Edges and Excitations for Graphene in the Quantum Hall Regime

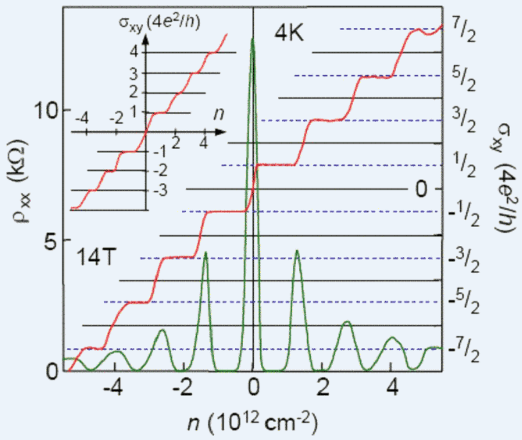
H.A. Fertig, Indiana University and Technion

I. Introduction: QHE in Graphene; Edge States
II. Edge States in Graphene: Zigzag and Armchair
III. Domain Wall at the Edge
III. Bulk Excitations: Excitons
V. Summary

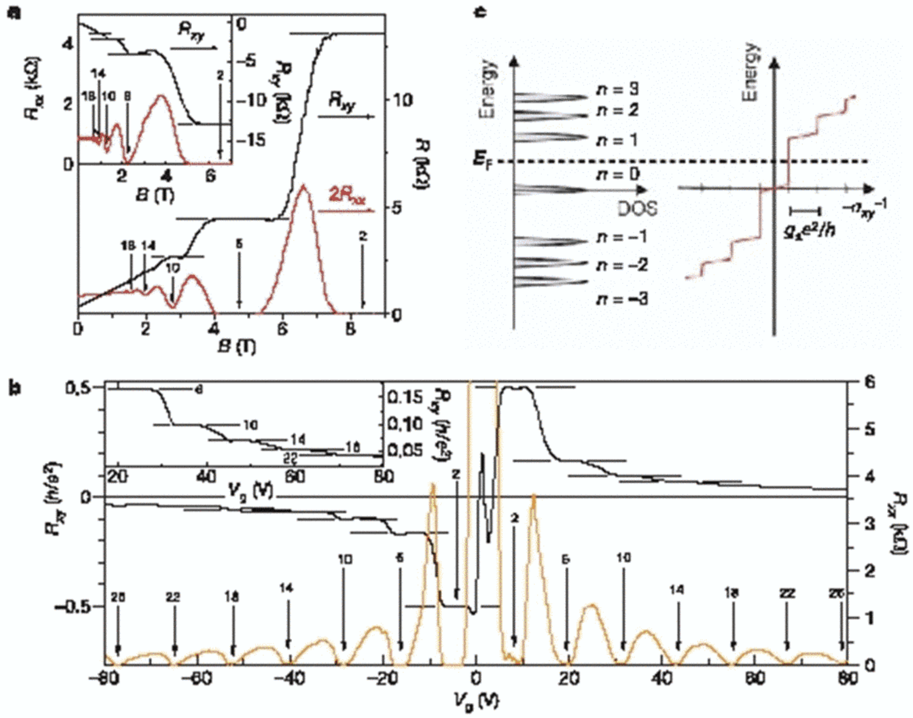
Collaborators: Luis Brey, CSIC, Madrid;
Drew Iyengar and Jianhui Wang, IU

Funding: NSF

I. Quantum Hall Effect in Graphene



From Novoselov et al.,
Nature (2005)



From Zhang et al., Nature (2005)

Electronic states for graphene in a magnetic field

1. k·P approximation: Write $\psi(\mathbf{r})=e^{iK(')\cdot\mathbf{r}}\varphi(\mathbf{r})$
2. Peierls substitution:

$$k_\mu \to -i\partial_\mu \to -i\partial_\mu - \frac{e}{c}A_\mu$$

3. Choose gauge:

$$A=(-By,0,0) \Rightarrow \quad b^+ = \frac{\ell}{\sqrt{2}}\left(i\partial_y + y\ell^2 - ik_x\right) \quad \text{with } \ell=\sqrt{\frac{\hbar c}{eB}}$$

$$\sqrt{3}\frac{a}{\ell}t\begin{pmatrix}0 & b\\ b^+ & 0\end{pmatrix}\begin{pmatrix}\phi_A(\vec{r})\\ \phi_B(\vec{r})\end{pmatrix}=\varepsilon\begin{pmatrix}\phi_A(\vec{r})\\ \phi_B(\vec{r})\end{pmatrix} \qquad \tau=+1 \qquad K \text{ valley}$$

$$\sqrt{3}\frac{a}{\ell}t\begin{pmatrix}0 & -b^+\\ -b & 0\end{pmatrix}\begin{pmatrix}\phi_A(\vec{r})\\ \phi_B(\vec{r})\end{pmatrix}=\varepsilon\begin{pmatrix}\phi_A(\vec{r})\\ \phi_B(\vec{r})\end{pmatrix} \qquad \tau=-1 \qquad K' \text{ valley}$$

