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.

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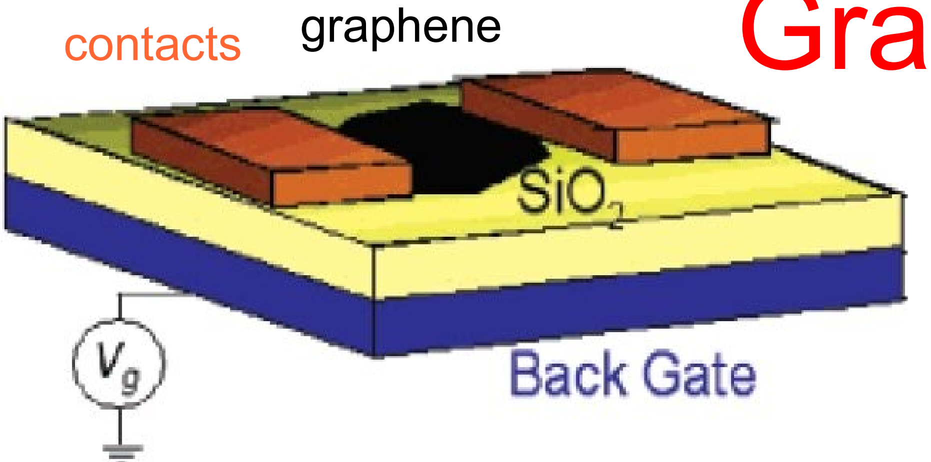
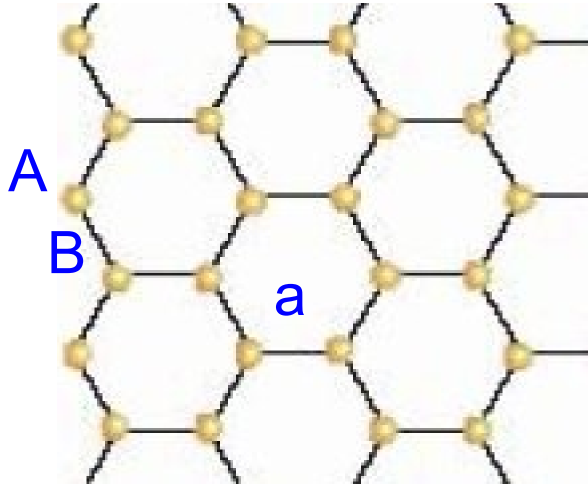
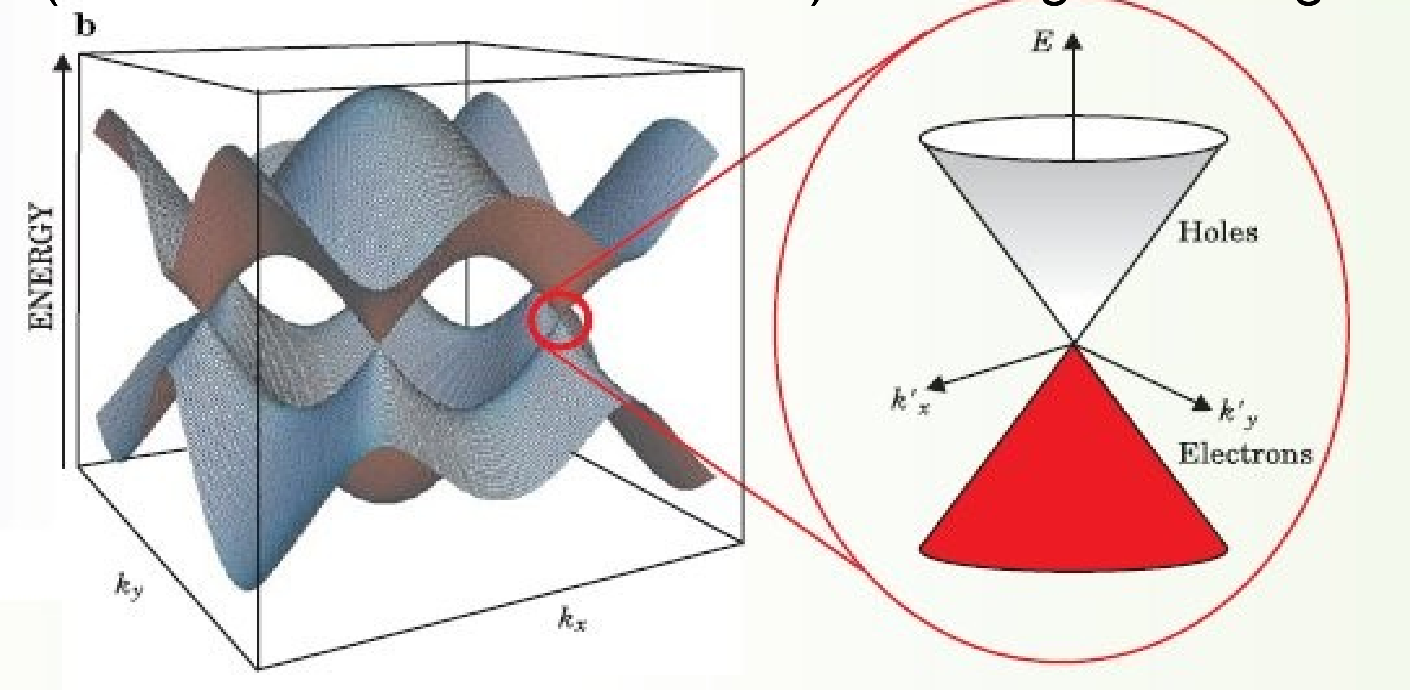


