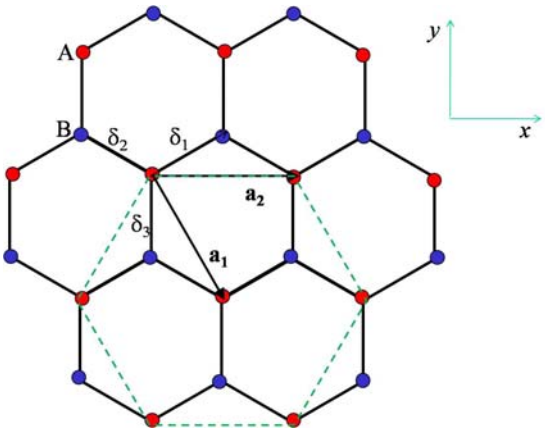
CHAPTER 1

# Hartree-Fock Hamiltonians for the chiral 2DEGs in graphene and bilayer graphene

## 1.1 Basic notions

- **Lattice structure**: honeycomb lattice of C atoms (triangular lattice with 2 C per unit cell: A and B)




The crystal structure of graphene.

- **Primitive vectors**:

$$\mathbf{a}_1 = a\left(\frac{1}{2}, -\frac{\sqrt{3}}{2}\right), \tag{1.1}$$

$$\mathbf{a}_2 = a\,(1,0)\,. \tag{1.2}$$

with $a = \sqrt{3}c$ where $c = 1.42$ Å is the spacing between carbons atoms.

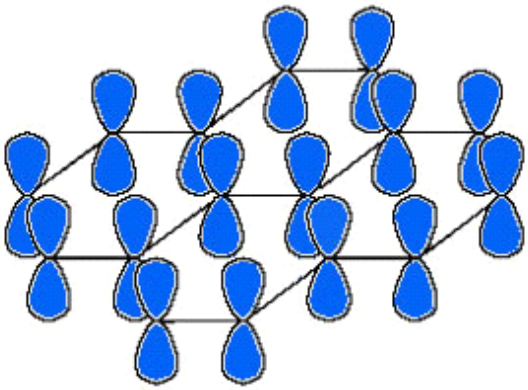
- **Nearest-neighbors**:

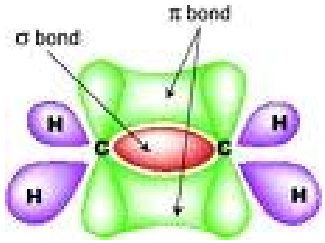
$$\boldsymbol{\delta}_1 = a\left(\frac{1}{2}, \frac{1}{2\sqrt{3}}\right), \tag{1.3}$$

$$\boldsymbol{\delta}_2 = a\left(-\frac{1}{2}, \frac{1}{2\sqrt{3}}\right), \tag{1.4}$$

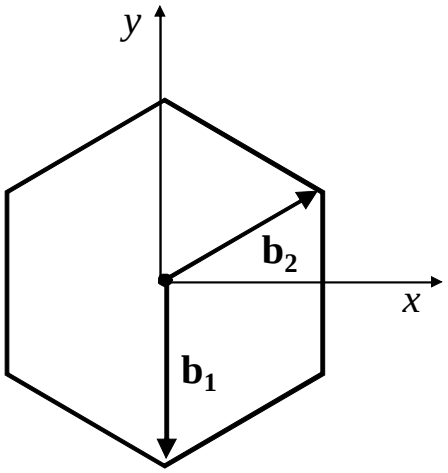
$$\boldsymbol{\delta}_3 = a\left(0, -\frac{1}{\sqrt{3}}\right). \tag{1.5}$$

- **$sp_2$ hybridization**, **$\sigma$ and $\pi$ bonds**






- **Reciprocal lattice:**

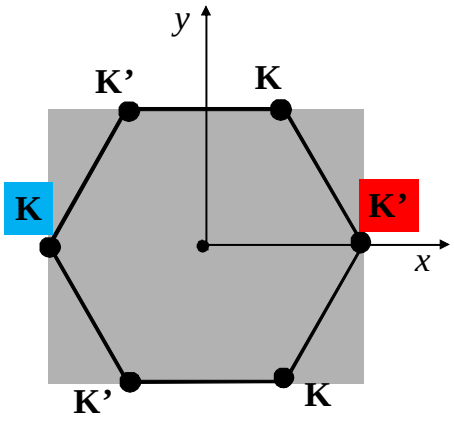



Reciprocal lattice of graphene.

