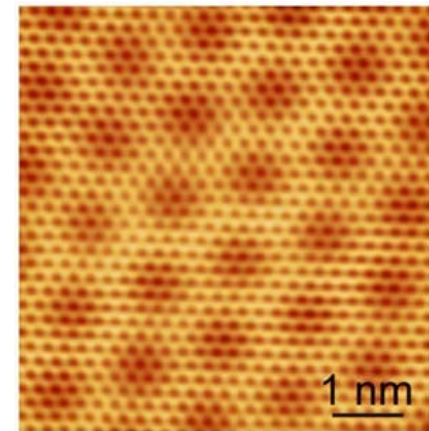
↑ lattice mismatch 1.8% for G/hBN ↑ misalignment



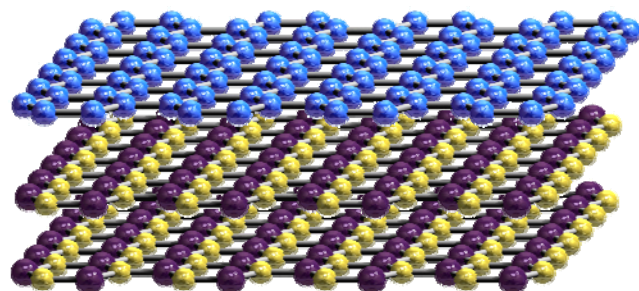
STM of graphene on Ir(111)
Busse et al
PRL 107, 036101 (2011)



STM of graphene on Ni
Arramel et al
Graphene 2, 102 (2013)

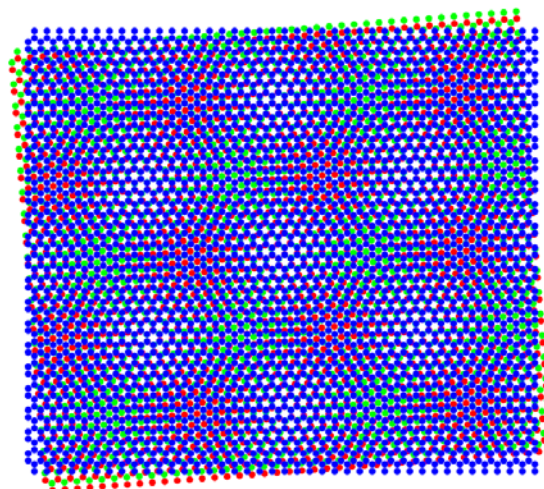


STM of G/hBN
Xue et al
Nature Mat. 10, 282–285 (2011)



highly oriented
graphene-BN:

$A \sim 15 \text{ nm}$



heterostructure
with new
electronic
properties

Highly oriented graphene-hBN heterostructures
(misalignment $\theta < 1^\circ$) have been produced
by groups of Geim & Novoselov (Manchester)

Ponomarenko, Gorbachev, Elias, Yu, Patel, Mayorov, Woods, Wallbank, Mucha-Kruczynski,
Piot, Potemski, Grigorieva, Guinea, Novoselov, VF, Geim - Nature 497, 594 (2013)

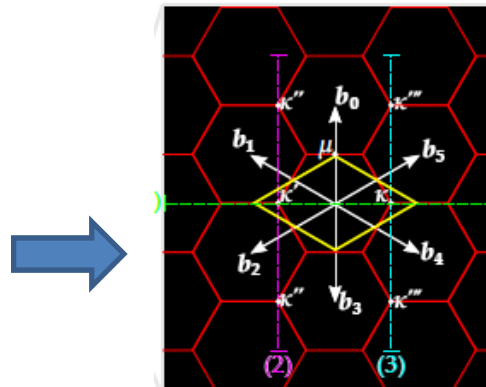
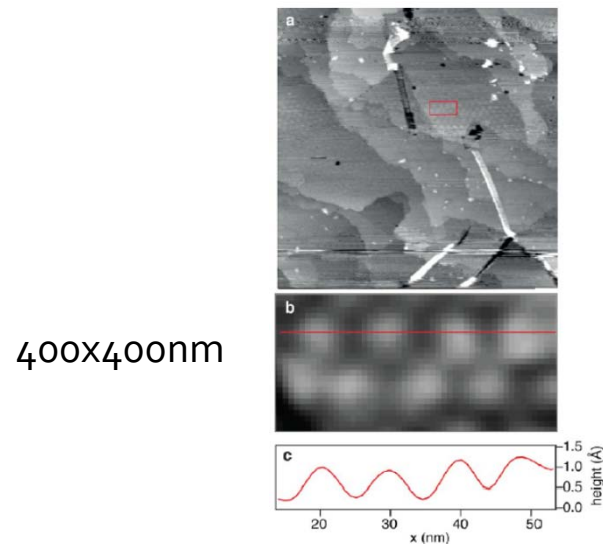
Jarillo-Herrero & Ashoori (MIT), Kim & Hone (Columbia)

B Hunt, et al - Science 340, 1427 (2013)

CR Dean, et al, Nature 497, 598 (2013)

Graphene grown on hBN

CVD: Usachov *et al.*, PRB 82, 075415 (2010); Roth *et al.*, Nano Letters 13, 2668 (2013);
 Yang *et al.*, Nature Mater. 12, 792 (2013),



superlattice with period $A \gg a$
 and reciprocal lattice (Bragg)
 vectors

$$\vec{b}_n = \vec{G}_n^G - \vec{G}_n^{hBN}$$

MBE: Summerfield, Davies, Cheng, Korolkov, Cho, Mellor, Foxon, Khlobystov, Watanabe,
 Taniguchi, Eaves, Novikov, Beton - Scientific Reports 6, 22440 (2016)

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moiré superlattice in van der Waals heterostructures

moiré minibands in G/hBN

Brown-Zak magnetic minibands in G/hBN

Separation between layers is larger than the lattice constant, hence, moiré perturbation is dominated by harmonics determined by simplest combinations of Bragg vectors of graphene and hBN (effect of higher harmonics is exponentially small)

Lopes dos Santos, Peres, Castro Neto - PRL 99, 256802 (2007)

Lopes dos Santos, Peres, Castro Neto - arXiv:1202.1088 (2012)

Bistritzer, MacDonald - PRB 81, 245412 (2010)

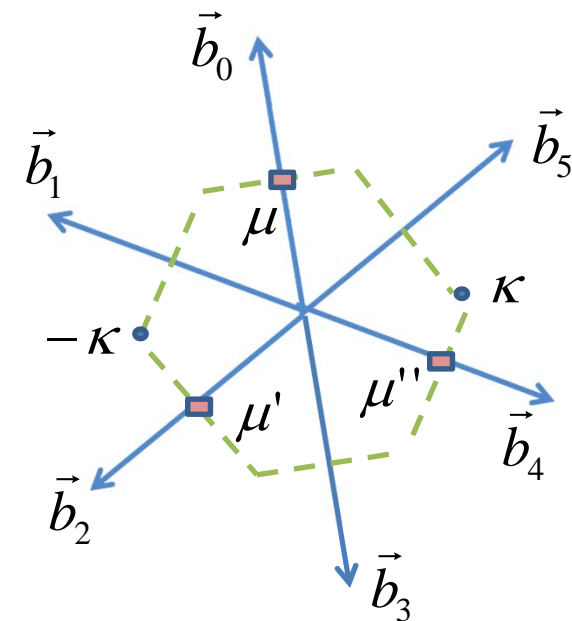
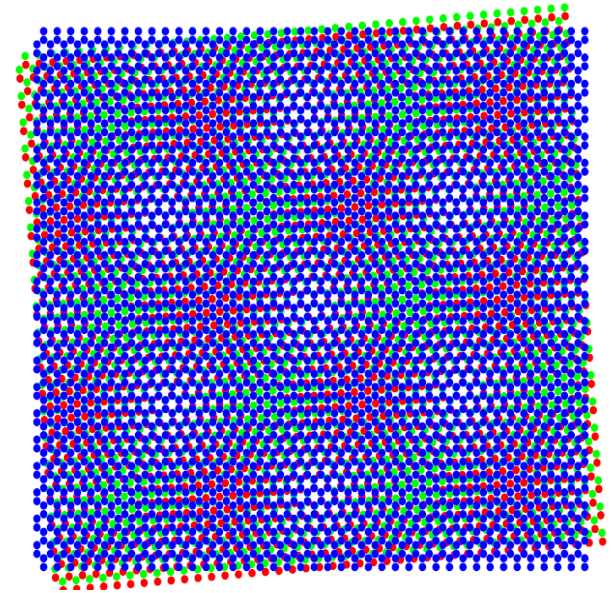
Kindermann, Uchoa, Miller - Phys. Rev. B 86, 115415 (2012)

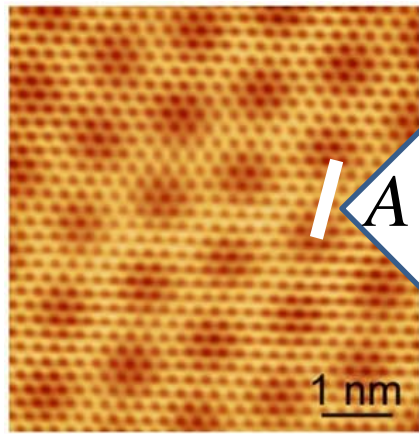
$$\vec{b}_0 = \vec{G}_G - \vec{G}_{BN} = \left[1 - (1 + \delta)^{-1} \hat{R}_\theta \right] \begin{pmatrix} \frac{4\pi}{3a} \\ 0 \end{pmatrix}$$

$$|\vec{b}_0| \equiv b \approx \frac{3\pi}{4a} \sqrt{\delta^2 + \theta^2}$$

lattice mismatch
1.8% for G/hBN

misalignment
<5°



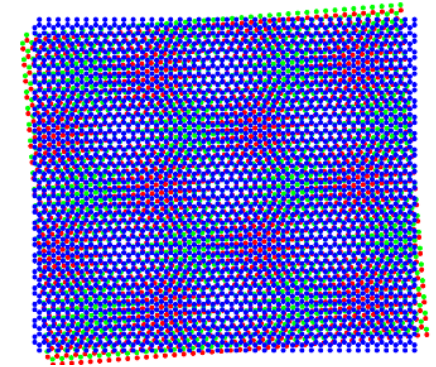


$$A \approx \frac{a}{\sqrt{\delta^2 + \theta^2}}$$

small misalignment

lattice mismatch

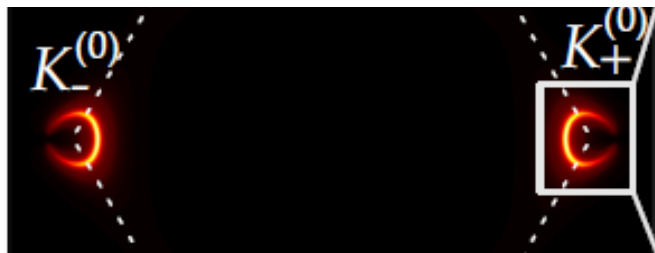
$\delta=0.018$ for non-strained graphene on hBN



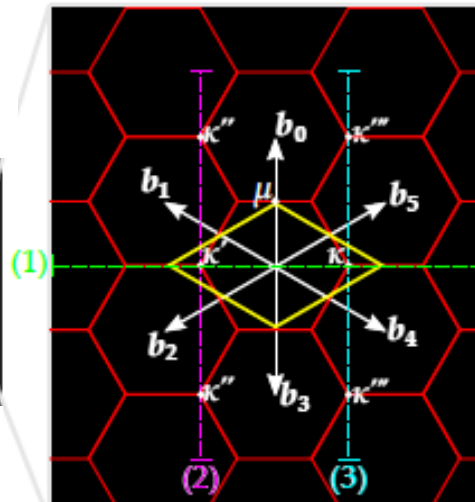
Xue, Sanchez-Yamagishi, Bulmash, Jacquod, Deshpande, Watanabe, Taniguchi, Jarillo-Herrero, LeRoy - Nature Mat 10, 282 (2011)

Long-period moiré patterns are generic for all G/hBN heterostructures, grown and mechanically transferred