Graphene at B=0



Tight-binding model on honeycomb lattice (triangular Bravais lattice with a 2 carbon atom basis: A and B) with hopping t = 3eV: Wallace, Phys. Rev. 1947
Relativistic like dispersion relation close to K and K' : $\varepsilon_k = \pm\hbar v_F|\mathbf{k}|$ with $\hbar v_F = 3ta/2$
2 valleys (or chiralities or pseudo-spin): α = ±1
2 spin states: σ = ±1
Half-filled big band (= valence+conduction bands) at zero gate voltage V_g= 0.



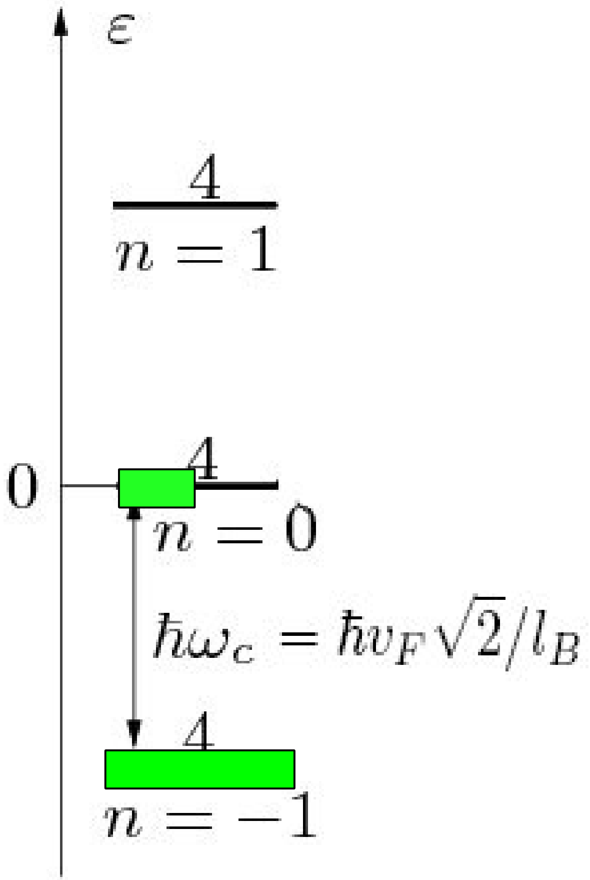
Graphene at small B: relativistic QHE

Integer n = LL index

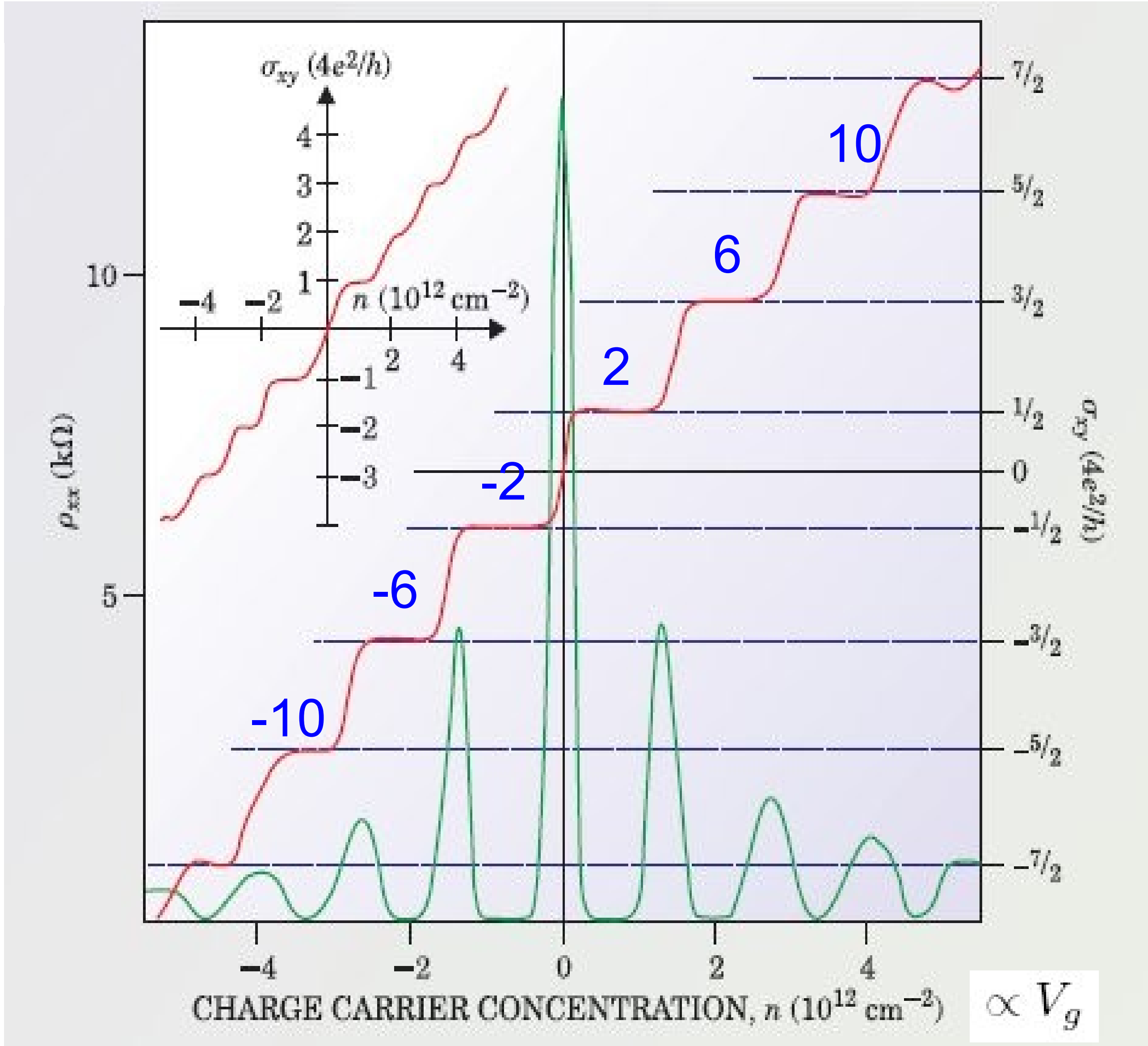
$$\varepsilon_n = \mathrm{sgn}(n)\sqrt{|n|}\frac{\hbar v_F\sqrt{2}}{l_B}$$

$$\mathrm{deg.} = 4N_\phi = 4B_\perp \mathcal{A}/\phi_0$$

McClure Phys. Rev. 1956.