Wavefunctions:

$$\Psi(+,n)=e^{ik_x x}\begin{pmatrix}\pm\phi_{n-1}(y-k_x\ell^2)\\ \phi_n(y-k_x\ell^2)\end{pmatrix} \quad \Psi(-,n)=e^{ik_x x}\begin{pmatrix}\pm\phi_{n}(y-k_x\ell^2)\\ \phi_{n-1}(y-k_x\ell^2)\end{pmatrix}$$

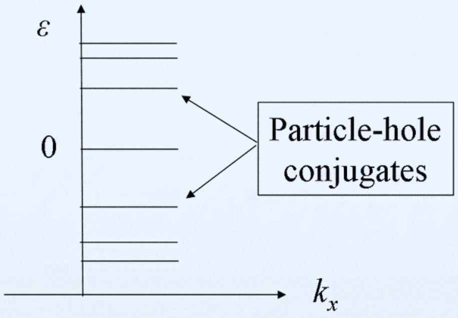
$$\Psi(+,0)=e^{ik_x x}\begin{pmatrix}0\\ \phi_0\end{pmatrix} \qquad \Psi(-,0)=e^{ik_x x}\begin{pmatrix}\phi_0\\ 0\end{pmatrix}$$

ϕ_n = harmonic oscillator state

Energies:

$$\boxed{\varepsilon(\tau,n)=\pm\sqrt{3\,n}\,\frac{a}{\ell}t}$$

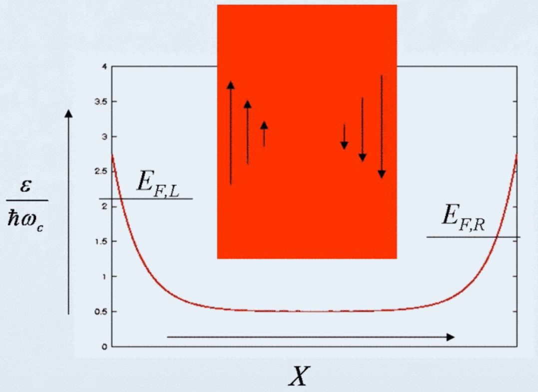
With valley and spin indices, each Landau level is 4-fold degenerate



Particle-hole conjugates

Explanation in terms of edges states:

- Real samples in experiments are very narrow (.1-1μm) ⇒ edges can have a major impact on transport
- Edge structure can be probed directly via STM at very small length scales. Nothing comparable is possible in standard 2DEG's (GaAs samples, Si MOSFET's)



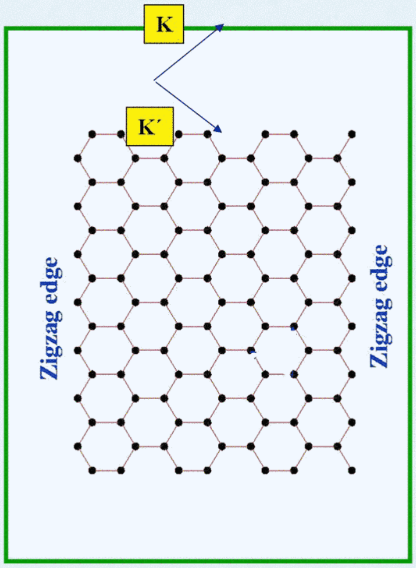
Hall resistance:

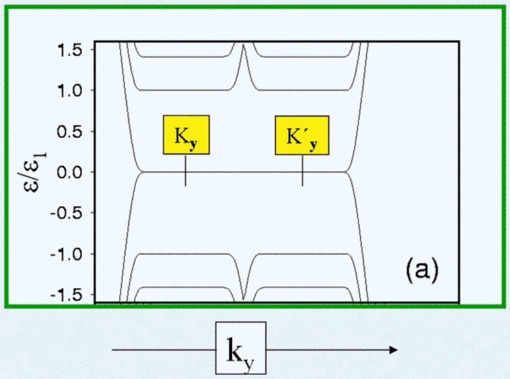
$$\boxed{R_H = V/NI = h/Ne^2}$$

with N the number of edge state pairs crossed by E_F

II. Edge States in Graphene

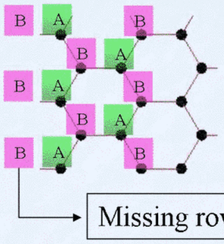
(1) Tight-binding results, zigzag edge





What happened to the n=0 edge states in the center?