Both graphene and hBN lattices are honeycomb,

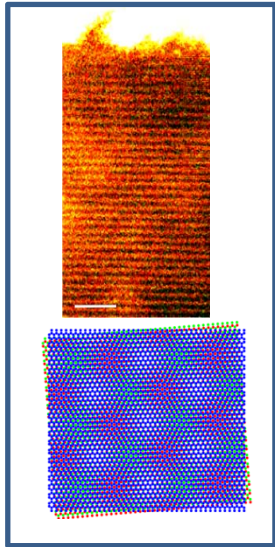


hence, moiré superlattice is hexagonal

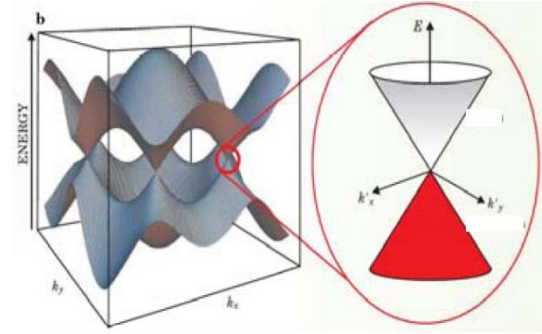


$$\vec{b} = \vec{G}^G - \vec{G}^{hBN} = \frac{2\pi}{4A}$$

$$b_n \approx \frac{3\pi}{4a} \sqrt{\delta^2 + \theta^2} \ll K, G^G$$



electrons in G/hBN moiré superlattices



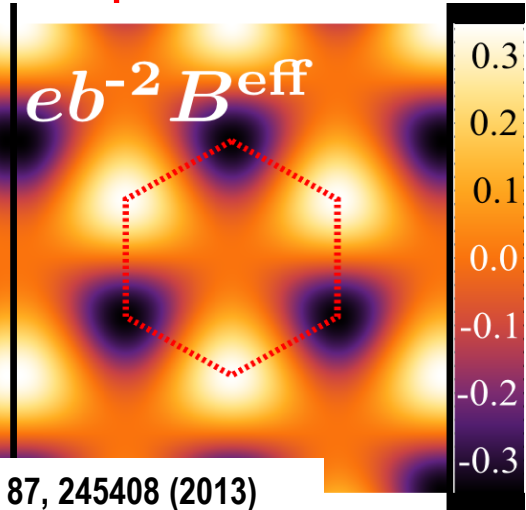
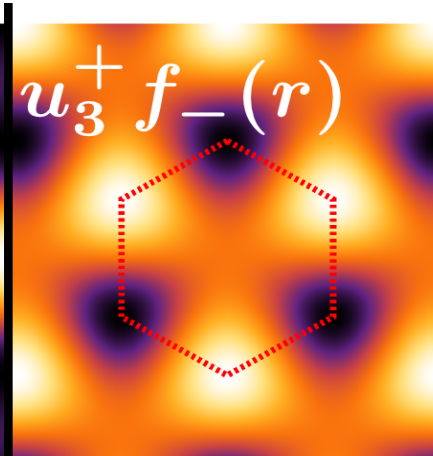
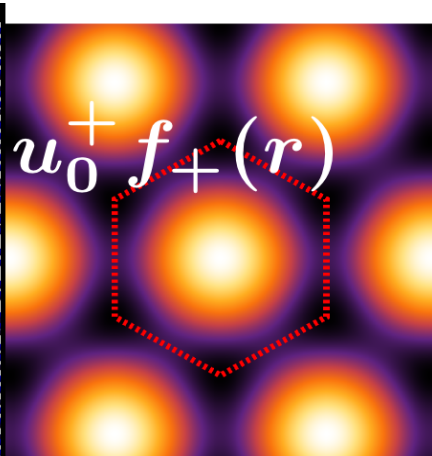
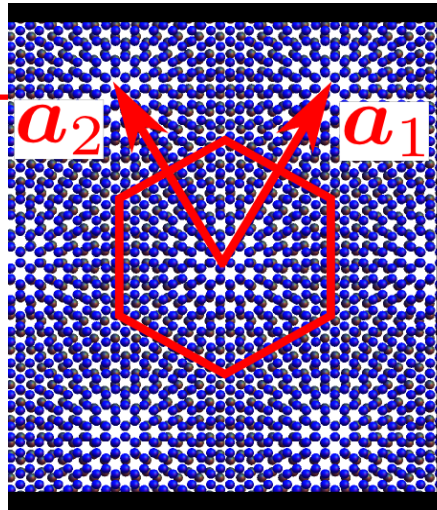
$$a_z > a \Rightarrow \text{only } \vec{b} = \vec{G}^G - \vec{G}^{hBN} \longrightarrow \delta H_{\text{moiré}}$$

electrostatic modulation

sublattice asymmetry

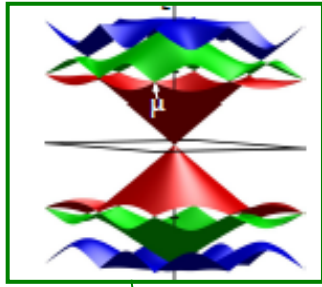
hopping between sublattices, leading to a pseudomagnetic field

$$\hat{H} = vp \cdot \sigma + u_0 v b f_1(r) + u_3 v b f_2(r) \sigma_3 \tau_3 + u_1 v [l_z \times \nabla f_2(r)] \cdot \sigma \tau_3 \quad \text{inversion symmetric}$$

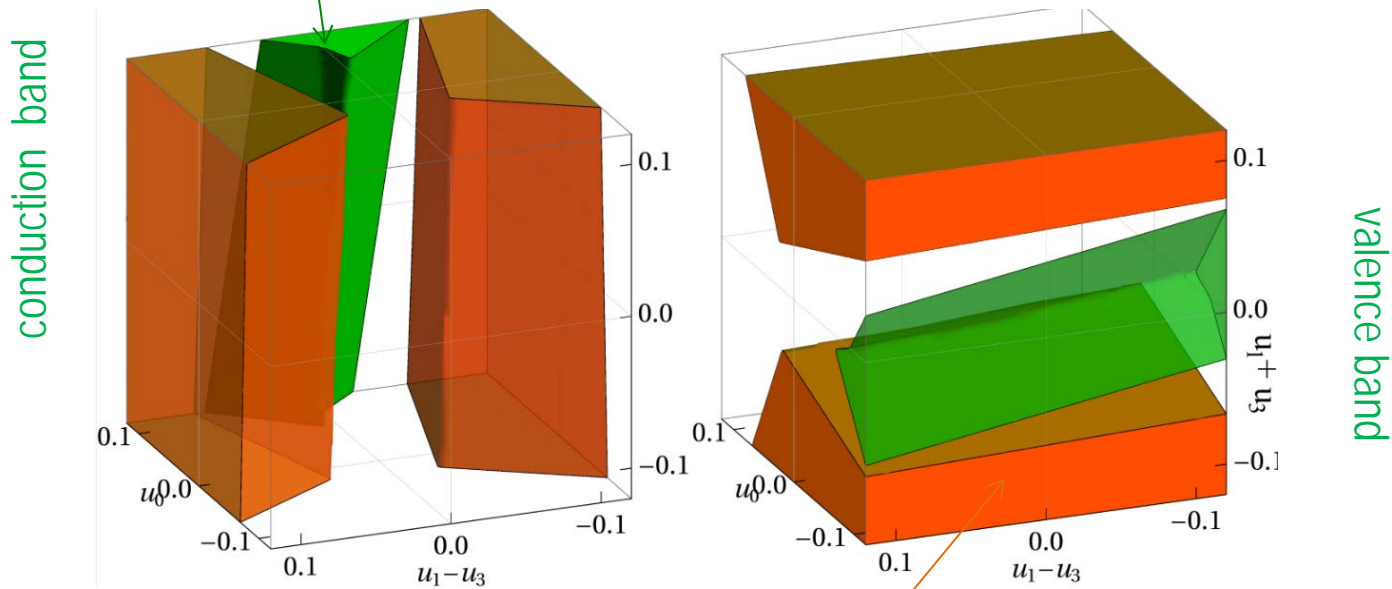


Wallbank, Patel, Mucha-Kruczynski, Geim, Fal'ko - PRB 87, 245408 (2013)

three mini-DPs
at the edge
of 1st miniband

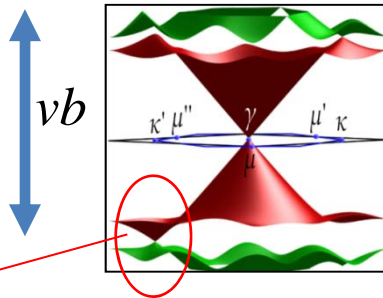


characteristic moiré miniband regimes:
no electron-hole symmetry



single mini-Dirac point at
the edge of 1st miniband

$$v_{mDP} \approx \frac{1}{2} v$$



G-hBN hopping model and electric
quadrupole moments on, e.g., nitrogen sites

$$\frac{1}{2} u \quad - \frac{vbu_0}{\sqrt{\delta^2 + \theta^2}} u \quad - \frac{vbu_1}{\sqrt{\delta^2 + \theta^2}} u \quad - \frac{vbu_3}{2} u$$

graphene sublattice

graphene valley

$$\hat{H} = vp \cdot \sigma + u_0 v b f_1(\mathbf{r}) + u_3 v b f_2(\mathbf{r}) \sigma_3 \tau_3 + u_1 v [l_z \times \nabla f_2(\mathbf{r})] \cdot \sigma \tau_3 + \tilde{u}_0 v b f_2(\mathbf{r}) + \tilde{u}_3 v b f_1(\mathbf{r}) \sigma_3 \tau_3 + \tilde{u}_1 v [l_z \times \nabla f_1(\mathbf{r})] \cdot \sigma \tau_3$$

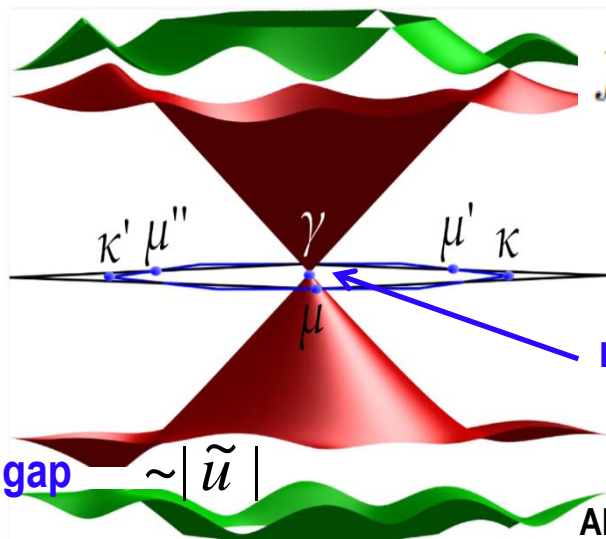
graphene lattice may adjust to the periodic modulation of vdW force

$$\vec{\ell}(\vec{r}) = \sum_m \vec{\ell}_m e^{i\vec{b}_m \vec{r}}$$

$$u_i = u_i(d + \ell_z)$$

$$f_1(\mathbf{r}) = \sum_{m=0\dots5} e^{i\mathbf{b}_m \cdot \mathbf{r}} e^{i\vec{G}_m \vec{\ell}(\vec{r})}$$

$$f_2(\mathbf{r}) = i \sum_{m=0\dots5} (-1)^m e^{i\mathbf{b}_m \cdot \mathbf{r}} e^{i\vec{G}_m \vec{\ell}(\vec{r})}$$



minigap at the band edge $\sim |\tilde{u}u| + |\vec{\ell}| |\tilde{u}|$

minigap $\sim |\tilde{u}|$

San-Jose, Gutierrez, Sturla, Guinea - PRB 90, 075428 (2014)

Cosma, Wallbank, Cheainov, Fal'ko - Faraday Discussion 173 (2014)

Kindermann, Uchoa, Miller - Phys. Rev. B 86, 115415 (2012)

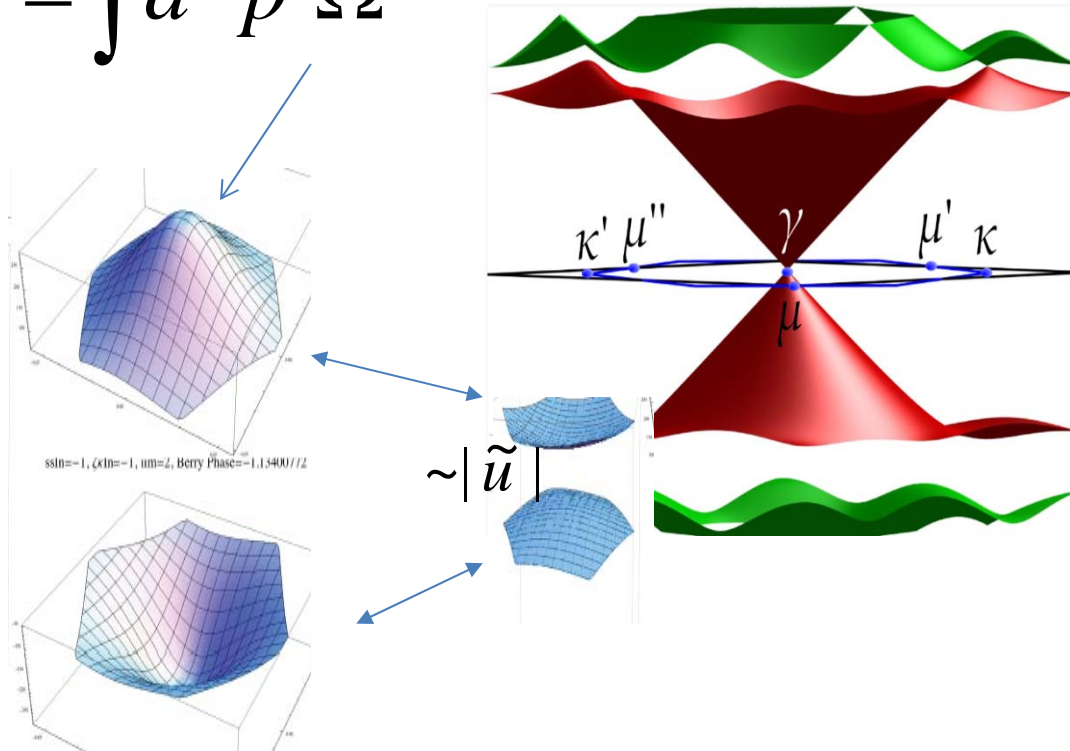
Abergel, Wallbank, Chen, Mucha-Kruczynski, Fal'ko - New J Phys 15, 123009 (2013)

