Spontaneous parity breaking of graphene in the quantum Hall regime

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**Topic:** QHE in graphene and especially the recently observed QH states at filling factor = 0;±1;±4.

**Main message:** The new QH states may result from a magnetic field driven out-of-plane lattice distortion.
Graphene at B=0

Tight-binding model on honeycomb lattice (triangular Bravais lattice with a 2 carbon atom basis: A and B) with hopping $t = 3\text{eV}$: Wallace, Phys. Rev. 1947

Relativistic like dispersion relation close to $K$ and $K'$:

$$\varepsilon_k = \pm \hbar v_F |k| \quad \text{with} \quad \hbar v_F = \frac{3ta}{2}$$

2 valleys (or chiralities or pseudo-spin): $\alpha = \pm 1$

2 spin states: $\sigma = \pm 1$

Half-filled big band (= valence+conduction bands) at zero gate voltage $V_g = 0$. 
Graphene at small B: relativistic QHE


\[ B \approx 10 \, \text{T} \]

Integer \( n = \) LL index

\[ \varepsilon_n = \text{sgn}(n) \sqrt{|n|} \frac{\hbar v_F \sqrt{2}}{l_B} \]

\[ \text{deg.} = 4N_\phi = 4B_{\perp} A / \phi_0 \]


\[ \hbar \omega_c = \hbar v_F \sqrt{2} / l_B \]

**Graphene at large B: extra QH states**

Th.: Landau levels + Zeeman: filling factor = $0; \pm 2; \pm 4; \pm 6; \pm 8$; etc.

Exp.: filling factor = $0; \pm 1; \pm 2; \pm 4; \pm 6$ but not filling factor = $\pm 3; \pm 5$

\[
\varepsilon_{n,\sigma} = \text{sgn}(n) \sqrt{|n|} \hbar \omega_c + \frac{g^*}{2} \mu_B B \text{tot} \sigma
\]

Mechanisms of valley splitting

1) Valley-Zeeman effect
- Uniaxial stress (e.g. applied via a piezo): doesn't lift the valley degeneracy in graphene.

2) Electron-electron interactions
- Exchange gap (QH valley ferromagnetism) \( \sim \frac{e^2}{\epsilon l_B} \)
- Excitonic gap (“magnetic catalysis”) \( \sim \frac{e^2}{\epsilon l_B} \)
- El.-el. Interactions at the lattice scale (QH valley “paramagnetism”) \( \sim \frac{e^2 a}{\epsilon l_B^2} \)

3) Electron-phonon interactions
- Magnetic field driven out-of-plane Peierls distortion
Parity breaking of the honeycomb lattice

If A and B atoms are different (e.g. boron nitride) then the honeycomb lattice's inversion symmetry is broken and the valley degeneracy is lifted (in n=0).

A and B carbon atoms are now assumed to be different. Tight-binding model with different on-site energies ±M (Haldane, PRL 1988):

Central Landau level (n=0): \( \alpha = +1 = A \) and \( \alpha = -1 = B \)

Not true for the other Landau levels (n≠0)

\[
\epsilon_{n,\sigma,\alpha} = \text{sgn}(n) \sqrt{M^2 + (\hbar\omega_c)^2|n|} + \frac{\Delta z}{2} \sigma \text{ if } n \neq 0
\]

\[
= \alpha M + \frac{\Delta z}{2} \sigma \text{ if } n = 0
\]
Magnetic field driven Peierls distortion

How can one have $A \neq B$?

Out-of-plane lattice distortion
AND substrate (SiO2) $\neq$ superstrate (air)

B moves towards the silicon dioxide substrate (-$\eta$)

A moves away from the substrate (+$\eta$)

Electronic energy (gain):
$$E_{n=0} = -N\phi (2 - |\nu|) M; \quad E_{n<0} = -0.7 \frac{N_p a}{\hbar v_F} M^2; \quad M = D\eta$$

Elastic energy (cost):
$$E_{\text{elastic}} = N_p G\eta^2 \text{ where } N_p = \text{ number of unit cells.}$$

Effective elastic energy:
$$E'_{\text{elastic}} = E_{\text{elastic}} + E_{n<0} = N_p G'\eta^2 \text{ with } G' = G - 0.7D^2 a / \hbar v_F$$

Total energy:
$$E_{\text{tot}} = E_{n=0} + E'_{\text{elastic}}$$

Minimizing the total energy:
$$\Delta_{\nu} = \frac{N\phi}{N_p} (2 - |\nu|) \frac{D^2}{G'} \propto B_\perp$$
**Estimate of the constants D and G**

G = elastic constant corresponding to the out-of-plane optical phonon mode (ZO)

\[ \frac{\omega_0}{2\pi c} \sim 800 \text{cm}^{-1} \quad \text{(for graphite)} \quad Ga^2 \approx \frac{m_c \omega_0^2 a^2}{4} \sim 14 \text{eV} \]

D = “deformation potential”, coupling to the substrate

Rough estimate of the coupling to the substrate via the Lennard-Jones interaction of a carbon atom with the substrate: \(Da \approx 1\) to \(14\) eV

No deformation when \(B=0\): \(G' > 0\) therefore \(Da < 9.8\) eV

Valley splitting is larger than Zeeman splitting if \(Da > 6.3\) eV

To explain the experiments, we choose \(Da \approx 7.8\) eV, therefore \(G'a^2 \approx 4.2\) eV

\[
\Delta_v = 2M \approx 4.2K \times (1 - |\nu|/2)B_\perp [T]
\]

\[\hbar \omega_c \approx 420K \times \sqrt{B_\perp [T]}\]

\[\Delta_Z = g^* \mu_B B_{\text{tot}} \approx 1.5K \times B_{\text{tot}} [T]\]

\[\Delta_{\text{imp}} \approx 30K\]
Conclusion: experimental tests

Experiments should decide which mechanism is responsible for lifting the valley degeneracy in graphene. Out-of-plane lattice distortion implies:

-- Valley gap as a function of the magnetic field: \( \Delta_v \propto B_\perp \)

-- Valley gap as a function of the gate voltage: \( \Delta_v \propto (2 - |\nu|) \) with \( \nu \propto V_g \)

-- Lattice distortion: X-ray diffraction at grazing incidence; STM; Helium surface diffraction; etc.

-- IR absorption spectroscopy of the ZO phonons

-- In a symmetric dielectric environment, the lattice distortion should vanish (e.g. for a suspended graphene sheet or for a sheet inside a polymer matrix, see R. Ruoff).
Thank you!