B ≈ 10 T

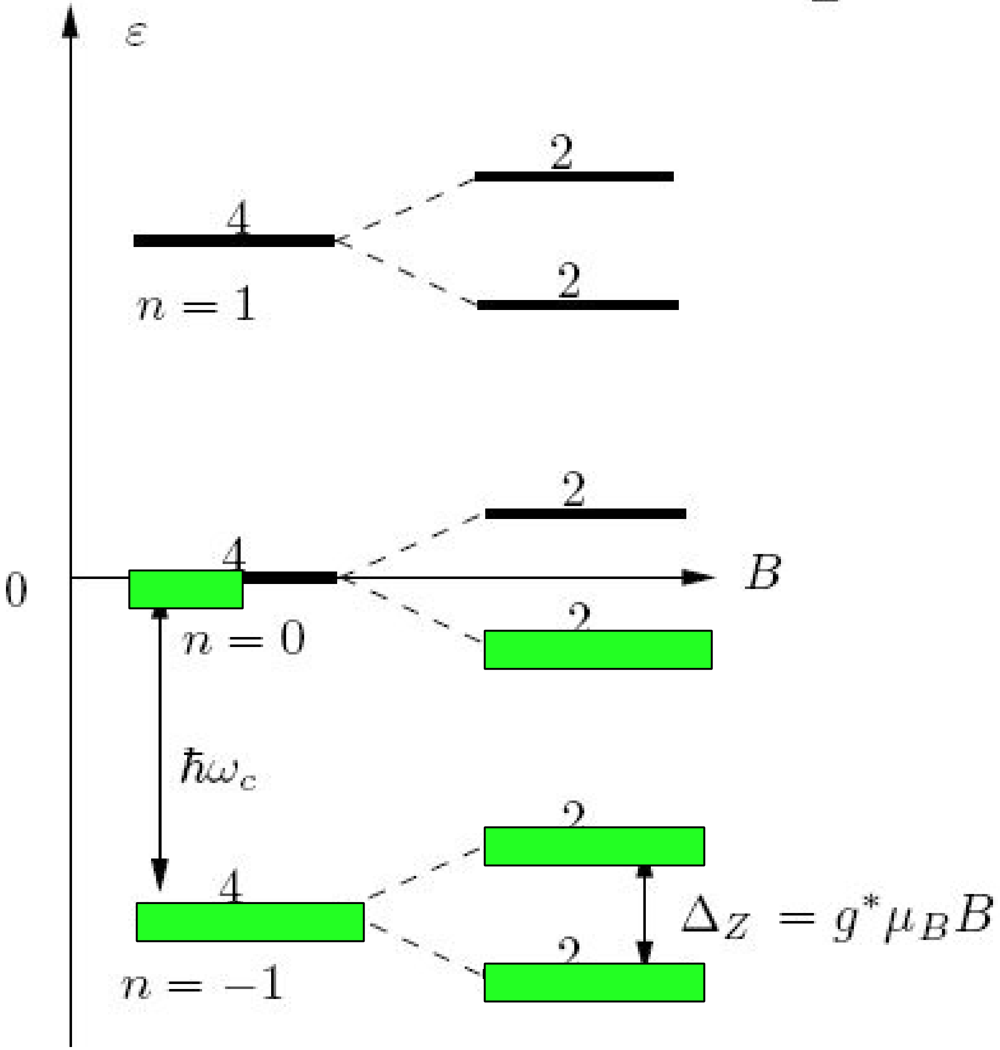


Novoselov et al., Nature 2005; Zhang et al., Nature 2005.