- **Valleys**:

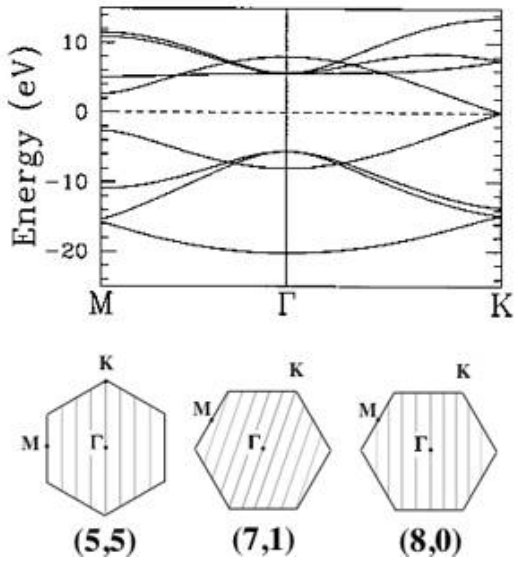
$$\mathbf{K}' = \left(\frac{2}{3}, 0\right)\frac{2\pi}{a}, \tag{1.6}$$

$$\mathbf{K} = \left(-\frac{2}{3}, 0\right)\frac{2\pi}{a}. \tag{1.7}$$




First Brillouin zone of graphene.

- **Band structure:** eith 2 C's per unit cell, we have 8 bandes: 6 $\sigma$ bands and 2 $\pi$ bands:




- **Fermi level:** valence of C is 4: 3 $\sigma$ and 1 $\pi$ bands are occupied in undoped graphene.

## 1.2 Tight-binding hamiltonian for the $\pi$ bands

- Hamiltonian for the $\pi$ bands:

$$H = -t \sum_{\langle i,j \rangle} \left( a_i^\dagger b_j + h.c. \right), \tag{1.8}$$

with $t \approx 2.8$ eV and $t' \approx 0.1$ eV, $t'' \approx 0.07$ eV.

- Fourier transform to $a_{\mathbf{k}}$ and $b_{\mathbf{k}}$ operators:

$$a_j = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_{j,A}} a_{\mathbf{k}}, \tag{1.9}$$

$$b_j = \frac{1}{\sqrt{N}} \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}_{j,B}} b_{\mathbf{k}}, \tag{1.10}$$

with

$$\left\{ a_{\mathbf{k}}, a_{\mathbf{k}'}^\dagger \right\} = \left\{ b_{\mathbf{k}}, b_{\mathbf{k}'}^\dagger \right\} = \delta_{\mathbf{k},\mathbf{k}'}. \tag{1.11}$$

- Hamiltonian:

$$H = \sum_{\mathbf{k}} \begin{pmatrix} a_{\mathbf{k}}^\dagger & b_{\mathbf{k}}^\dagger \end{pmatrix} \begin{pmatrix} 0 & \Lambda(\mathbf{k}) \\ \Lambda^*(\mathbf{k}) & 0 \end{pmatrix} \begin{pmatrix} a_{\mathbf{k}} \\ b_{\mathbf{k}} \end{pmatrix}, \tag{1.12}$$

where

$$\Lambda(\mathbf{k}) = -t \sum_{\boldsymbol{\delta}} e^{i\mathbf{k}\cdot\boldsymbol{\delta}}. \tag{1.13}$$