San-Jose, Gutierrez, Sturla, Guinea - PRB 90, 115152 (2014)

Wallbank, Mucha-Kruczynski, Chen, Fal'ko - Ann. Phys. 527, 359 (2015)

Berry phase and Berry curvature for gapped secondary DPs:

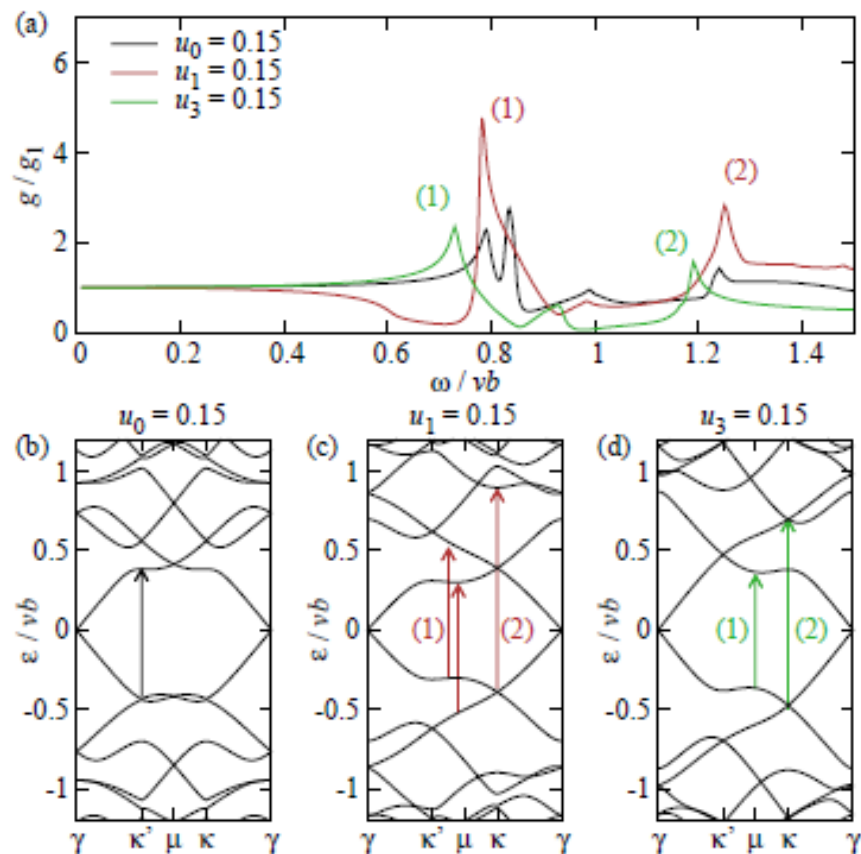
$$\Phi = \int d^2 p \Omega$$



$$\Omega(\tilde{u} \rightarrow 0) \rightarrow \pm \pi \delta(\vec{p} - \vec{K})$$

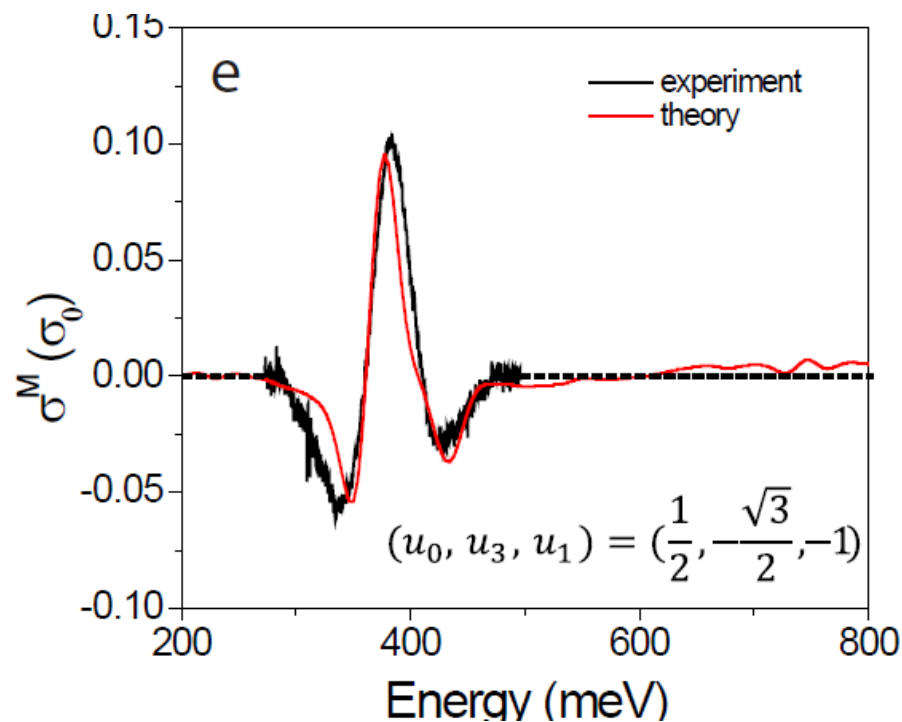
$$\Phi(\tilde{u} \rightarrow 0) \rightarrow \pm \pi$$

Optical signature of moiré minibands



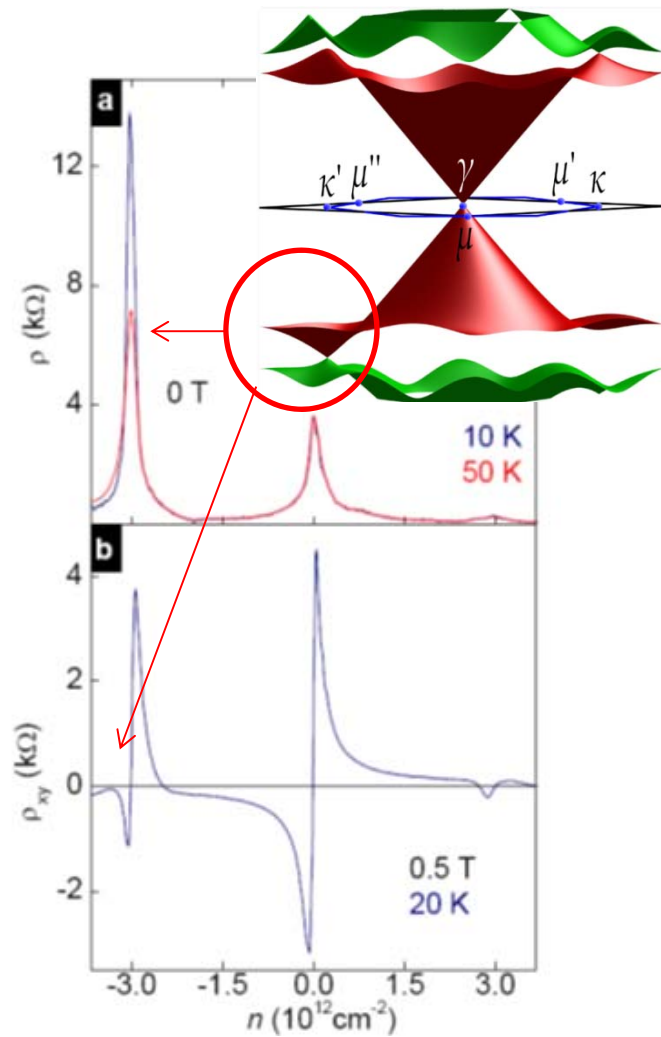
For better visibility should be enhanced by differentiation with respect to gate voltage/density

Abergel, Wallbank, Chen, Mucha-Kruczynski, Fal'ko
New J Phys 15, 123009 (2013)

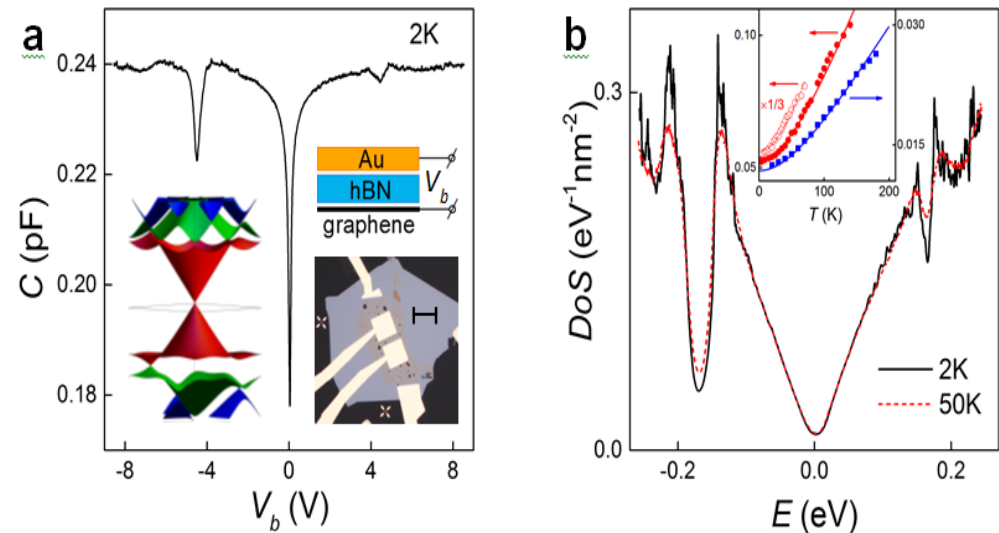


Shi, Jin, Yang, Ju, Horng, Lu, Bechtel, Martin, Fu, Wu, Watanabe, Taniguchi, Zhang, Bai, Wang, Zhang, Wang
Nature Physics 10, 743 (2014)