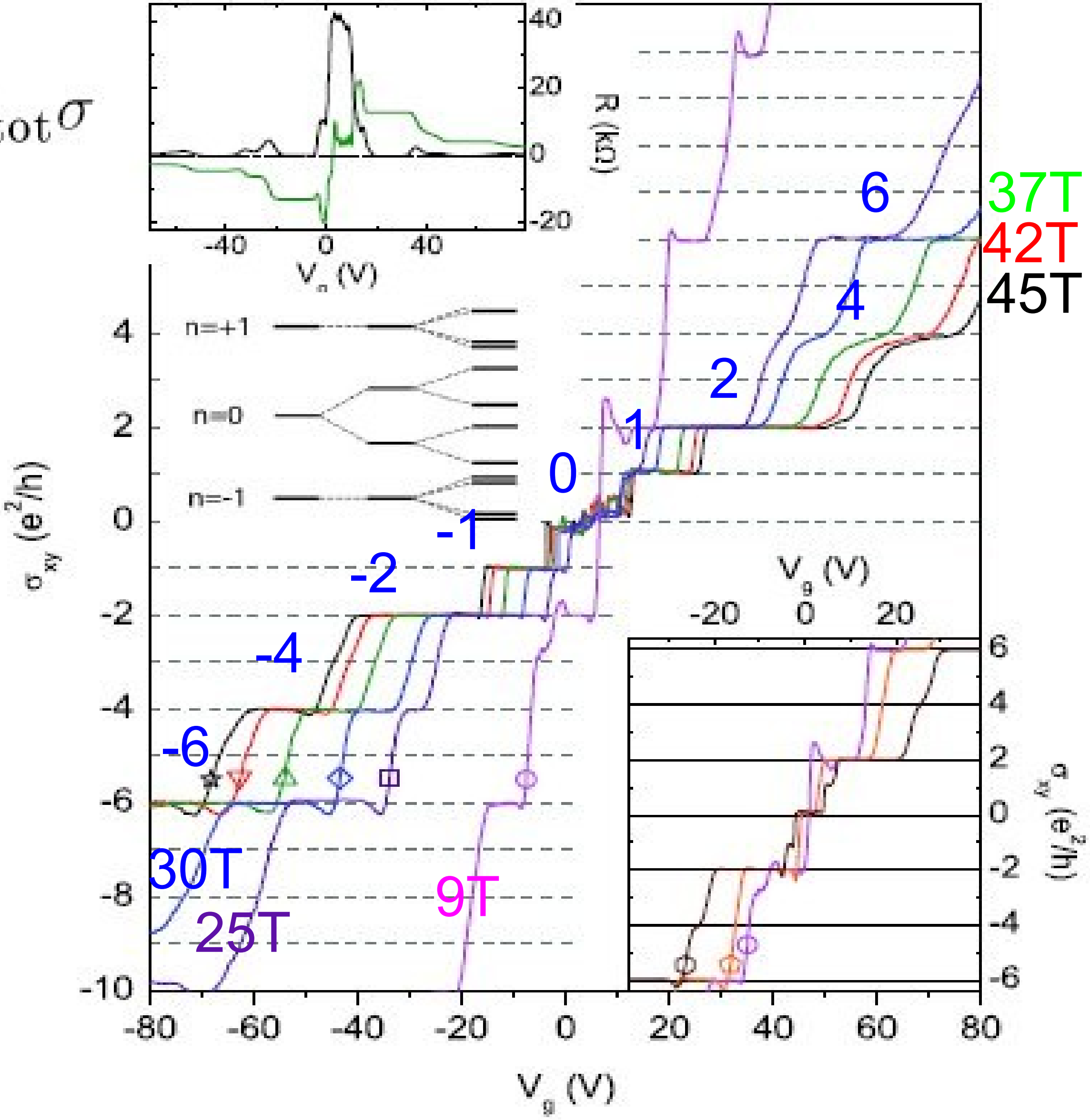
Graphene at large B: extra QH states

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

$$\varepsilon_{n,\sigma} = \mathrm{sgn}(n)\sqrt{|n|}\hbar\omega_c + \frac{g^*}{2}\mu_B B_{\mathrm{tot}}\sigma$$



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



Zhang et al., Phys. Rev. Lett. 2006.

Mechanisms of valley splitting

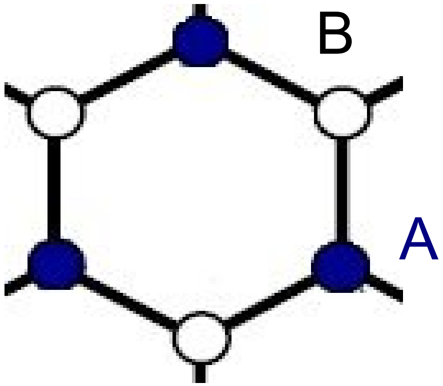
1) Valley-Zeeman effect
- Uniaxial stress (e.g. applied via a piezo): doesn't lift the valley degeneracy in graphene.