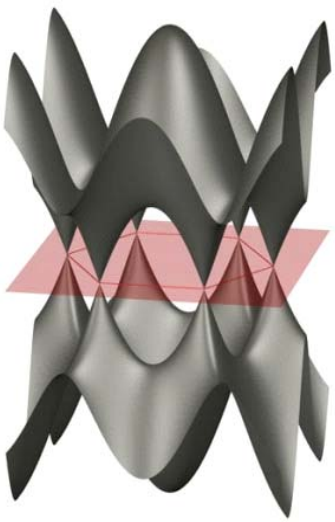
The TB Hamiltonian is diagonalized to give:

$$H = \sum_{\mathbf{k}} E_c(\mathbf{k}) \, c_{c,\mathbf{k}}^\dagger c_{c,\mathbf{k}} + \sum_{\mathbf{k}} E_v(\mathbf{k}) \, c_{v,\mathbf{k}}^\dagger c_{v,\mathbf{k}}, \tag{1.14}$$

- Band structure:

$$E_c(\mathbf{k}) = +\sqrt{\Lambda(\mathbf{k})\Lambda^*(\mathbf{k})} = +t\sqrt{1 + 4\cos^2\left(\frac{k_x a}{2}\right) + 4\cos\left(\frac{k_x}{2}a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right)}, \tag{1.15}$$

$$E_v(\mathbf{k}) = -\sqrt{\Lambda(\mathbf{k})\Lambda^*(\mathbf{k})} = -t\sqrt{1 + 4\cos^2\left(\frac{k_x a}{2}\right) + 4\cos\left(\frac{k_x}{2}a\right)\cos\left(\frac{\sqrt{3}}{2}k_y a\right)}. \tag{1.16}$$



## 1.3 Continuum approximation

We consider that the doping is small so that the Fermi level is near energy $E = 0$ and we can use the band structure around the valley points $K_\pm$. Expanding to linear order in $p$, we get the linear dispersion:

$$E(\mathbf{p}) = \pm\hbar v_F |\mathbf{p}| . \tag{1.17}$$

where the Fermi velocity is

$$v_F = \frac{3ct}{2\hbar} \simeq 1 \times 10^6 \mathrm{m/s}. \tag{1.18}$$

For the Hamiltonians (basis $A, B$)

$$H_K(\mathbf{p}) = -v_F \begin{pmatrix} 0 & pe^{-i\theta} \\ pe^{i\theta} & 0 \end{pmatrix} = -v_F \boldsymbol{\sigma}\cdot\mathbf{p}, \tag{1.19}$$

$$H_{K'}(\mathbf{p}) = +v_F \begin{pmatrix} 0 & pe^{i\theta} \\ pe^{-i\theta} & 0 \end{pmatrix} = +v_F \boldsymbol{\sigma}^*\cdot\mathbf{p}, \tag{1.20}$$

where:

$$\tan\theta = \frac{p_y}{p_x}. \tag{1.21}$$

The eigenspinors give the wave function on site $A$ and $B$. For the $K$ and $K'$ valleys and the conduction (C) and valence (B) bands:

$$\psi_C^K(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta(\mathbf{p})/2} \\ -e^{i\theta(\mathbf{p})/2} \end{pmatrix}, \psi_V^K(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta(\mathbf{p})/2} \\ e^{i\theta(\mathbf{p})/2} \end{pmatrix}, \tag{1.22}$$

$$\psi_C^{K'}(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta(\mathbf{p})/2} \\ e^{-i\theta(\mathbf{p})/2} \end{pmatrix}, \psi_V^{K'}(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\theta(\mathbf{p})/2} \\ -e^{-i\theta(\mathbf{p})/2} \end{pmatrix}. \tag{1.23}$$

If we use the basis $(A, B)$ for $K$ and $(B, A)$ for $K'$, then: ($\xi = +1$ for $K$ and $\xi = -1$ for $K'$)

$$H_{\xi K}(\mathbf{p}) = -\xi v_F \begin{pmatrix} 0 & pe^{-i\theta} \\ pe^{i\theta} & 0 \end{pmatrix} = -\xi v_F \boldsymbol{\sigma}\cdot\mathbf{p} \tag{1.24}$$

and we have for the **sublattice** spinors

$$\psi_C^{\xi K}(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{-i\theta(\mathbf{p})/2} \\ -\xi e^{i\theta(\mathbf{p})/2} \end{pmatrix} \tag{1.25}$$

$$\psi_V^{\xi K}(\mathbf{p}) = \frac{1}{\sqrt{2}} \begin{pmatrix} \xi e^{-i\theta(\mathbf{p})/2} \\ e^{i\theta(\mathbf{p})/2} \end{pmatrix}, \tag{1.26}$$