Manifestation of minibands in magneto-transport and capacitance spectroscopy

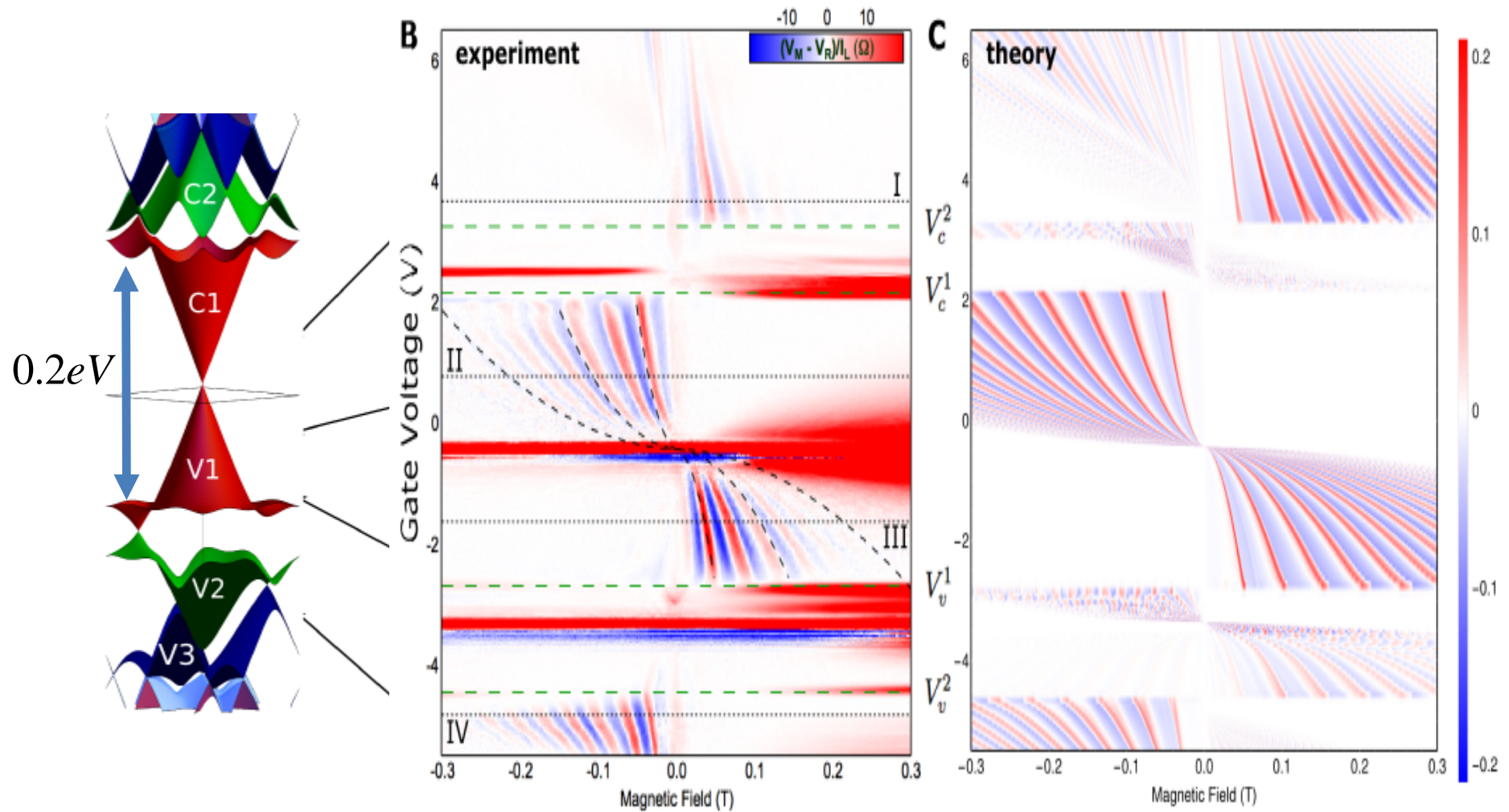


Ponomarenko, Gorbachev, Elias, Yu, Patel, Mayorov, Woods, Wallbank, Mucha-Kruczynski, Piot, Potemski, Grigorieva, Guinea, Novoselov, Fal'ko, Geim
 Nature 497, 594 (2013)
 Wallbank, Patel, Mucha-Kruczynski, Geim, Fal'ko
 PRB 87, 245408 (2013)



Yu, Gorbachev, Tu, Kretinin, Cao, Jalil, Withers, Ponomarenko, Chen, Piot, Potemski, Elias, Watanabe, Taniguchi, Grigorieva, Novoselov, Fal'ko, Geim, Mishchenko
 Nature Physics 10, 525 (2014)

Transverse magnetic focusing of electrons in moiré minibands in almost aligned G/hBN



Lee, Wallbank, Gallagher, Watanabe, Taniguchi, Fal'ko, Goldhaber-Gordon - Science 353, 1526 (2016)

Landau levels of Dirac electrons in a magnetic field

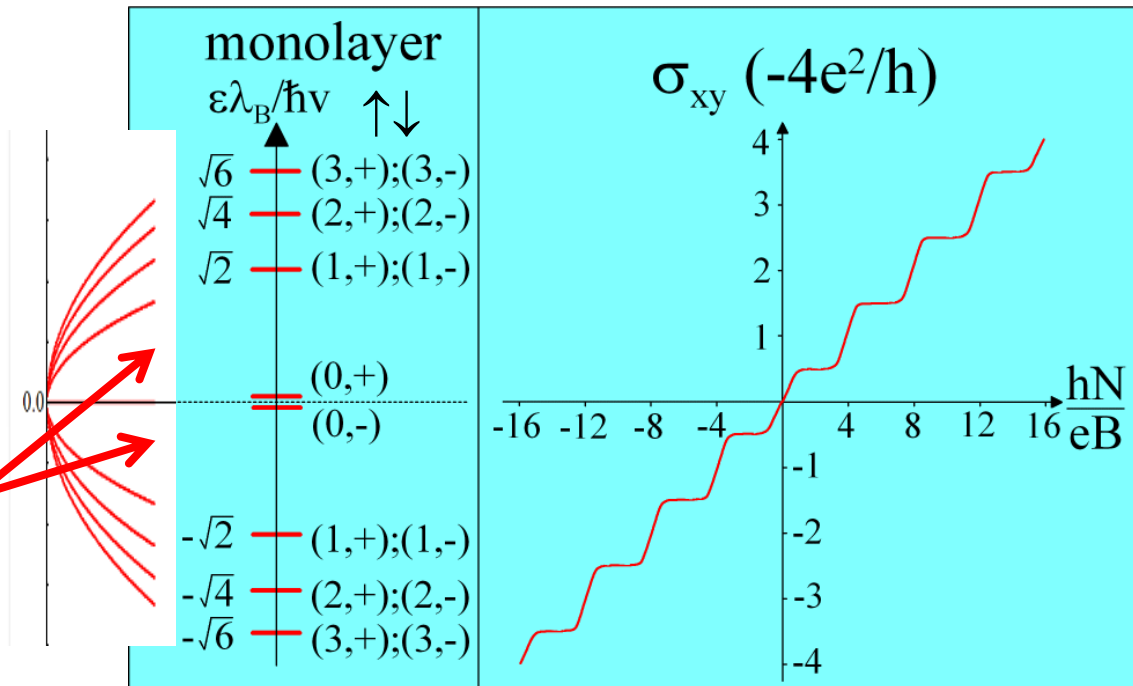
$$H = v(\vec{p} - \frac{e}{c}\vec{A}) \cdot \vec{\sigma} \Rightarrow$$

$$\varepsilon^\pm = \pm \sqrt{2n} \frac{v}{\lambda_B} \propto \sqrt{n \cdot B}$$

with 4-fold degenerate
Landau level

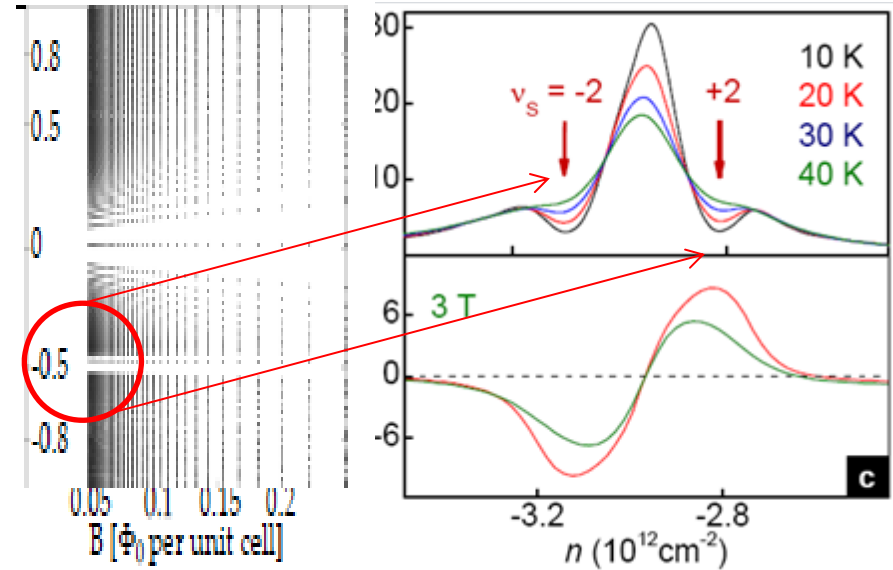
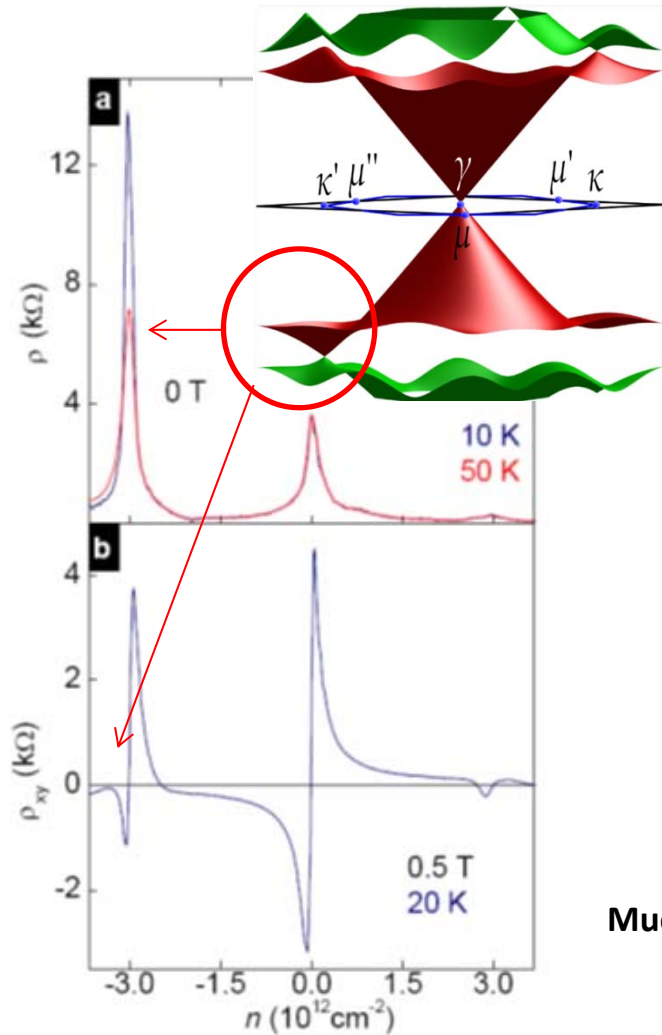
McClure - Phys. Rev. 104, 666 (1956)

**the largest gaps in
the LL spectrum**



**Should be the same for the secondary Dirac electrons
at the edge of the 1st moiré miniband**

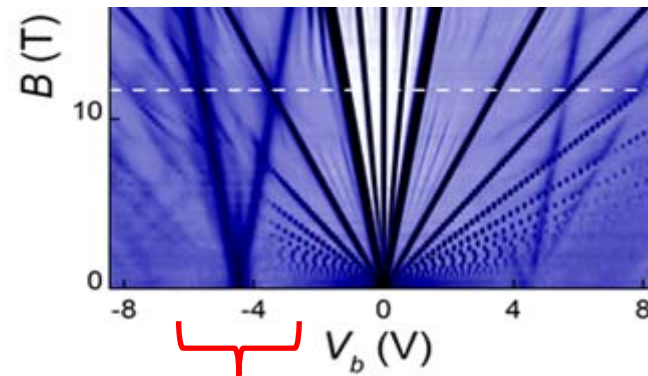
Magneto-transport in oriented graphene-BN heterostructures



Wallbank, Patel, Mucha-Kruczynski, Geim, Fal'ko - PRB 87, 245408 (2013)
 Ponomarenko, Gorbachev, Elias, Yu, Patel, Mayorov, Woods, Wallbank,
 Mucha-Kruczynski, Piot, Potemski, Grigorieva, Guinea, Novoselov, Fal'ko, Geim
 Nature 497, 594 (2013)

Magneto-capacitance

Yu, Gorbachev, Tu, Kretinin, Cao, Jalil, Withers, Ponomarenko, Chen,
 Piot, Potemski, Elias, Watanabe, Taniguchi, Grigorieva, Novoselov,
 Fal'ko, Geim, Mishchenko Nature Physics 10, 525 (2014)



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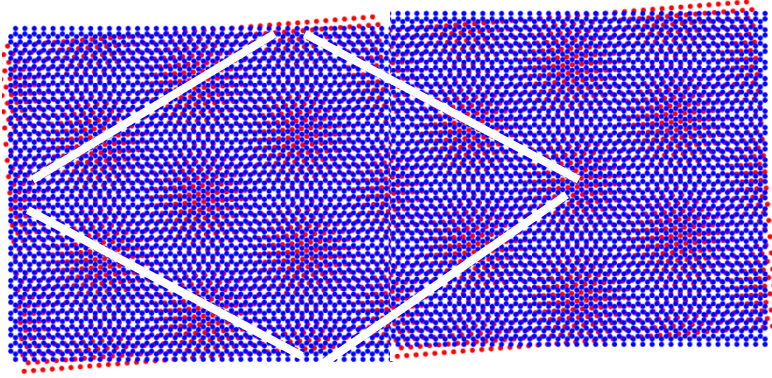
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Brown-Zak magnetic minibands in G/hBN

Brown, PR 133, A1038 (1964); Zak, PR 134, A1602 & A1607 (1964)



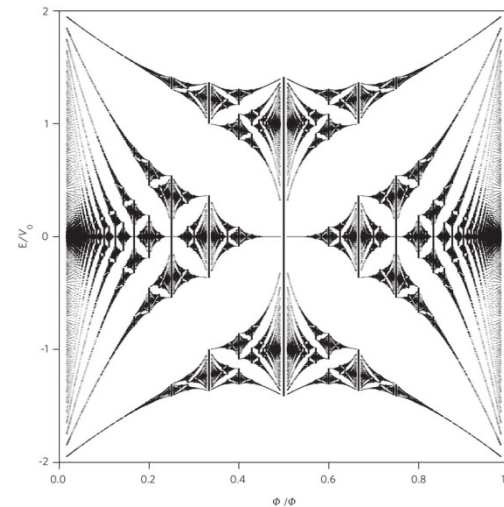
$$\phi \equiv BS = \frac{p}{q} \phi_0, \quad \phi_0 = \frac{h}{e}$$

Magnetic minibands at rational values of magnetic field flux per super-cell

‘Magnetic lattice’ with a q^2 times bigger effective supercell and q^2 times smaller mini Brillouin zone.