Edge states from Dirac equation:



Boundary condition:
$\phi_B(x=0)=0$

Missing row of atoms all from same sublattice

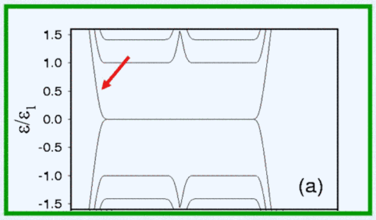
Acting on wavefunctions *twice* with Hamiltonian gives scalar equations:

$$\boxed{\begin{array}{c}\frac{2\gamma^2 a_0^2}{\ell^2} b^\dagger b \varphi_B = \varepsilon^2 \varphi_B \\ \varphi_A = b\varphi_B/\varepsilon\end{array}} \quad \boxed{\begin{array}{c}\frac{2\gamma^2 a_0^2}{\ell^2} b b^\dagger \varphi'_A = \varepsilon^2 \varphi'_A \\ \varphi'_B = -b\varphi'_A/\varepsilon\end{array}} \qquad \gamma = \frac{\sqrt{3}}{2}t$$

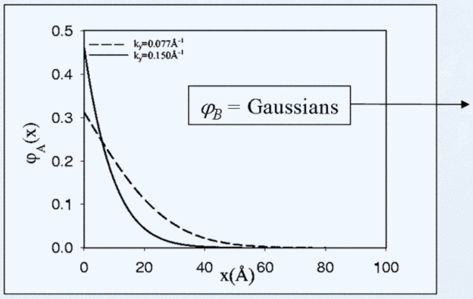
- For high Landau levels, problem essentially identical to GaAs case
- For n=0, **K** and **K´** wavefunctions behave differently

K-valley: Current Carrying Edge States

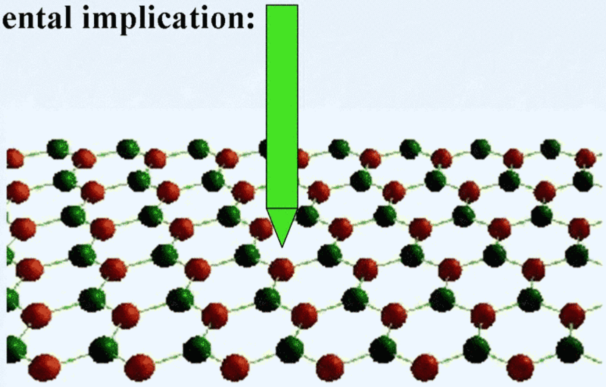
$$\boxed{\begin{array}{c}\frac{2\gamma^2 a_0^2}{\ell^2} b^\dagger b \varphi_B = \varepsilon^2 \varphi_B \\ \varphi_A = b\varphi_B/\varepsilon\end{array}}$$



- For $k_y l^2$ not too close to edge, φ_B very similar to a bulk LLL state. Only significant difference is at $x=0$.
- Since b annihilates a LLL state, φ_A strongly localized near $x=0$!
- When $k_y l^2$ close to edge, tunneling between A and B becomes significant and hole-like and particle-like states disperse.



Possible experimental implication:



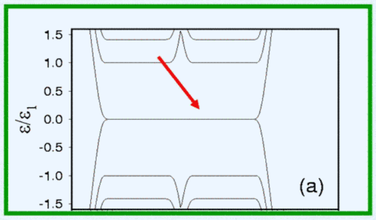
May be able to observe oscillations when injecting electrons with an STM tip near a zigzag edge. Oscillation period depends on distance from edge.

$$\boxed{\begin{array}{c}\frac{2\gamma^2 a_0^2}{\ell^2} b b^{\dagger} \varphi_A' = \varepsilon^2 \varphi_A' \\ \varphi_B' = -b\varphi_A'/\varepsilon\end{array}}$$

K′-valley: Dispersionless Edge States

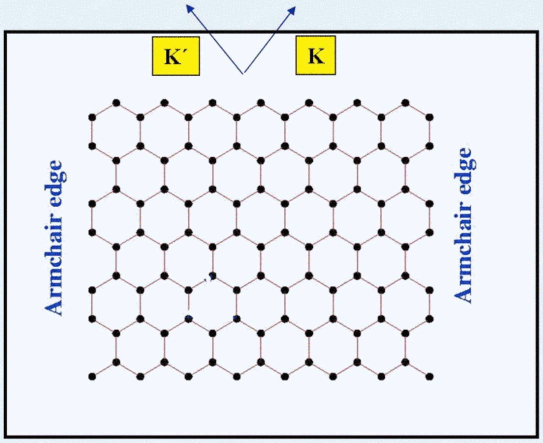
- Equations satisfied for φ'_B=0 and φ'_A a LLL state, even when guiding center is off edge of system ⇒ φ'_A the tail of a Gaussian, and $\varepsilon = 0$

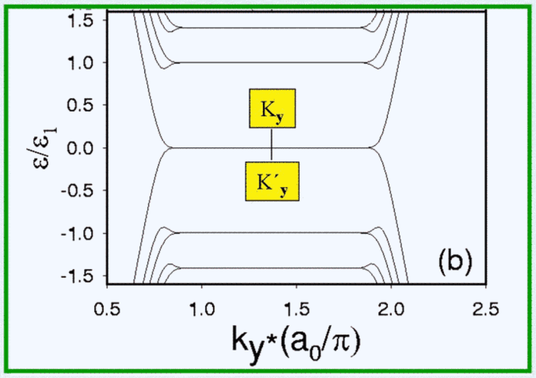
- These states carry no current!