## 1.4 Helicity

A general spin 1/2 spinor is given by

$$|+\rangle_{\mathbf{u}} = \cos\left(\frac{\varphi}{2}\right) e^{-i\theta/2} |+\rangle + \sin\left(\frac{\varphi}{2}\right) e^{+i\theta/2} |-\rangle , \tag{1.27}$$

$$|-\rangle_{\mathbf{u}} = \sin\left(\frac{\varphi}{2}\right) e^{-i\theta/2} |+\rangle - \cos\left(\frac{\varphi}{2}\right) e^{+i\theta/2} |-\rangle . \tag{1.28}$$

For $\varphi = \pi/2$ :

$$|+\rangle_{\mathbf{u}} = \frac{1}{\sqrt{2}} \left[ e^{-i\theta/2} |+\rangle + e^{+i\theta/2} |-\rangle \right], \tag{1.29}$$

$$|-\rangle_{\mathbf{u}} = \frac{1}{\sqrt{2}} \left[ e^{-i\theta/2} |+\rangle - e^{+i\theta/2} |-\rangle \right]. \tag{1.30}$$

With the correspondence

$$|A\rangle \rightarrow |+\rangle, \tag{1.31}$$
$$|B\rangle \rightarrow |-\rangle, \tag{1.32}$$

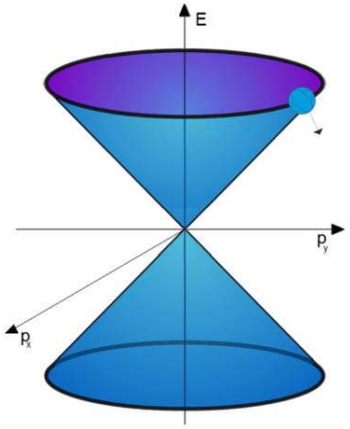
we have

$$\left|\psi_C^K(\mathbf{p})\right\rangle = |-\rangle_{\mathbf{u}}, \left|\psi_V^K(\mathbf{p})\right\rangle = |+\rangle_{\mathbf{u}}, \tag{1.33}$$
$$\left|\psi_C^{K'}(\mathbf{p})\right\rangle = |+\rangle_{\mathbf{u}}, \left|\psi_V^{K'}(\mathbf{p})\right\rangle = |-\rangle_{\mathbf{u}}, \tag{1.34}$$

where

$$\mathbf{u} = \widehat{\mathbf{p}} \tag{1.35}$$

The sublattice spinor is in (or opposite) the direction of the electronic momentum. For $K'$ :




The helicity is defined as the projection of the pseudospin onto the direction of propagation

$$\eta = \boldsymbol{\sigma} \cdot \frac{\mathbf{p}}{|\mathbf{p}|}. \tag{1.36}$$

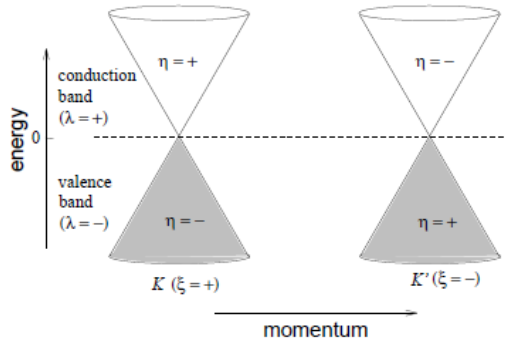
In graphene

$$H_K(\mathbf{p}) = -v_F \boldsymbol{\sigma} \cdot \mathbf{p} = -v_F |\mathbf{p}| \eta \tag{1.37}$$

and so

$$\eta_K = \frac{H_K(\mathbf{p})}{-v_F |\mathbf{p}|} = -1 \text{ (c.b.) and } +1 \text{ (v.b.)} \tag{1.38}$$
$$\eta_{K'} = \frac{H_{K'}(\mathbf{p})}{v_F |\mathbf{p}|} = +1 \text{ (c.b.) and } -1 \text{ (v.b.)} \tag{1.39}$$

(in this picture, $K$ and $K'$ are inverted w.r.t. my definitions)



- The chirality is equivalent to the helicity only for masless particle.