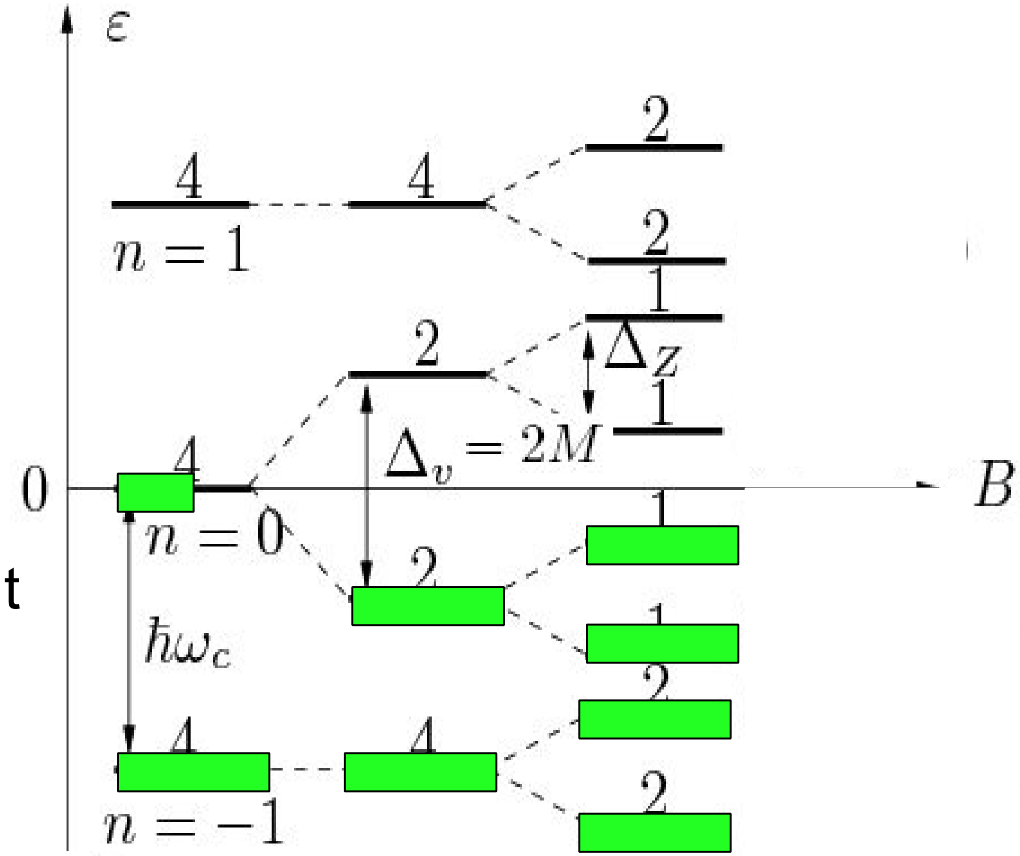
2) Electron-electron interactions
- Exchange gap (QH valley ferromagnetism) $\sim e^2/\epsilon l_B$
- Excitonic gap ("magnetic catalysis") $\sim e^2/\epsilon l_B$
- El.-el. Interactions at the lattice scale (QH valley "paramagnetism") $\sim e^2 a/\epsilon l_B^2$

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):

$$\begin{aligned} \varepsilon_{n,\sigma,\alpha} &= \mathrm{sgn}(n)\sqrt{M^2 + (\hbar\omega_c)^2|n|} + \frac{\Delta_Z}{2}\sigma \text{ if } n \neq 0 \\ &= \alpha M + \frac{\Delta_Z}{2}\sigma \text{ if } n = 0 \end{aligned}$$

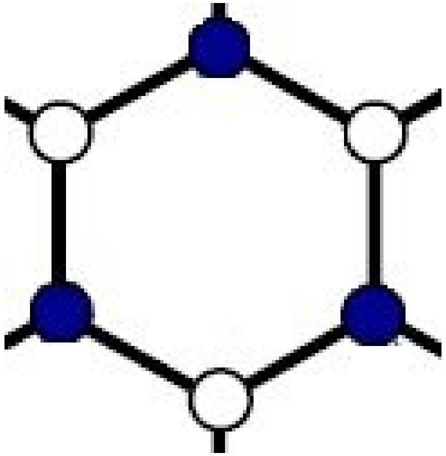
Central Landau level (n=0): α = +1 = A and α = -1 = B
Not true for the other Landau levels (n≠0)

Magnetic field driven Peierls distortion

How can one have A ≠ B?

Out-of-plane lattice distortion

AND substrate (SiO2) ≠ superstrate (air)



B moves towards the silicon dioxide substrate (-η)

A moves away from the substrate (+η)

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

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

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

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

Minimizing the total energy: $\Delta_v = \dfrac{N_\phi}{N_p}(2-|\nu|)\dfrac{D^2}{G'} \propto B_\perp$

Estimate of the constants D and G

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

$\omega_0/2\pi c \sim 800\mathrm{cm}^{-1}$ (for graphite) $\quad Ga^2 \approx m_c\omega_0^2 a^2/4 \sim 14\mathrm{eV}$

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 ≈ 1 to 14 eV

No deformation when B=0: G' > 0 therefore Da < 9,8eV

Valley splitting is larger than Zeeman splitting if Da > 6.3eV

To explain the experiments, we choose Da ≈ 7.8 eV, therefore $G'a^2 \approx 4{,}2\mathrm{eV}$

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

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

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

$$\Delta_{\mathrm{imp}} \approx 30\mathrm{K}$$

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 environnement, the lattice distortion should vanish (e.g. for a suspended graphene sheet or for a sheet inside a polymer matrix, see R. Ruoff).

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Thank you!