Lifshitz transition in gapped BLG
Magnetic (Brown-Zak) minibands due to moiré superlattice in monolayer and bilayer graphene
Bilayer graphene with a gap


hBN allows for better quality and larger $E_z$

skew inter-layer hopping

\[ v_3 = -\frac{\sqrt{3}}{2} \frac{\gamma \alpha a}{\hbar} \sim 0.1v \]

\[ \pi = p_x + ip_y = pe^{i\varphi} \]

\[ H = \begin{pmatrix}
\frac{1}{2}u & v_3 \pi & 0 & v\pi \\
v_3 \pi^* & -\frac{1}{2}u & v\pi^* & 0 \\
0 & v\pi & -\frac{1}{2}u & \gamma_1 \\
v\pi^* & 0 & \gamma_1 & \frac{1}{2}u
\end{pmatrix} \begin{pmatrix} A \\ \tilde{B} \\ \tilde{A} \\ B \end{pmatrix} \]

\[ \epsilon_{\alpha}^2 = \frac{\gamma_1^2}{2} + \frac{u^2}{4} + \left( v^2 + \frac{v_3^2}{2} \right) p^2 + (-1)^{\alpha} \sqrt{\Gamma} \]

\[ \Gamma = \frac{1}{4}(\gamma_1^2 - v_3^2 p^2)^2 + v^2 p^2 [\gamma_1^2 + u^2 + v_3^2 p^2] 
+ 2\xi \gamma_1 v_3 v^2 p^3 \cos 3\varphi, \]

McCann, VF - PRL 96, 086805 (2006)
Gapped BLG: intricate band features due to trigonal warping

\[
\frac{\varepsilon_F}{\frac{1}{2} u} = -1 + \frac{1}{2} \left( \frac{u}{\gamma_1} \right)^2 + \sqrt{2} \frac{u}{\gamma_1} \frac{\nu_3}{\nu}
\]

\[
\frac{\varepsilon_F}{\frac{1}{2} u} = -1 + \frac{1}{2} \left( \frac{u}{\gamma_1} \right)^2 - \sqrt{2} \frac{u}{\gamma_1} \frac{\nu_3}{\nu}
\]
Lifshitz transition in metals

- Topology of the Fermi surface changes, DoS diverges
- Cyclotron orbits in magnetic field change circulation
- Magnetic breakdown - field mixes disconnected parts of Fermi surfaces, at $\delta p \sim 1/\lambda_B$.

\[ \frac{\varepsilon_F}{\frac{1}{2} u} = -1 + \frac{1}{2} \left( \frac{u}{\gamma_1} \right)^2 + \sqrt{2} \frac{u}{\gamma_1} \frac{v_3}{v} \]

\[ \frac{\varepsilon_F}{\frac{1}{2} u} = -1 + \frac{1}{2} \left( \frac{u}{\gamma_1} \right)^2 - \sqrt{2} \frac{u}{\gamma_1} \frac{v_3}{v} \]
Lifshitz transition, magnetic breakdown, and phase transitions between QHFM states
Dirac point generates
a 4-fold degenerate $\epsilon=0$ Landau level

McClure - PR 104, 666 (1956)

$$\epsilon_{\pm} = \pm \sqrt{2n} \frac{v}{\lambda_B}$$

$$\bar{p} = -i\hbar \nabla - \frac{e}{c} \vec{A}, \quad \text{rot} \vec{A} = B \vec{l}_z$$

$$\pi = p_x + ip_y; \quad \pi^+ = p_x - ip_y$$

descending/raising operators in LL orbitals

8-fold degenerate $\epsilon=0$ Landau level, which splits when inversion symmetry is broken.

McCann, VF - PRL 96, 086805 (2006)
$$H = \begin{pmatrix}
\frac{1}{2}u & \nu_3\pi & 0 & \nu\pi \\
\nu_3\pi^+ & -\frac{1}{2}u & \nu\pi^+ & 0 \\
0 & \nu\pi & -\frac{1}{2}u & \gamma_1 \\
\nu\pi^+ & 0 & \gamma_1 & \frac{1}{2}u
\end{pmatrix}$$

$u = 0.08 \text{eV}$
6-fold (2 x spin and 3 x orbital) degenerate LL at small magnetic fields

\[ \nu = -3 \text{ spin polarised (ferromagnetic) QHE state} \]

\[ \nu = -6 \text{ unpolarised QHE state} \]
magnetic breakdown
Landau level crossing

\( \nu = -3, -5 \) QHFM gaps vanish and \( \nu = -4 \) undergoes ferromagnetic transition.

\( \nu = 0, -1, -2 \) ferromagnetic and normal QHE

Polarised

\( \nu = -3, -5 \)

\( \nu = -4, -6 \) QHE
Highly oriented hBN-graphene heterostructures

Geim (Manchester)      Jarillo-Herrero (MIT)

highly oriented graphene-BN:

heterostructure with new electronic properties

highly oriented BLG-hBN heterostructures

Kim (Harvard) & Hone (Columbia)
Due to a separation between layers larger than distance between atoms within the layers, moiré perturbation is dominated by the simplest spatial spatial harmonics.