- The eigenstates of the Dirac Hamiltonian are also eigenstates of the chirality operator and so chirality is a good quantum number. It is conserved. Chirality is a quantum number that is conserved in elastic scattering processes induced by impurity potentials $V_{imp} = V(\mathbf{r})\, I$ ($I$ is the unit matrix) that vary smoothly on the lattice scale. This type of potential does not permit inter-valley scattering and so $\xi$ is fixed and $\lambda = \xi\eta$ is conserved. This effect gives rise to the absence of backscattering in graphene and is at the origin of the Klein tunneling (perfect transmission through a high potential barrier at normal incidence).

- Note that chirality is a good number only in the vicinity of the Dirac points. If we include higher-order corrections, it is no longer conserved.

- The rotation operator by an angle $\alpha$ about an axis $\mathbf{u}$ for a spin 1/2 particle is given by

$$R_{\mathbf{u}}(\alpha) = e^{-i\alpha\frac{\boldsymbol{\sigma}}{2}\cdot\mathbf{u}} = \cos\left(\frac{\alpha}{2}\right) - i\boldsymbol{\sigma}\cdot\mathbf{u}\sin\left(\frac{\alpha}{2}\right). \tag{1.40}$$

  We see that a rotation **in the spin space** by $\alpha = 2\pi$ gives a phase factor of $\pi$. This means, in our case, that if the particule circles around the Dirac cone, the vector $p$ turns by $2\pi$ and so does the sublattice pseudospin. The eigenstate thus acquires a $-1$ sign.

- The chiral nature of low-energy electrons in graphene places an additional constraint on their scattering properties. If a given potential doesn't break the A-B symmetry, then it is unable to influence the pseudospin degree of freedom which must, therefore, be conserved upon scattering. Considering only the pseudospin part of the chiral wave function $\psi_{\pm}$, the probability to scatter in a direction $\theta = 0$, where $\theta = 0$ is the forwards direction, is proportional to $w(\theta) = \left|\left\langle\psi_{\pm}(\theta)\,|\psi_{\pm}(0)\right\rangle\right|^2$. For monolayer graphene, $w(\theta) = \cos^2(\theta/2)$. This is anisotropic, and displays an absence of backscattering $w(\pi) = 0$]: scattering into a state with opposite momentum is prohibited because it requires a reversal of the pseudospin. Such conservation of pseudospin is at the heart of anisotropic scattering at potential barriers in graphene monolayers, known as Klein tunneling.

### 2.7.2 Chirality factor and the absence of backscattering

Here, we discuss an important consequence of the pseudo-spin, first discovered by Ando and coworkers in the context of carbon nanotubes [25,26]. Consider a massless Dirac electron, which is incident on an impurity whose potential is smooth on the lattice scale such that intervalley scattering is suppressed and the problem can be described within a single valley model (see Sect. 2.3). The impurity potential is therefore $\hat{V}_{\rm imp}(\boldsymbol{r}) \approx U(\boldsymbol{r})\hat{1}$ [25,26]. For simplicity, though the argument can be made much more general (see [25,26] and the next paragraph), we will compute the scattering probability using the first order Born approximation. It is given by

$$P(\theta) \propto |\langle \boldsymbol{k}', \alpha' | U(\boldsymbol{r})\hat{1} | \boldsymbol{k}, \alpha \rangle|^2 \tag{21}$$