Each state in this mini Brillouin zone is q times degenerate.

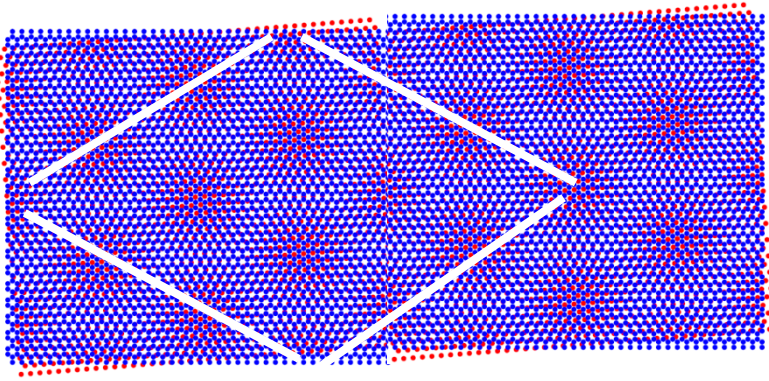
Branded as fractal ‘Hofstadter butterfly’ spectrum.



Example for the tight-binding model on a square lattice

Hofstadter
PRB 14, 2239
(1976)

Brown - PR 133, A1038 (1964)
 Zak - PR 134, A1602 & A1607 (1964)

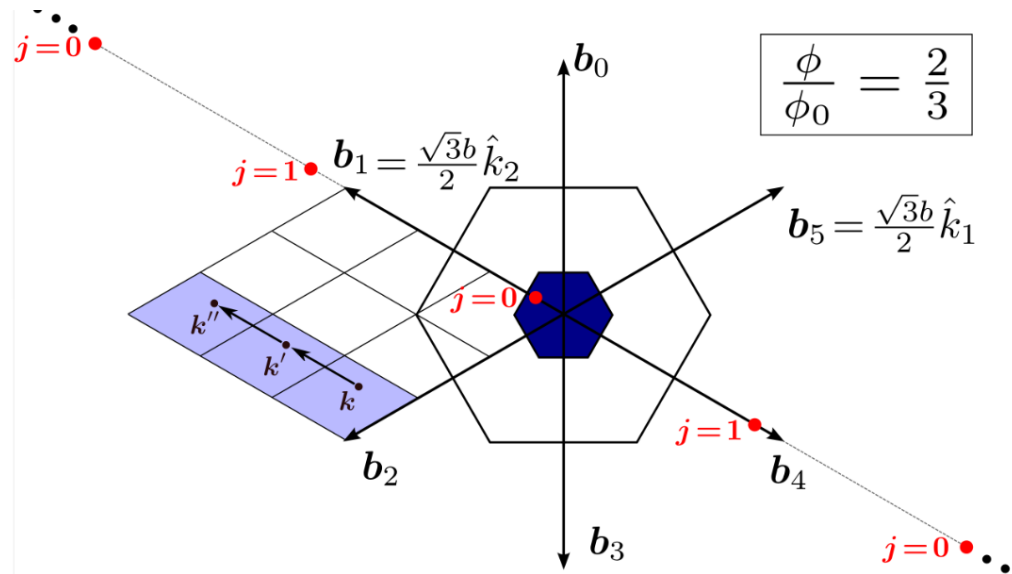


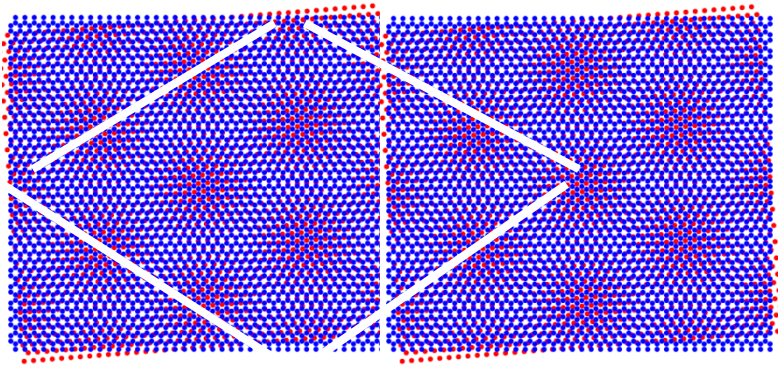
Zak-Brown magnetic minibands

$$\phi \equiv BS = \frac{p}{q} \phi_0$$

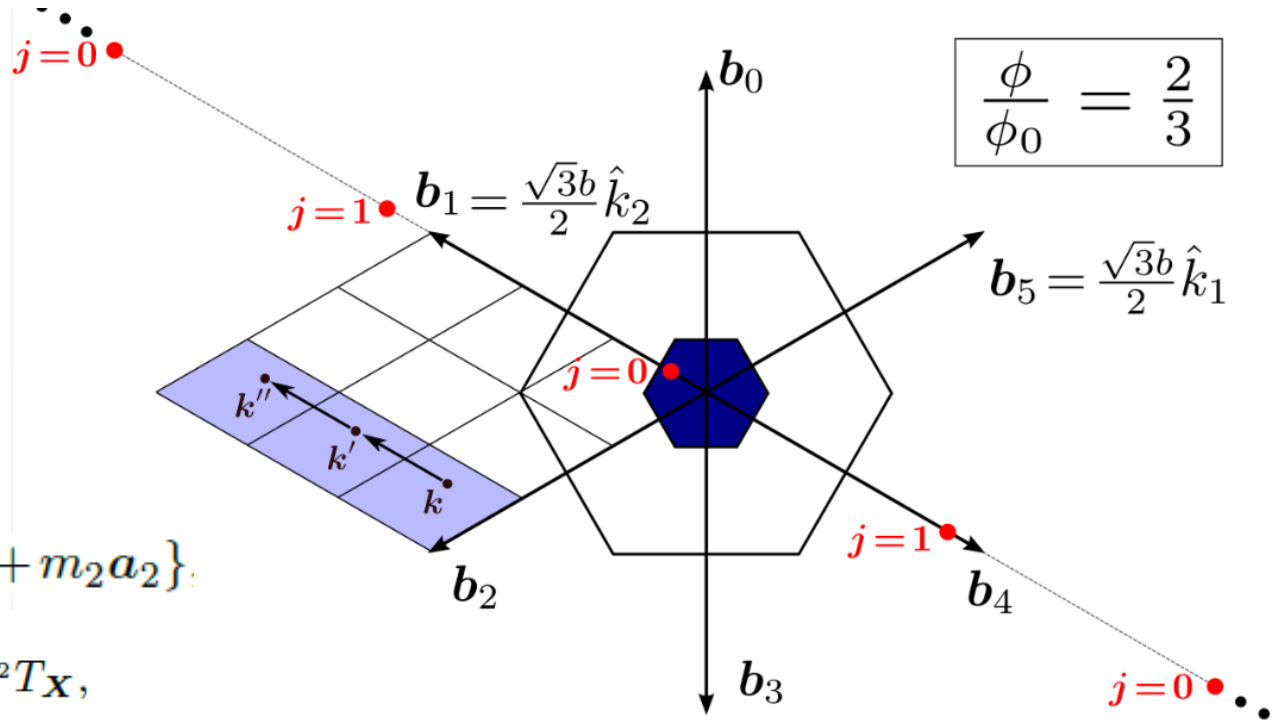
‘Magnetic lattice’ with a q^2 times bigger effective supercell and q^2 times smaller Brillouin mini-zone (over-folded).

Each state in this Brillouin mini-zone is q times degenerate.





‘Magnetic lattice’
with a **9** times bigger
effective supercell



$$G_M = \{\Theta_X, X = m_1 a_1 + m_2 a_2\}$$

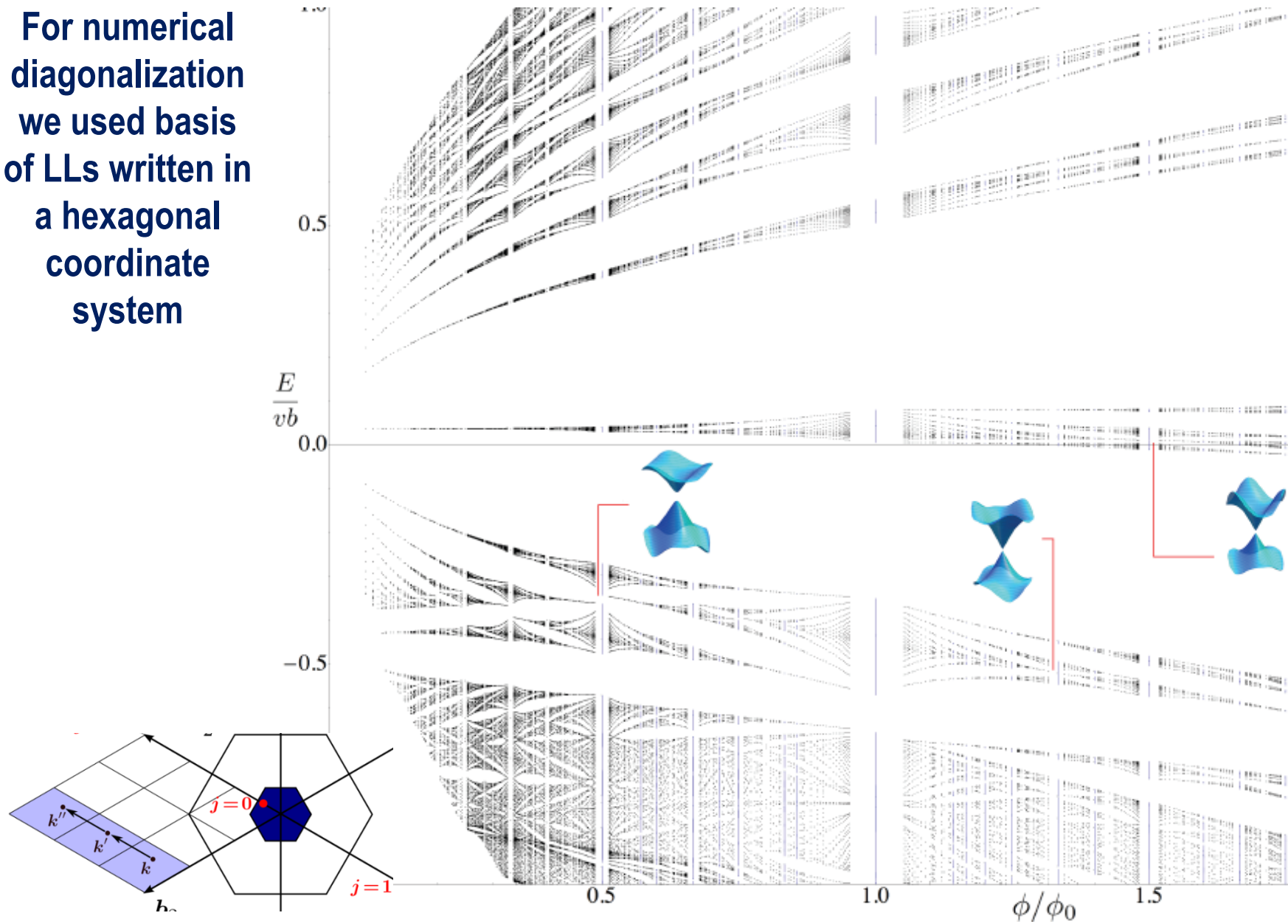
$$\Theta_X \equiv e^{-ieBm_1 a \frac{\sqrt{3}}{2} x_2} T_X,$$