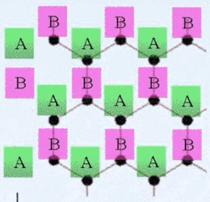
⇒ n=0 Hall conductance is half as large as steps for larger n

(2) Tight-binding results, armchair edge





Two sets of edge states for n>0, one for n=0.



Boundary conditions:
$\phi_B(x=0)+\phi'_B(x=0)=0$
$\phi_A(x=0)+\phi'_A(x=0)=0$
Admixes valleys

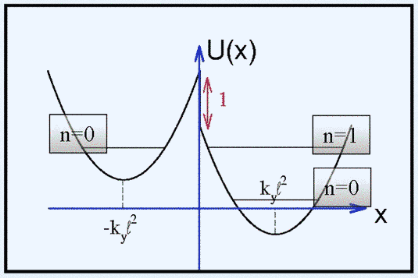
Missing row of atoms with equal number of atoms from both sublattices

$$\varphi_A = b\varphi_B/\varepsilon$$

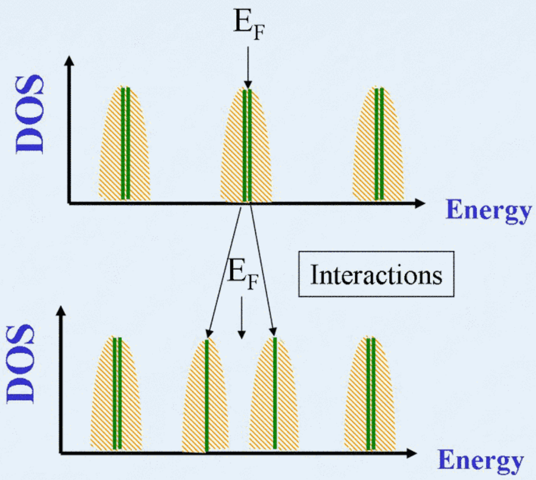
$$\varphi'_A = -b^\dagger \varphi'_B/\varepsilon \quad \Rightarrow \quad \partial_x\varphi_B(x=0) + \partial_x\varphi'_B(x=0) = 0$$

Trick: define wavefunction
for $-\infty < x < \infty$:

$$\Psi(x) = \varphi_B(x)\theta(x)$$
$$+\varphi'_B(-x)\theta(-x)$$



III. Quantum Hall Ferromagnetism and the Graphene Edge



- Exchange tends to force electrons into the same level even when bare splitting between levels is small
- Renormalizes gap to much larger value than expected from non-interacting theory (even if bare gap is zero!)