where $|\boldsymbol{k}, \alpha\rangle$ and $|\boldsymbol{k}', \alpha'\rangle$ are the initial and the final states respectively and $\theta$ is the angle between the final and initial wavevectors. As the collision is elastic $k' = k$ and $\alpha' = \alpha$. Therefore the only freedom in the final state is the angle $\theta \equiv \phi_{\boldsymbol{k}'} - \phi_{\boldsymbol{k}}$ that $\boldsymbol{k}'$ makes with $\boldsymbol{k}$. We are now in a position to compute the matrix element:

$$\langle \boldsymbol{k}', \alpha' | U(\boldsymbol{r})\hat{1} | \boldsymbol{k}, \alpha \rangle = \frac{1 + e^{i\theta}}{2} \bar{U}(\boldsymbol{k}' - \boldsymbol{k}) \tag{22}$$

where $\bar{U}(\boldsymbol{q}) \equiv \int d^2 r U(\boldsymbol{r}) \exp(i\boldsymbol{q} \cdot \boldsymbol{r})$ is the Fourier transform of the potential $U(\boldsymbol{r})$. Note that the transferred momentum is $q = 2k \sin(\theta/2)$. Therefore, the scattering probability reads:

$$P(\theta) \propto |\bar{U}(\boldsymbol{q})|^2 \cos^2 \frac{\theta}{2} = |\bar{U}(\boldsymbol{q})|^2 \frac{1 + \cos\theta}{2}. \tag{23}$$

The first term $|\bar{U}(\boldsymbol{q})|^2$ is the usual result of the Born approximation and the second $\cos^2 \frac{\theta}{2}$ is due to the sublattice pseudo-spin and is called the "chirality factor". The latter is just the square of the scalar product between the incoming and outgoing bispinors: $(1, e^{i\phi_{\boldsymbol{k}}})/\sqrt{2}$ and $(1, e^{i\phi_{\boldsymbol{k}'}})/\sqrt{2}$. The effect of the chirality factor is quite dramatic as it kills backscattering ($\boldsymbol{k}' = -\boldsymbol{k}$):

$$P(\theta = \pi) \propto |\bar{U}(\boldsymbol{q})|^2 \cos^2 \frac{\pi}{2} = 0 \text{ with } q = 2k. \tag{24}$$

An intuitive explanation of this absence of backscattering is the following: if the electron tries to backscatter

$\boldsymbol{k}' = -\boldsymbol{k}$ it also has to reverse its sublattice pseudo-spin $\boldsymbol{\sigma} \rightarrow -\boldsymbol{\sigma}$ as the pseudo-spin direction is tied to that of the momentum (indeed remember that away from the impurity $\hat{H}_{\text{kin}} = \boldsymbol{k} \cdot \hat{\boldsymbol{\sigma}}$). However, the potential $U(\boldsymbol{r})\hat{1}$ does not act in sublattice space (it is the unit matrix) and can therefore not reverse the pseudo-spin. Therefore backscattering is impossible. This has profound physical consequences on the transport properties of massless Dirac electrons, such as weak antilocalization [27–29].

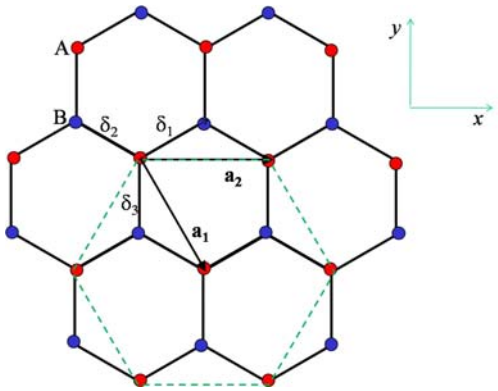
(From P.E. Allain and J. N. Fuchs: Klein tunneling in graphene, Eur. Phys. J. B. 83, 201 (2011)). (Note : $\alpha$ is the band index in this text.)