Bistritzer, MacDonald - PRB 81, 245412 (2010)

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

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

lattice mismatch 1.8% for G/hBN
misalignment <2°
Effective low-energy ‘Dirac theory’ for electrons
Phenomenological approach to classify generic miniband structure caused by a moiré perturbation.
\[
\hat{H} = v_p \cdot \sigma + u_0 v b f_1(r) + u_3 v b f_2(r) \sigma_3 \tau_3 + u_1 v [l_z \times \nabla f_2(r)] \cdot \sigma \tau_3 \\
+ \tilde{u}_0 v b f_2(r) + \tilde{u}_3 v b f_1(r) \sigma_3 \tau_3 + \tilde{u}_1 v [l_z \times \nabla f_1(r)] \cdot \sigma \tau_3
\]

\[
f_2(r) = i \sum_{m=0...5} (-1)^m e^{i b_m \cdot r} \quad f_1(r) = \sum_{m=0...5} e^{i b_m \cdot r}
\]

Wallbank, Patel, Mucha-Kruczynski, Geim, VF - PRB 87, 245408 (2013)
Chen, Wallbank, Patel, Mucha-Kruczyński, McCann, VF - PRB 89, 075401 (2014)
Magnetic minibands at rational values of magnetic field flux per super-cell

\[ \phi = \frac{p}{q} \phi_0, \phi_0 = \frac{h}{e} \]

Each state in this Brillouin minizone is \( q \) times degenerate.

‘Magnetic lattice’ with a \( q^2 \) times bigger supercell and \( q^2 \) times smaller Brillouin minizone.

Branded as ‘Hofstadter butterfly’ spectrum.
‘Magnetic lattice’ with a 9 times bigger supercell

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

\[ \Theta_X \equiv e^{-ieBm_1 a_1 \frac{\sqrt{3}}{2} x_2} T_X, \]

\[ \Theta_X \Theta_{X'} = e^{-i2\pi \frac{p}{q} m_1 m_2} \Theta_{X+X'}, \]

\[ \Theta_X \Theta_{X'} = e^{-i2\pi \frac{p}{q} (m_1 m_2 - m_1 m_2')} \Theta_{X'} \Theta_X. \]

\[ G_{qM} = \{ \Theta_R, R = qm_1 \tilde{a}_1 + qm_2 \tilde{a}_2 \} \subset G_M \]
Generations of Dirac electrons in Zak’s magnetic minibands in moiré superlattices
Magnetic minibands at $\phi = \frac{p}{q} \phi_0$ - gapped Dirac electrons

$$H_{\text{Dirac}} = v_{mDP} \left( \vec{k} - \frac{e}{c} \delta \vec{A} \right) \cdot \vec{\sigma} + \frac{1}{2} u \sigma_z$$

Chen, Wallbank, Patel, Mucha-Kruczyński, McCann, VF - PRB 89, 075401 (2014)
Quantum Hall ferromagnetism in moiré superlattices

capacitance spectroscopy

Yu, Gorbachev, Tu, Kretinin, Cao, Jalil, Withers, Ponomarenko, Chen, Piot, Potemski, Elias, Watanabe, Taniguchi, Grigorieva, Novoselov, VF, Geim, Mishchenko (2014)
$\nu = 0, \nu_L = 0$

$E_c \quad \nu = 0, \nu_L = 0$

$N = 0$

$B_{1/1}$

$B$
\[ B_c \approx n \nu \]

Reverse Stoner transition
Highly oriented hBN-caged bilayer graphene
BLG-hBN heterostructures

Substrate affecting one layer produces inversion non-symmetric moiré superlattice potential.

For encapsulated BLG, different misalignment between BLG and top/bottom hBN layers has the same effect (low-energy electronic properties are determined by the moiré pattern due to the better aligned hBN layer.)
$H_{\text{eff}} = -\frac{v^2}{\gamma_1} \begin{pmatrix} 0 & \pi^+ \pi^2 \\ \pi^2 & 0 \end{pmatrix} \tau_z$

$\hat{\pi} = k_x + i k_y$

$H_{(K')} = \begin{pmatrix} vbg_+(r) & \frac{v^2 b}{\gamma_1} g^*(r) \pi^+ \\ \frac{v^2 b}{\gamma_1} \pi^2 g(r) & \frac{v^3 b}{\gamma_1^2} \pi^2 g^*(r) \pi^+ \end{pmatrix}$

$H_{(K'')} = \begin{pmatrix} \frac{v^3 b}{\gamma_1^2} \pi^+ g^*(r) \pi^+ & \frac{v^2 b}{\gamma_1} \pi^+ g(r) \\ \frac{v^2 b}{\gamma_1} g^*(r) \pi^+ & vbg_+(r) \end{pmatrix}$

$g_\pm(r) = \sum_m e^{ib_m \cdot r} (u_0 \pm i u_3 (-1)^m)$,

$g(r) = (u_2 + i u_1 \tau_z) \sum_m (-1)^m e^{ib_m \cdot r} (b_m^x + i b_m^y \tau_z)$

Mucha-Kruczynski, Wallbank, VF - PRB 88, 205418 (2013)
Inversion symmetry is broken because moire perturbation is applied only to one layer: this promotes gaps at the 1st miniband edge.

BLG-hBN heterostructures

Mucha-Kruczynski, Wallbank, VF - PRB 88, 205418 (2013)
Zak’s minibands in BLG-hBN heterostructures

Chen, Mucha-Kruczynski, Wallbank, VF (2014)
Zoom in to 0th LL only

MLG K

Zoom in to 0th and 1st LL

BLG K'

Zoom in to 0th LL only
hBN-caged graphene

Marcin Mucha-Kruczynski, Xi Chen, John Wallbank, Vladimir Falko
Andre Geim & National Graphene Institute @Manchester
Klaus Ensslin group @ETH

- Lifshitz transition in gapped BLG
- Magnetic (Brown-Zak) minibands due to moiré superlattice in monolayer and bilayer graphene