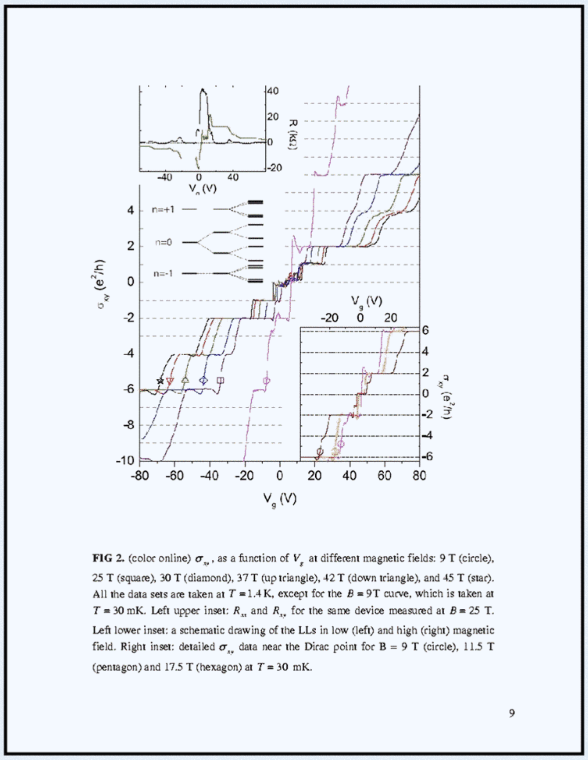


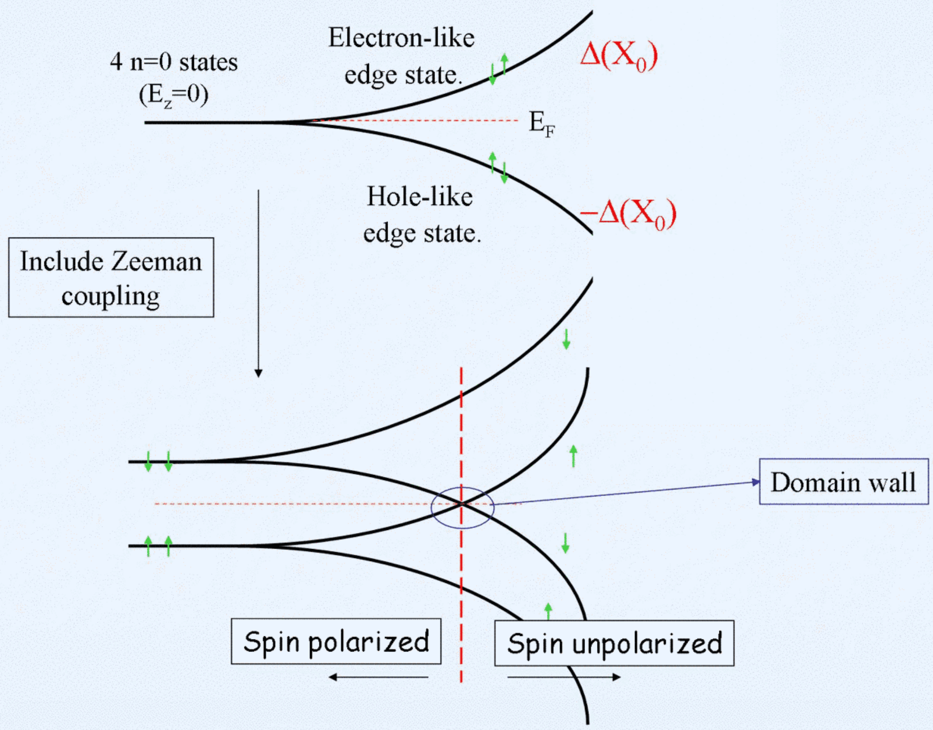
FIG 2. (color online) σ_{xy}, as a function of V_g at different magnetic fields: 9 T (circle), 25 T (square), 30 T (diamond), 37 T (up triangle), 42 T (down triangle), and 45 T (star). All the data sets are taken at $T = 1.4$ K, except for the $B = 9$T curve, which is taken at $T = 30$ mK. Left upper inset: R_{xx} and R_{xy} for the same device measured at $B = 25$ T. Left lower inset: a schematic drawing of the LLs in low (left) and high (right) magnetic field. Right inset: detailed σ_{xy} data near the Dirac point for B = 9 T (circle), 11.5 T (pentagon) and 17.5 T (hexagon) at $T = 30$ mK.

9

This does happen in graphene (Zhang et al., 2006).

- Plateaus at ν=0,±1.
- System is a *pseudospin ferromagnet.*

Consequences for edge states:



4 n=0 states (E_z=0)

Electron-like edge state.

$\Delta(X_0)$

E_F

Hole-like edge state.

$-\Delta(X_0)$

Include Zeeman coupling

Domain wall

Spin polarized

Spin unpolarized

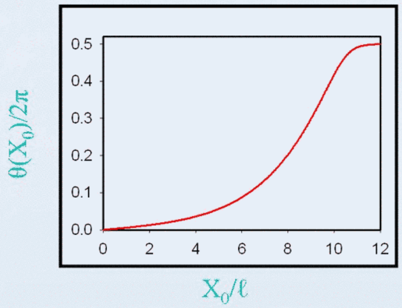
Description of the domain wall:

$$\boxed{|\Psi\rangle = \prod_{X_0<L}\left[\cos\frac{\theta(X_0)}{2}C^{+}_{+,X_0,\uparrow} + \sin\frac{\theta(X_0)}{2}C^{+}_{-,X_0,\downarrow}\right]C^{+}_{-,X_0,\uparrow}|0>}$$

$$X_0 \to -\infty \quad \theta = 0; \quad X_0 \to L \quad \theta = \pi$$

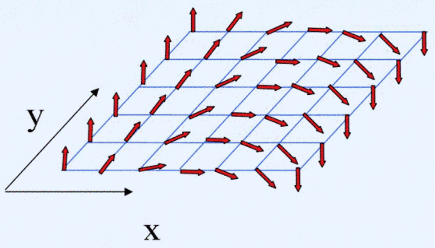
$$E = \pi\ell^2 \rho_s \sum_{X_0<L}\left(\frac{d\theta}{dX_0}\right)^2 + \sum_{X_0<L}(E_z - \Delta(X_0))\cos\theta(X_0)$$

Pseudospin stiffness

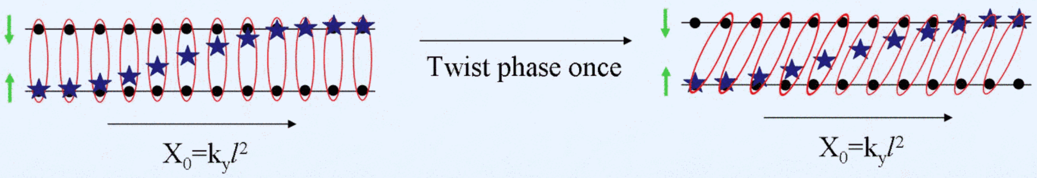


Result of minimizing energy. Width of domain wall set by strength of confinement.