$$\Theta_X \Theta_{X'} = e^{-i2\pi \frac{p}{q} m'_1 m_2} \Theta_{X+X'},$$

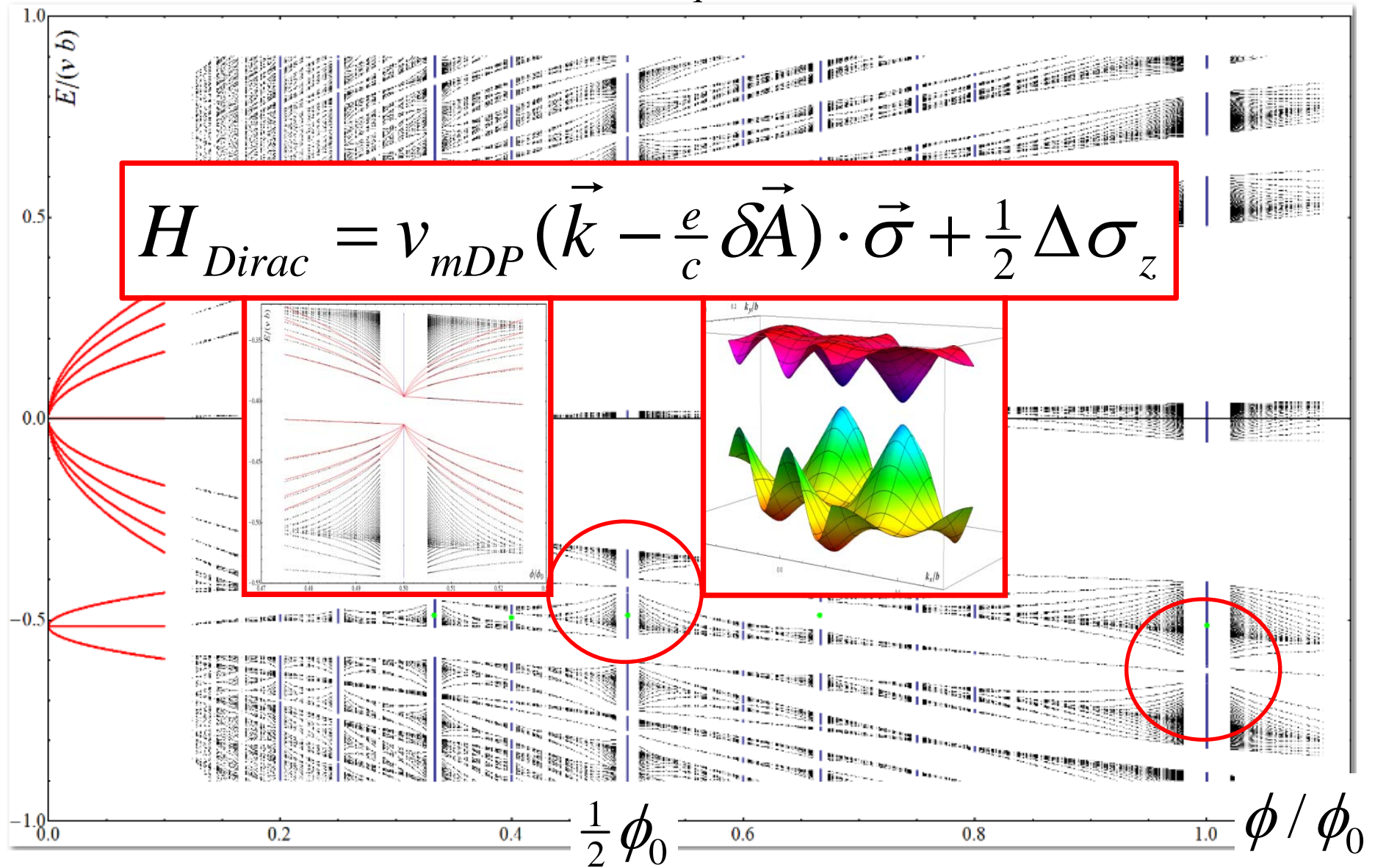
$$\Theta_X \Theta_{X'} = e^{-i2\pi \frac{p}{q} (m'_1 m_2 - m_1 m'_2)} \Theta_{X'} \Theta_X.$$

$$G_{qM} = \{\Theta_R, R = qm_1 \vec{a}_1 + qm_2 \vec{a}_2\} \subset G_M$$

For numerical diagonalization we used basis of LLs written in a hexagonal coordinate system



Magnetic minibands at $\phi = \frac{p}{q} \phi_0$ - gapped Dirac electrons

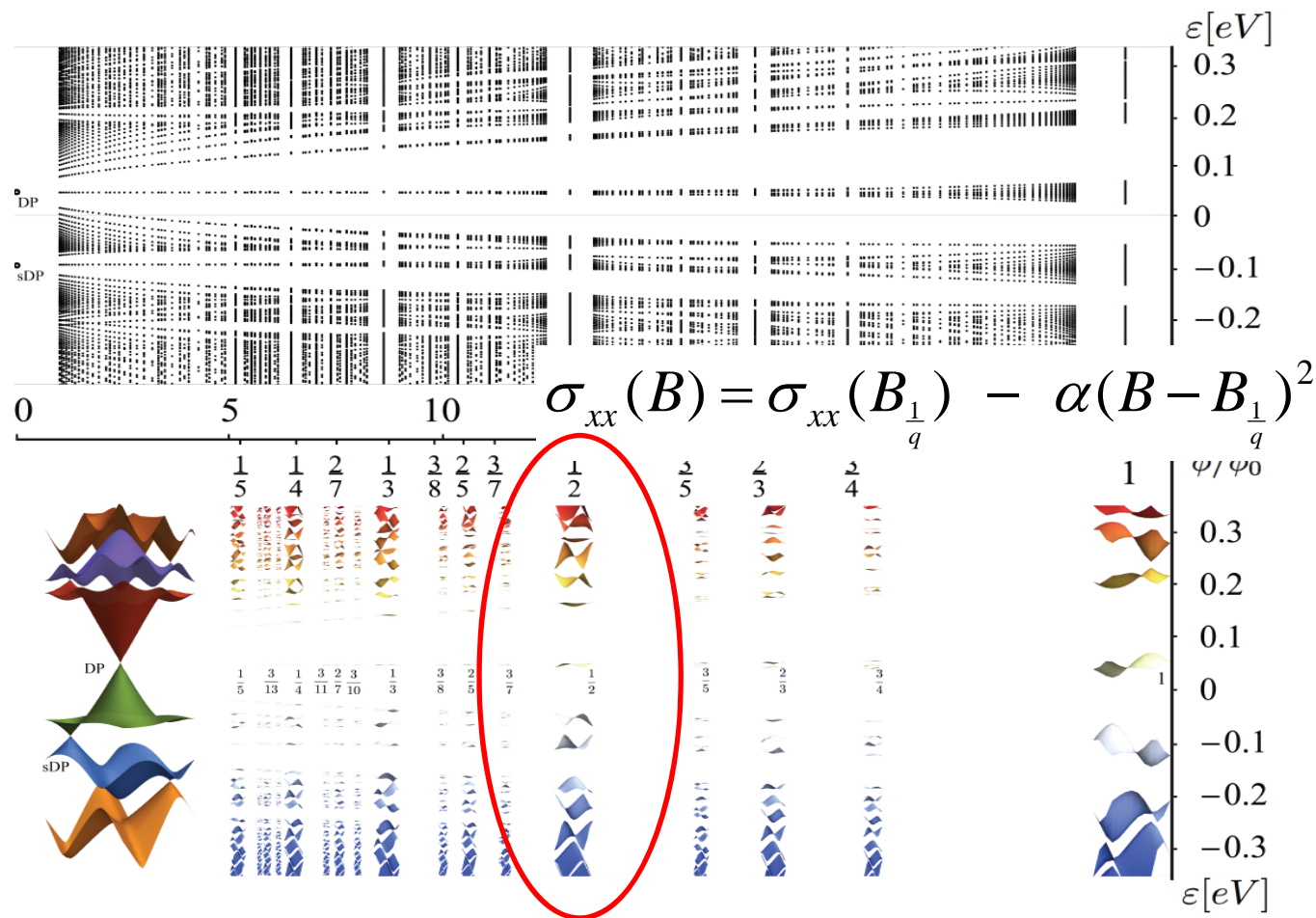


High-temperature Brown-Zak oscillations

Hierarchy of Brown-Zak minibands:

widest minibands at $1/N$ fractions; then at $2/(2N+1)$

all others are much smaller.



$$\sigma_{xx} = \frac{1}{2} e^2 \gamma \tau v^2 \quad \Rightarrow \quad \frac{2e^2}{h} \frac{\epsilon_{FT} \tau}{\hbar} \frac{\langle v^2 \rangle}{v_F^2}$$

$T \gg \epsilon_{band}, \hbar \omega_c$

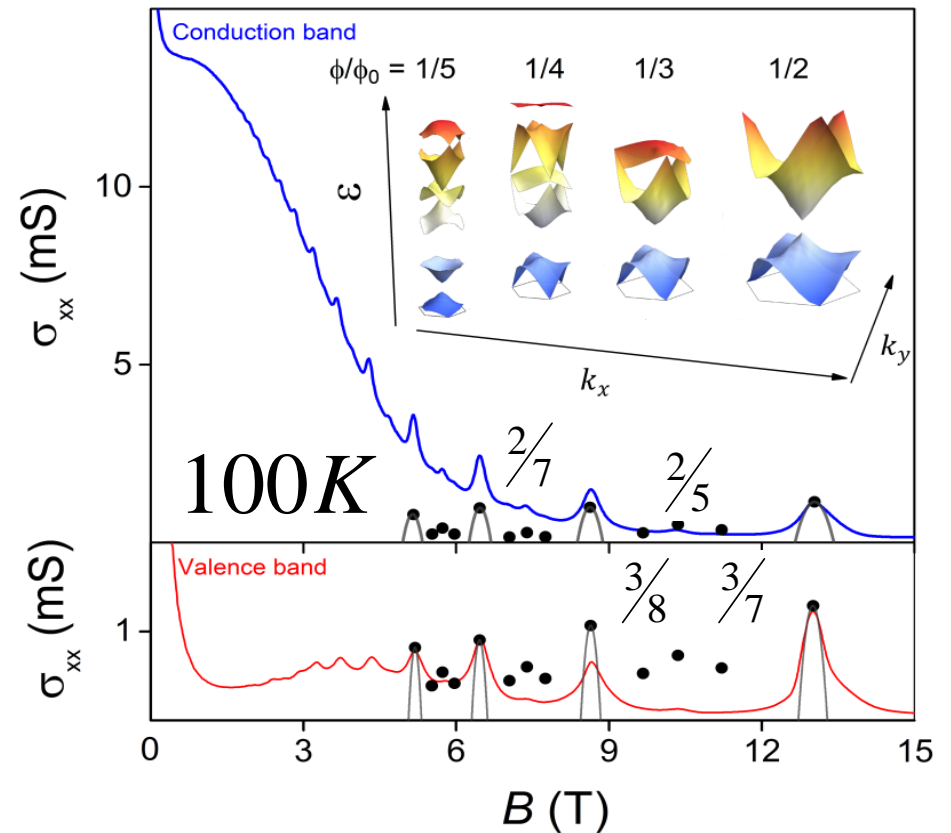
High-temperature Brown-Zak oscillations

$$50 \div 200 K > \varepsilon_{band}, \hbar \omega_c$$

- calculated

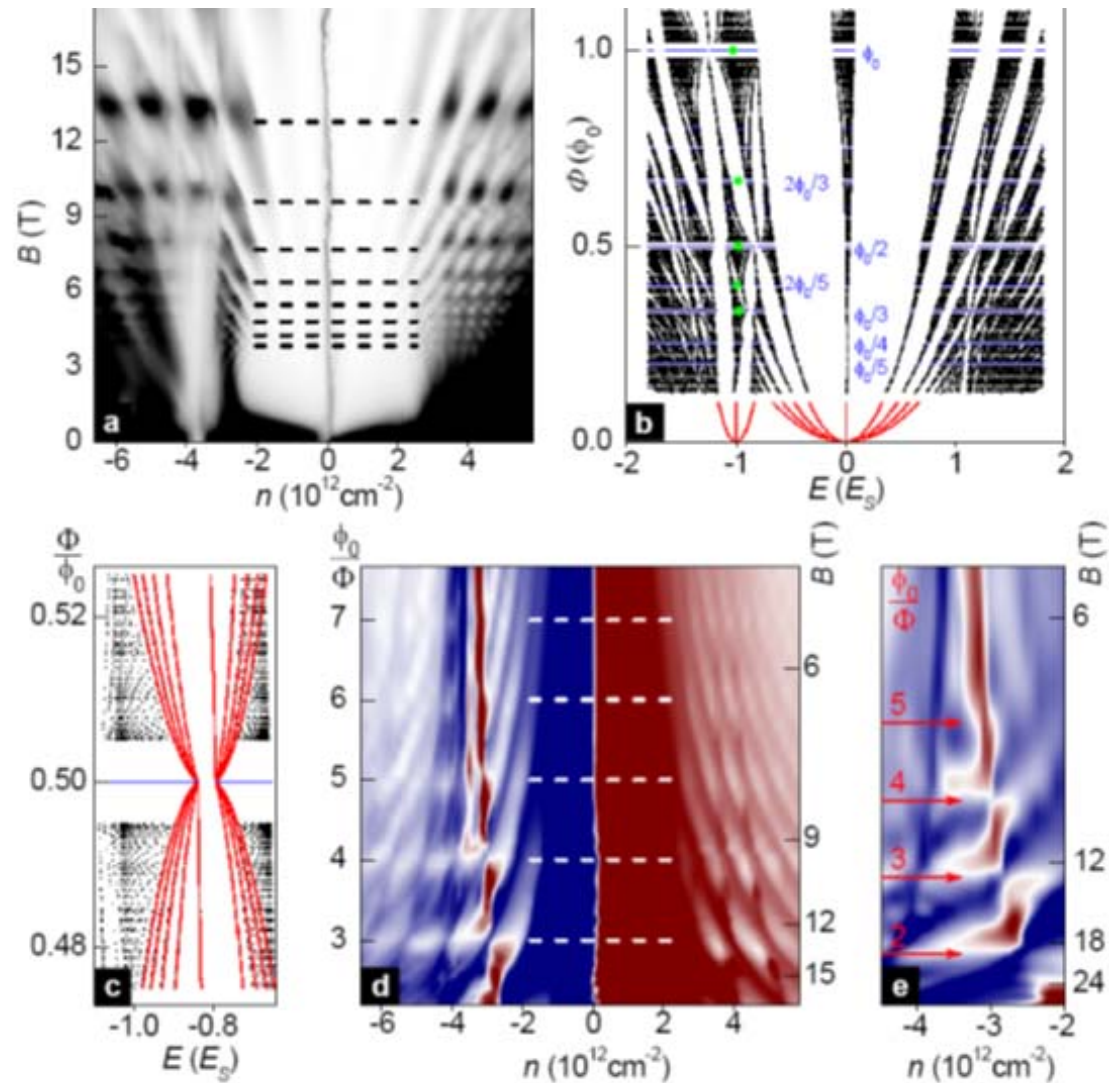
$$\sigma_{xx}(B_{p/q}) = \frac{2e^2}{h} \frac{\varepsilon_F \tau}{\hbar} \frac{\langle v^2 \rangle}{v_F^2}$$