## 1.5 Family of chiral 2DEGs

- In graphene (monolayer) $H_\xi(\mathbf{p})$ can be written as

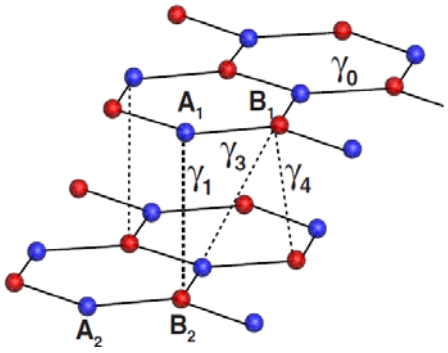
$$H_\xi^{(J)} = -\xi^J \hbar v_F p_c \left(\frac{p}{p_c}\right)^J \left[\cos(J\theta)\,\sigma_x + \sin(J\theta)\,\sigma_y\right], \tag{1.41}$$

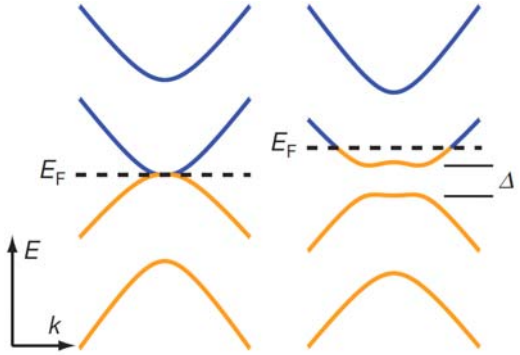
with $J = 1$ where $J$ is the chirality index. $E(p) \sim p$.




- In Bernal-stacked bilayer graphene, a low-energy Hamiltonian ($E << \gamma_1$) can be constructed where $A_2, B_1$ are the low-energy sites. The minimal Hamiltonian is given by $H_\xi^{(2)}$ i.e. $J = 2$ and $E(p) \sim p^2$.

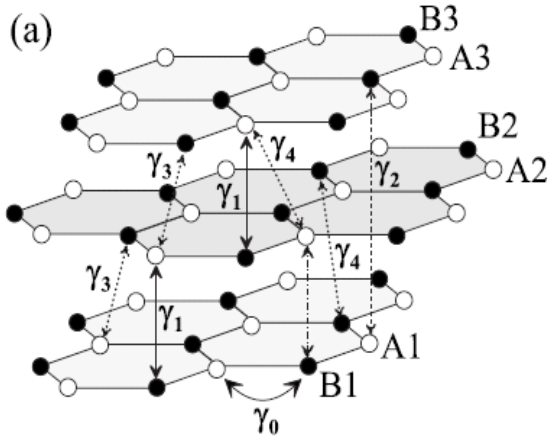
$$\begin{pmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \end{pmatrix} \rightarrow \begin{pmatrix} A_1 \\ B_2 \end{pmatrix} \tag{1.42}$$

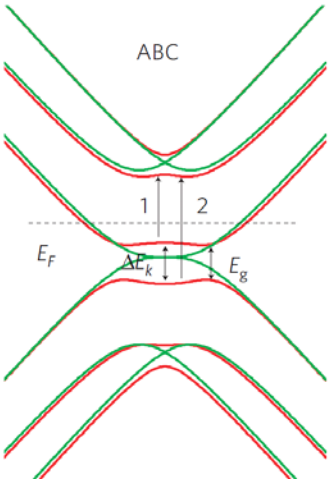



- In ABC-stacked trilayer graphene, the effective two-band model involves the low-energy sites $A_1, B_3$ and $J = 3$ i.e. $E(p) \sim p^3$.

$$\begin{pmatrix} A_1 \\ B_1 \\ A_2 \\ B_2 \\ A_3 \\ B_3 \end{pmatrix} \rightarrow \begin{pmatrix} A_1 \\ B_3 \end{pmatrix} \tag{1.43}$$






## 1.6 Example of the importance of the spinor structure

In second-quantization, we define the field operators as

$$\Psi_{\xi K}(\mathbf{r}) = \frac{1}{\sqrt{2S}} \sum_{\xi} \sum_{\mathbf{p}} e^{i\mathbf{p}\cdot\mathbf{r}} \begin{pmatrix} e^{-i\theta(\mathbf{p})/2} \\ -\xi e^{i\theta(\mathbf{p})/2} \end{pmatrix} c_{K,\mathbf{p},\boldsymbol{\xi}}. \tag{1.44}$$