Properties of the domain wall

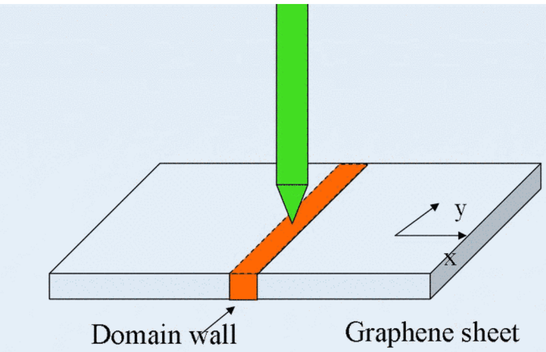


1. Broken U(1) symmetry ⇒ gapless collective mode
2. Spin-charge coupling ⇒ gapless charged excitations!

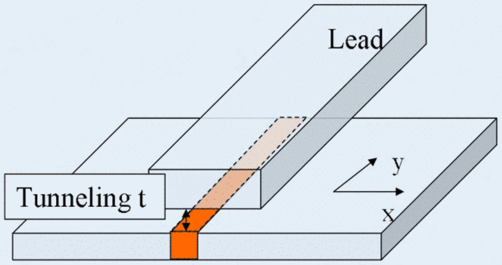


★ = weight in w/f

3. Tunneling from STM
tip: power law IV
⇒ not a Fermi liquid!
Power law exponent a function
of confinement potential



4. Tunneling from a
bulk lead:
possibility of a quantum
phase transition
(into 3D metal).



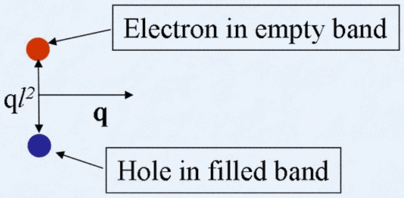
$$\frac{dt^2}{dl} = -(\kappa - 2)t^2 \quad \kappa = (x + 1/x)/2 \quad x = 4\pi\sqrt{\rho/\Gamma}$$

ρ = U(1) spin stiffness
Γ ~ confinement potential

IV. Inter-Landau Level Excitations (Magnetoplasmons)

Low-lying excited states = particle-hole pairs

Standard 2DEG:



cf. Kallin and
Halperin, 1984

- Measurable in cyclotron resonance, inelastic light scattering.
- This picture is largely the same for graphene, just need to be careful about spinor structure of particle and hole states.

Two-Body Problem

$$\boxed{H_0 = \underbrace{(\mathbf{p}_1 - \mathbf{A}_1) \cdot \sigma}_{\text{Electron}} \otimes \mathbf{1} + \mathbf{1} \otimes \underbrace{(\mathbf{p}_2 + \mathbf{A}_2) \cdot \sigma}_{\text{Hole}}}$$

(ħ=ω$_c$=l=1)

To diagonalize (**A**= -*By***x**):

1. Adopt center and relative coordinate **R**=($\mathbf{r}_1$+$\mathbf{r}_2$)/2, **r**= $\mathbf{r}_1$-$\mathbf{r}_2$
2. Apply unitary transformation H'_0 = U^+H_0U with

$$U = e^{i\vec{p}\cdot(\hat{z}\times\vec{P})}e^{-ixY}$$

$\vec{P}$ = center of mass momentum

$$\boxed{\rightarrow H_0' = \sqrt{2}\left[-\mathbf{1}\otimes\begin{pmatrix}0 & c_-\\ c_-^\dagger & 0\end{pmatrix} + \begin{pmatrix}0 & c_+^\dagger\\ c_+ & 0\end{pmatrix}\otimes\mathbf{1}\right]}$$

with

$$\boxed{\begin{aligned} c_+^\dagger &= \frac{i}{\sqrt{2}}(-2\partial_z + \bar{z}/2) \\ c_-^\dagger &= \frac{i}{\sqrt{2}}(-2\partial_{\bar{z}} + z/2) \end{aligned}}$$

z=x+iy

Wavefunctions constructed from:

$$\boxed{\varphi_{n_+,n_-}(z,\bar{z}) = \frac{(c_+^\dagger)^{n_+}}{\sqrt{n_+!}}\frac{(c_-^\dagger)^{n_-}}{\sqrt{n_-!}}\varphi_{0,0}(z,\bar{z})}$$

with

$$\boxed{\varphi_{0,0}(z,\bar{z}) = (2\pi)^{-1/2}e^{-\frac{1}{4}z\bar{z}}}$$

Wavefunctions are 4-vectors $|n_+,n_->$ constructed from φ_{n_+,n_-} with energies