scattering time
determined by fitting
one point, at $\Phi = 1/2 \Phi_0$



Krishna Kumar, Chen, Auton, Mishchenko, Bandurin, Morozov, Cao, Khestanova, Ben Shalom, Kretinin, Novoselov, Eaves, Grigorieva, Ponomarenko, Fal'ko, Geim - Science 357, 181 (2017)

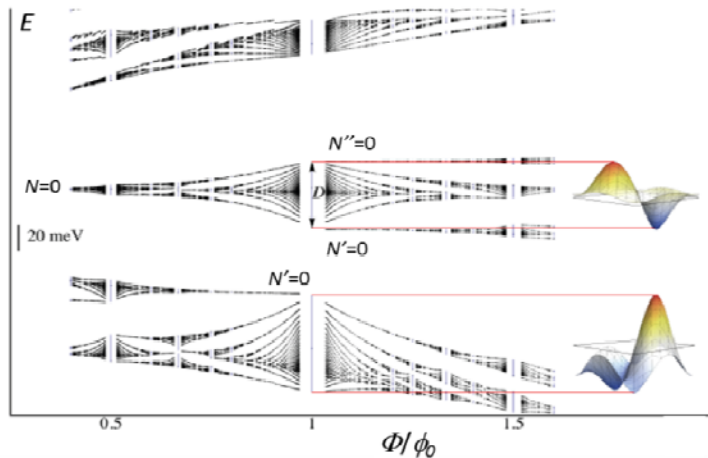
Low-T magneto-transport and gaps between magnetic minibands



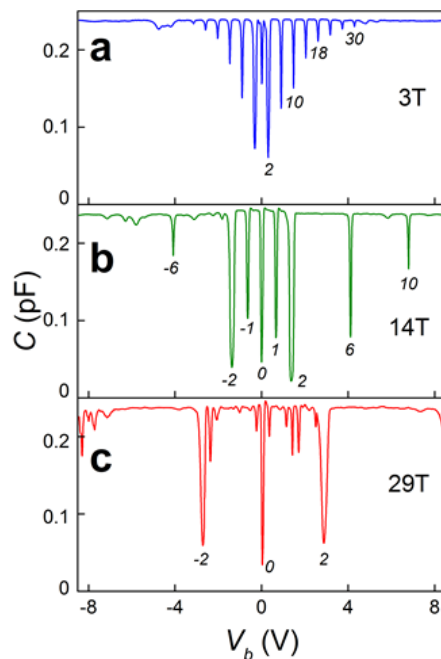
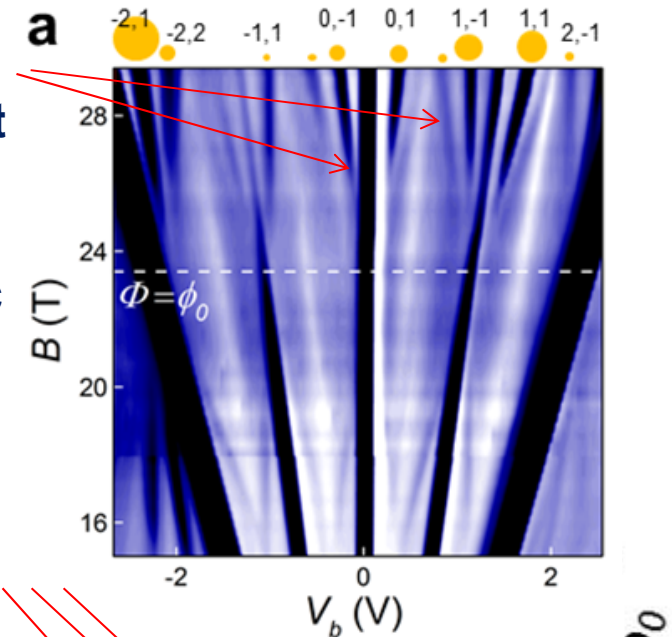
Ponomarenko, Gorbachev, Elias, Yu, Patel, Mayorov, Woods, Wallbank, Mucha-Kruczynski, Piot, Potemski, Grigorieva, Guinea, Novoselov, Fal'ko, Geim - Nature 497, 594 (2013)

Capacitance spectroscopy of gaps between magnetic minibands

Yu, Gorbachev, Tu, Kretinin, Cao, Jalil, Withers, Ponomarenko, Chen, Piot, Potemski, Elias, Watanabe, Taniguchi, Grigorieva, Novoselov, VF, Geim, Mishchenko - Nature Physics 10, 525 (2014)

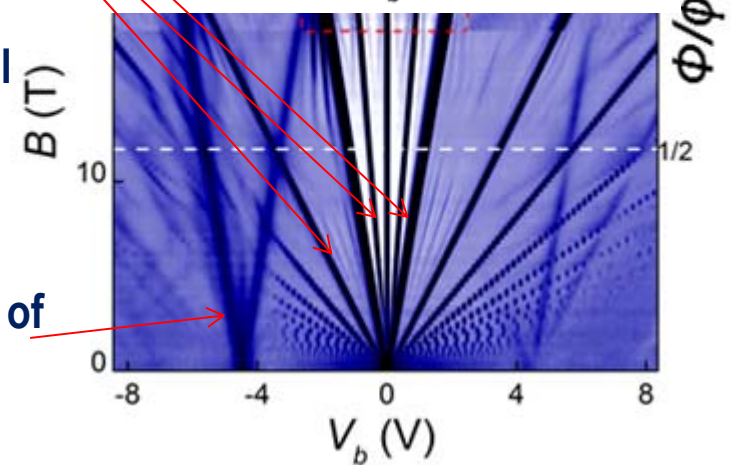


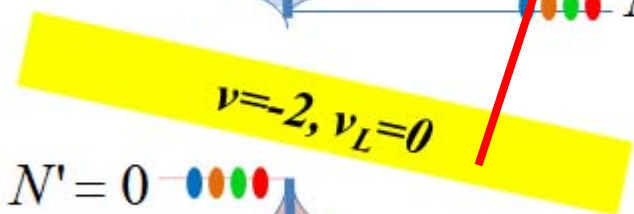
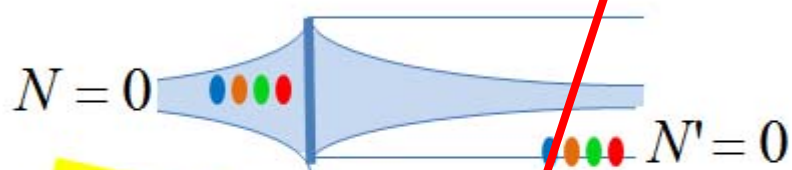
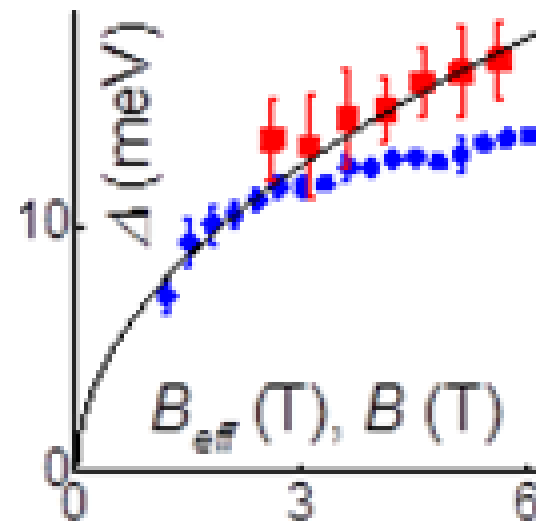
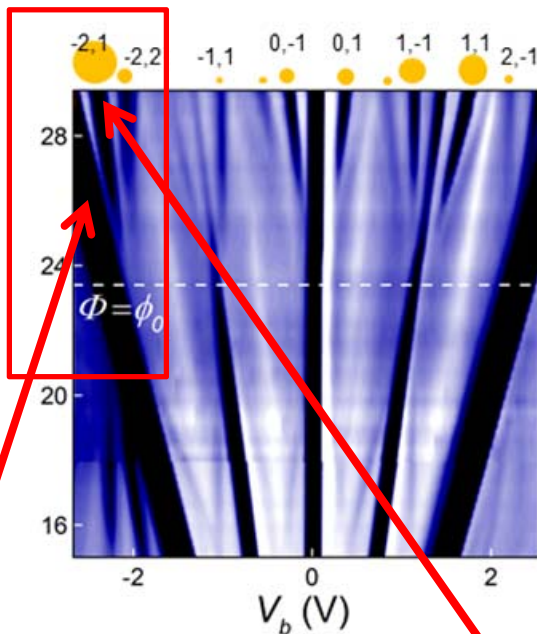
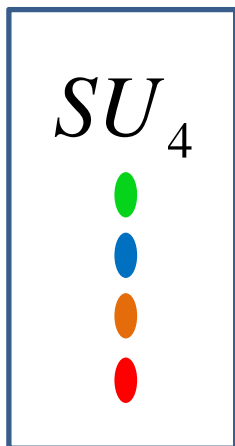
Ferromagnetic quantum Hall effect states in Landau levels of the third generation of Dirac electrons



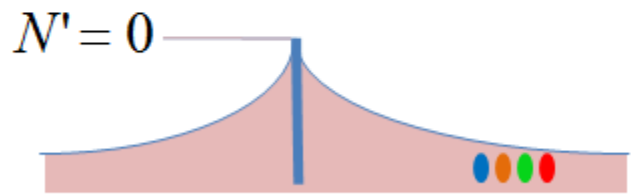
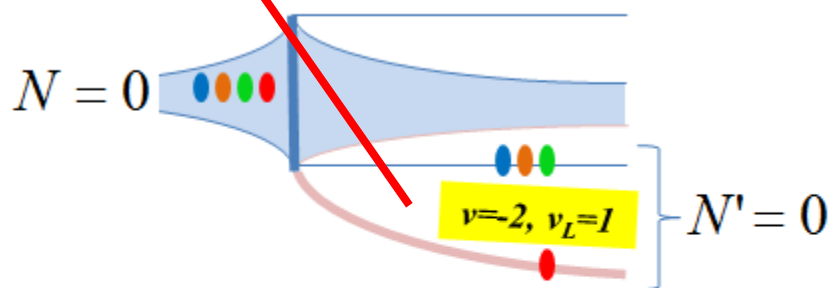
Gaps between Landau levels and incompressible ferromagnetic quantum Hall states of primary Dirac electrons