$$\boxed{E = \sqrt{2}[s_+\sqrt{|n_+|} - s_-\sqrt{|n_-|}]}$$

$s_+ = 1, \quad s_- = -1$

Electron Hole

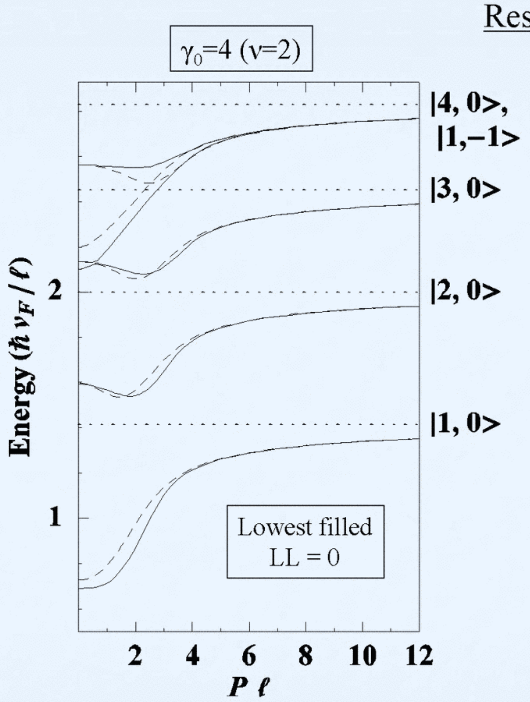
3. Apply unitary transformation to interaction H_1:

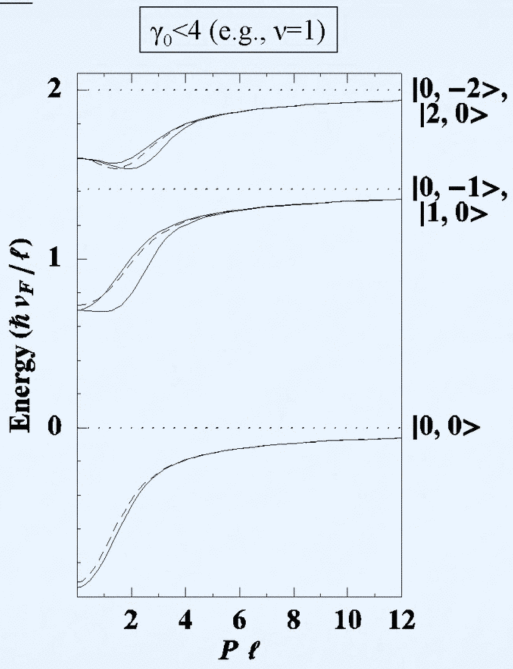
$$\boxed{H_1' = -e^2/(\epsilon\,|\mathbf{r} - \hat{\mathbf{z}}\times\mathbf{P}|)\,\mathbf{1}\otimes\mathbf{1}}$$

4. Compute eigenvalues of $< n_+', n_-'|H_0' + H_1'|n_+, n_- >$

⇒ two-body eigenenergies with fixed **P**

Results:

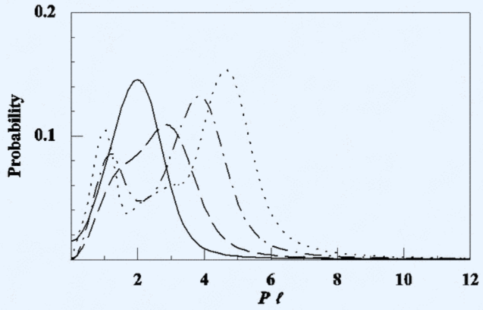




Interaction scale: $\beta=(e^2/\varepsilon l)/(\hbar v_F/l) \approx (c/v_F\varepsilon)/137 = 0.73$

Comments:

1. Negative energies because we have not included loss of exchange self-energy ⇒ many-body approach needed
2. Landau level mixing relatively small



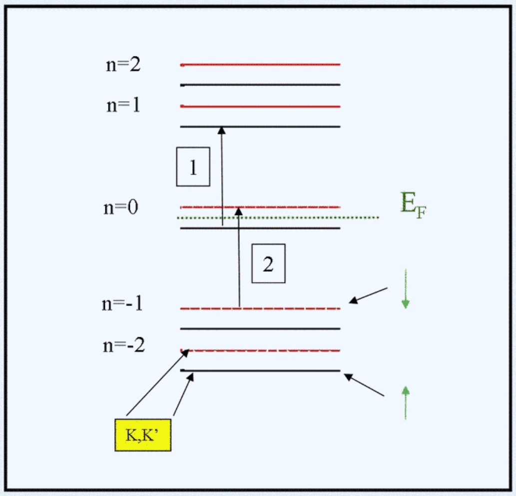
Note however for $\beta \approx 1$, LL mixing becomes much more pronounced
⇒ system on cusp between weakly and strongly interacting

Many-Body Particle-Hole Approach

$$|\mathbf{q}>= \rho_{\tau,\sigma,n;\tau',\sigma',n'}(\mathbf{q})|\mathrm{GS}>$$

$$\rho_{\tau,\sigma,n;\tau',\sigma',n'}(\mathbf{q}) = \frac{1}{N_\phi}\sum_X e^{-\frac{i}{2}q_x(2X+q_y)}C^+_{\tau,\sigma,n,X}C_{\tau',\sigma',n',X+q_y}$$

Must watch out for degeneracies:



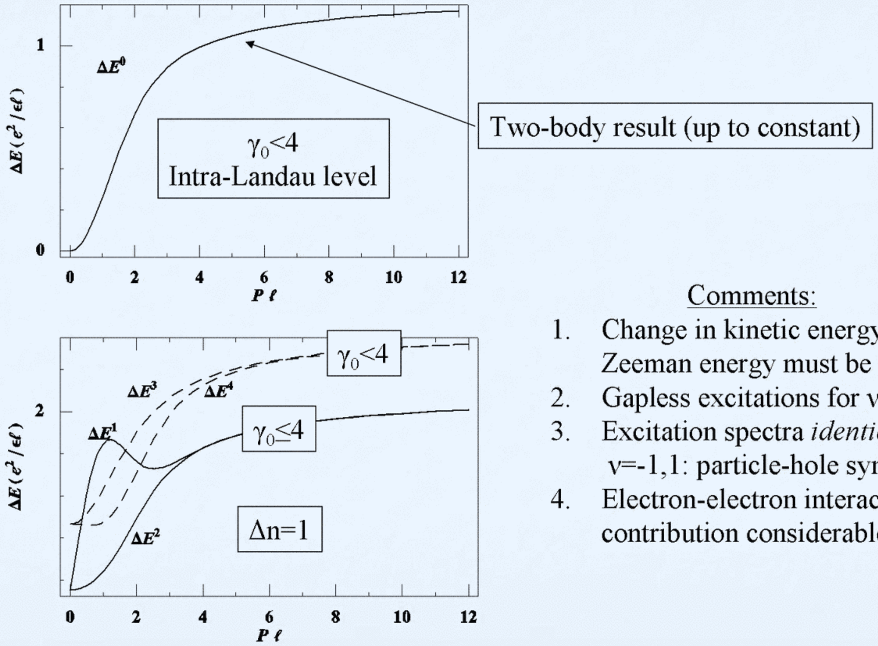
$$\boxed{|\mathbf{q}>= [c_1\rho_1(\mathbf{q})+c_2\rho_2(\mathbf{q})]|\mathrm{GS}>}$$

$$\boxed{|c_1|^2+|c_2|^2=1}$$

$$\boxed{\Delta E =< \mathbf{q}|H|\mathbf{q}> -E_0}$$

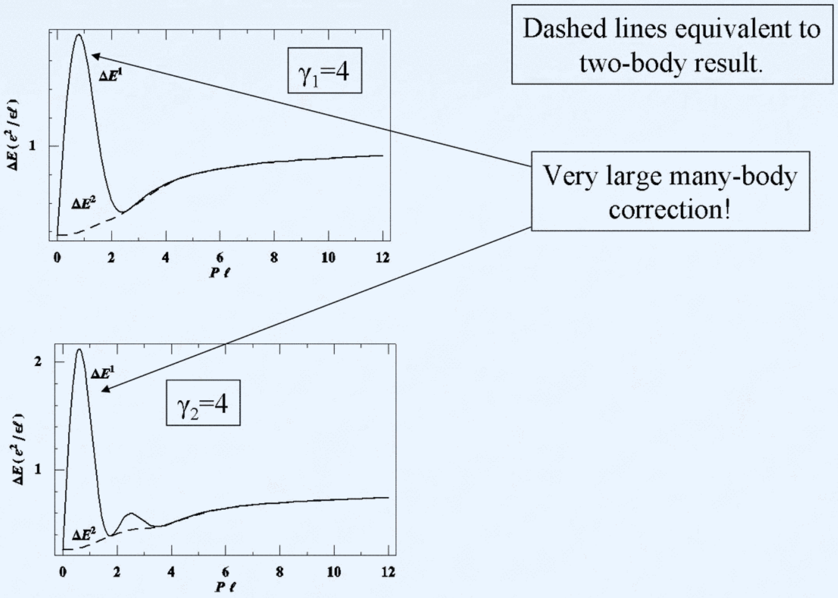
- Minimize with respect to c_1 and c_2
- Excitations characterized by ΔS_z and $\Delta\tau_z$

Results: N=0



Comments:

1. Change in kinetic energy and Zeeman energy must be added in
2. Gapless excitations for ν=-1,1
3. Excitation spectra *identical* for ν=-1,1: particle-hole symmetry
4. Electron-electron interaction contribution considerable



Dashed lines equivalent to two-body result.

Very large many-body correction!

- Minima/maxima may be visible in inelastic light scattering or microwave absorption.

Summary

- Graphene in quantum Hall regime supports unusual edge states
- Zigzag edge: current-carrying and dispersionless edges states in LLL
- Armchair edge: admixing of two valleys
- Clean system is likely a quantum Hall ferromagnet.
- Armchair edges: oppositely dispersing spin up and down bands
  $\Rightarrow$ domain wall
- Domain wall supports gapless collective excitations, and gapless charged excitations through pseudospin texture.
- Domain wall supports power law IV (Luttinger liquid).
- Domain wall may undergo quantum phase transition when coupled to a bulk lead.

- Collective inter-Landau level excitations = excitons
- Many-body corrections split and distort dispersions found in two-body problem