Gaps between Landau levels of secondary Dirac electrons

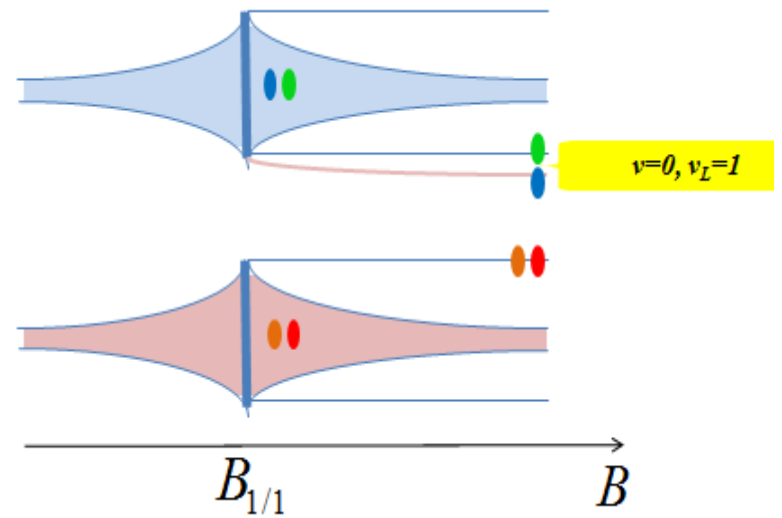
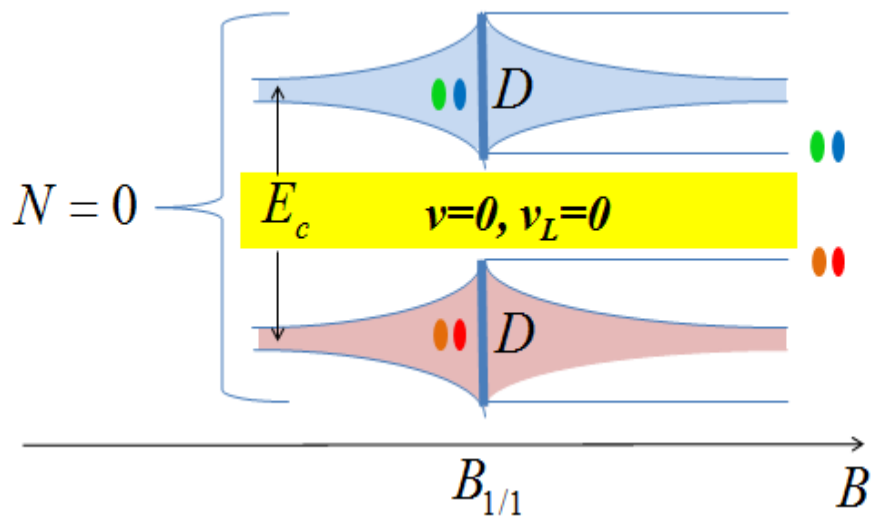
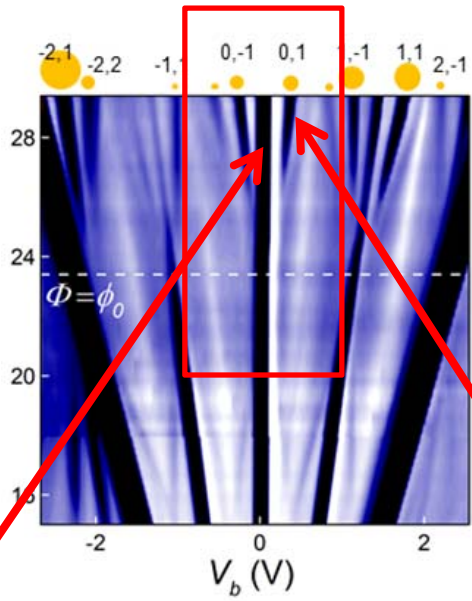
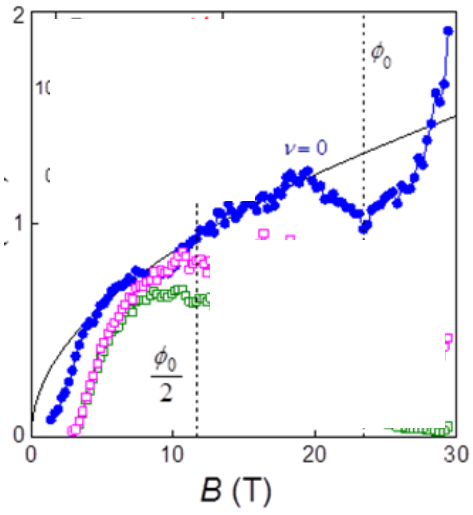


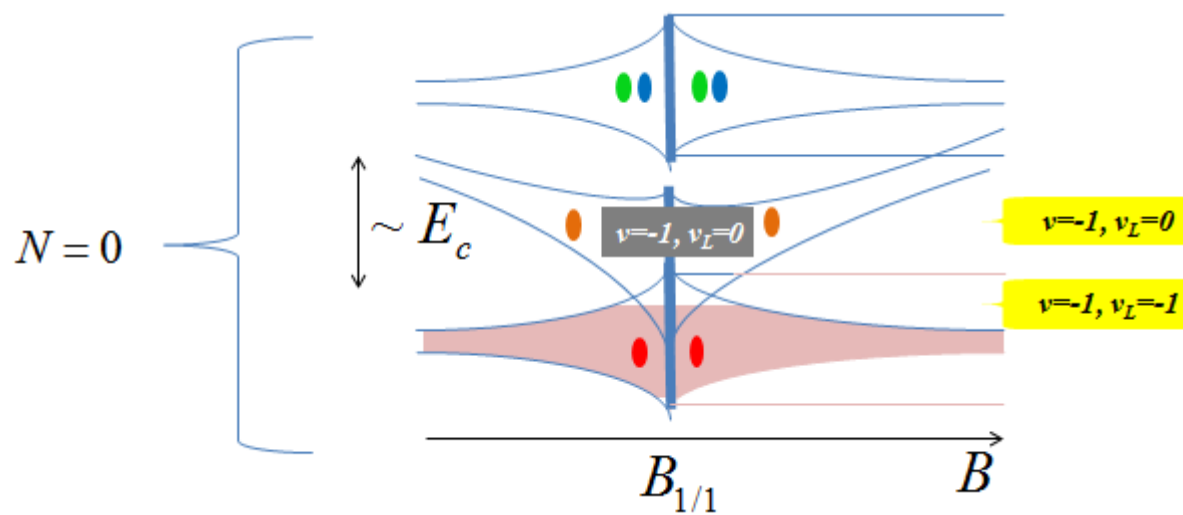
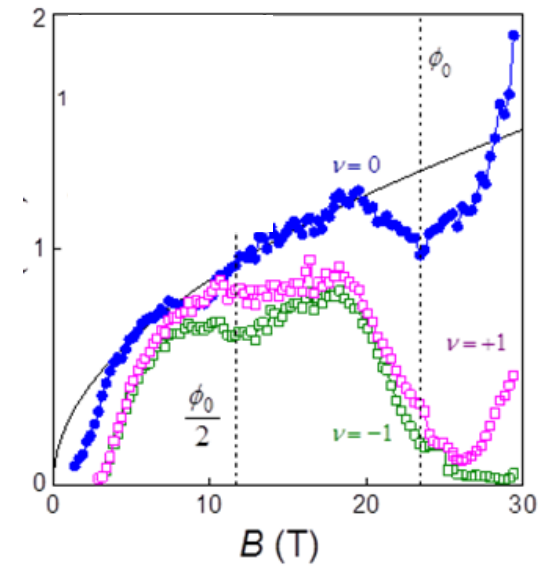
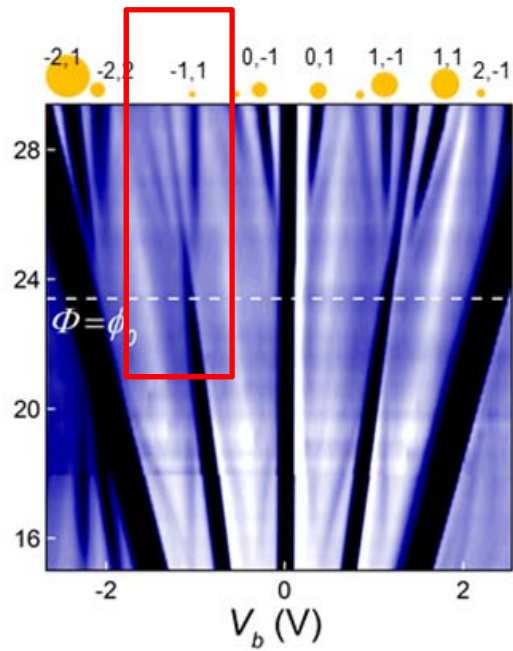


$B_{1/1}$ B



$B_{1/1}$ B





**Reverse
Stoner
transition**

Extreme quantum physics in moiré superlattice:

- ✓ moiré minibands for electrons
- ✓ Zak-Brown magnetic minibands / 'Hofstadter butterfly'

Xi Chen (NGI)

John Wallbank (NGI)

Marcin Mucha-Kruczynski (Bath)

David Abergel (Nordita)

Andre Geim (NGI)

Marek Potemski (CNRS-Grenoble)

David Goldhaber-Gordon (Stanford)

Takashi Taniguchi (NIMS)

EPSRC



GRAPHENE FLAGSHIP

honeycomb graphene
on weakly-coupled
insulating honeycomb
hBN

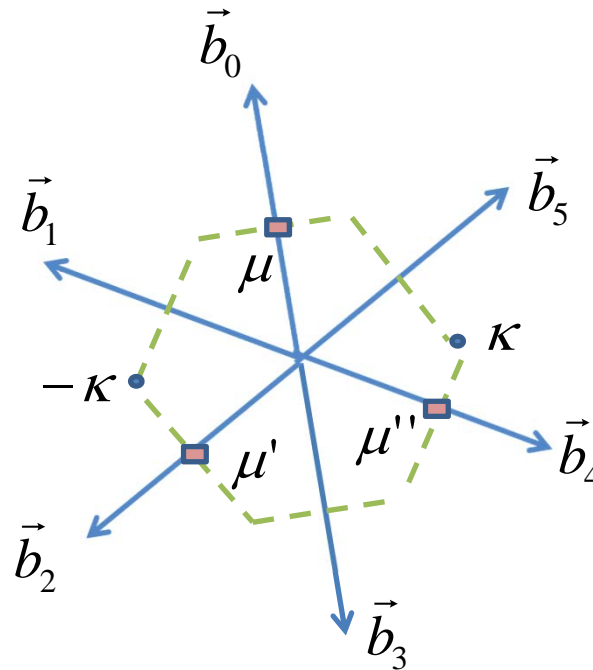


one of the atoms
in the unit cell affects
graphene orbitals
stronger than the other.

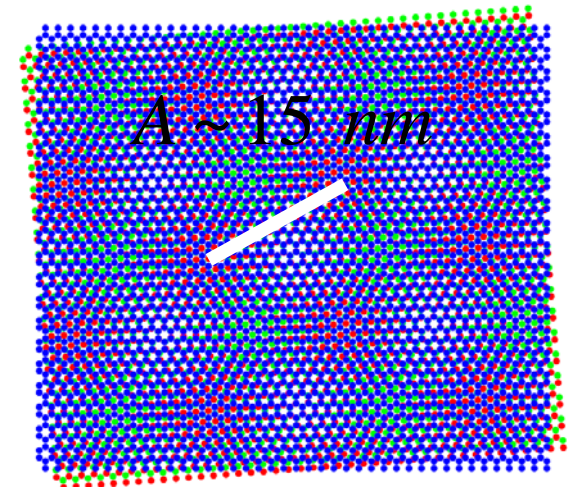


one sublattice defines
a simple hexagonal
lattice.

**inversion
non-symmetric**

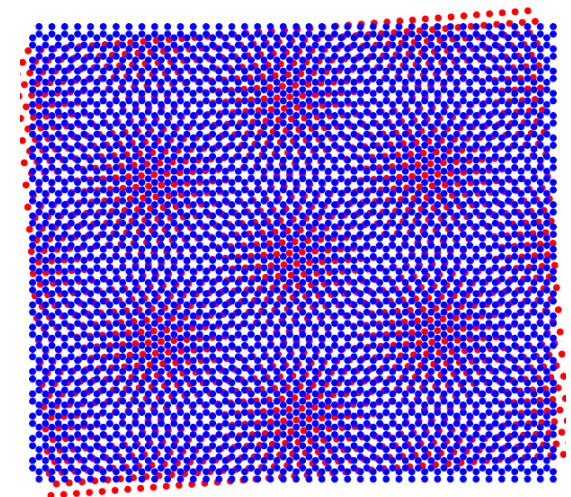


**inversion symmetric
with a small
asymmetric addition**



$$A \approx \frac{a}{\sqrt{\delta^2 + \theta^2}}$$

↑ misalignment
↑ lattice mismatch
1.8% for G/hBN



$$\hat{H} = vp \cdot \sigma + u_0 v b f_1(r) + u_3 v b f_2(r) \sigma_3 \tau_3 + u_1 v [l_z \times \nabla f_2(r)] \cdot \sigma \tau_3$$

3 mini-DPs at the
edge of 1st miniband
no e-h symmetry

single mini-DP at the
edge of 1st miniband
e-h symmetry

single mini-DP at the
edge of 1st miniband
in both c/v bands

generic:
single mini-DP at the
edge of 1st miniband
no e-h symmetry