The spinor structure modifies properties of the C2DEG wrt to the ordinary 2DEG. For example:

- Non-chiral 2DEG: retarded density response function is given by

$$\chi^R_{HF,nn}(\mathbf{q},\omega) = 2\frac{1}{\hbar S} \sum_{\mathbf{k}} \frac{f(E_{\mathbf{k}-\mathbf{q}}) - f(E_{\mathbf{k}})}{\omega + i\delta - (E(\mathbf{k}) - E(\mathbf{k}-\mathbf{q}))/\hbar}, \tag{1.45}$$

- Chiral 2DEG:

$$\begin{aligned} \chi^R_{nn}(\mathbf{q},\omega) &= \frac{1}{S\hbar} \sum_{s,s'} \sum_{\mathbf{k}} (1 + ss' \cos((\theta_{\mathbf{k}} - \theta_{\mathbf{k}-\mathbf{q}}))) \\ &\times \frac{f(E_{s,\mathbf{k}-\mathbf{q}}) - f(E_{s',\mathbf{k}})}{\omega + i\delta - (E_{s'}(\mathbf{k}) - E_s(\mathbf{k}-\mathbf{q}))/\hbar}. \end{aligned} \tag{1.46}$$

  where $s = \pm 1$ for the conduction and valence bands. This affects the dielectric function

$$\varepsilon(\mathbf{q},\omega) = 1 - \frac{2\pi e^2}{q} \chi^R_{nn}(\mathbf{q},\omega). \tag{1.47}$$

- Similar form factors appear in the conductivity response functions (and so in the calculation of the optical properties).

## 1.7 C2DEGs in a magnetic field

Peierls substitution

$$\mathbf{p} \to \mathbf{P} = \mathbf{p} + e\mathbf{A}/\hbar c \tag{1.48}$$

where $\nabla \times \mathbf{A} = \mathbf{B} = B_z \widehat{\mathbf{z}}$ with $B_z > 0$. We get

$$H = -v_F \begin{pmatrix} 0 & P_x - iP_y \\ P_x + iP_y & 0 \end{pmatrix} \tag{1.49}$$

with the commutation relation

$$P_x, P_y = -i\frac{\hbar^2}{\ell^2}, \tag{1.50}$$

where

$$\ell^2 = \frac{\hbar c}{eB_z} \tag{1.51}$$

is the magnetic length.

## 1.8 Landau levels and eigenfunctions

Ladder operators

$$a = \frac{\ell}{\sqrt{2}\hbar}\left(P_x - iP_y\right), \tag{1.52}$$

$$a^\dagger = \frac{\ell}{\sqrt{2}\hbar}\left(P_x + iP_y\right), \tag{1.53}$$

obeying the commutation relation

$$\left[a, a^\dagger\right] = 1 \tag{1.54}$$

The Hamiltonian is now:

$$H_K = -\frac{\sqrt{2}\hbar v_F}{\ell}\begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix}. \tag{1.55}$$

Landau gauge $\mathbf{A} = Bx\widehat{\mathbf{y}}$. Solutions are

$$E_n^{(K)} = sgn(n)\frac{\sqrt{2}\hbar v_F}{\ell}\sqrt{|n|} \tag{1.56}$$

with

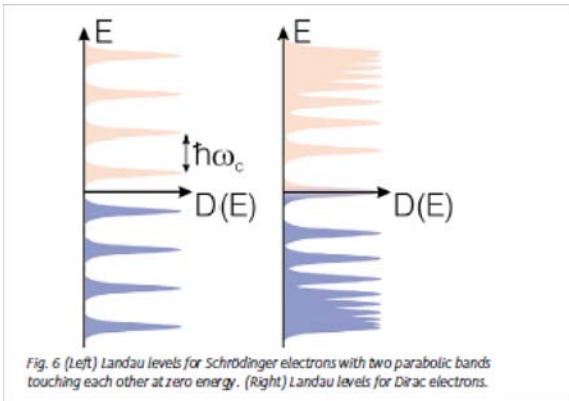
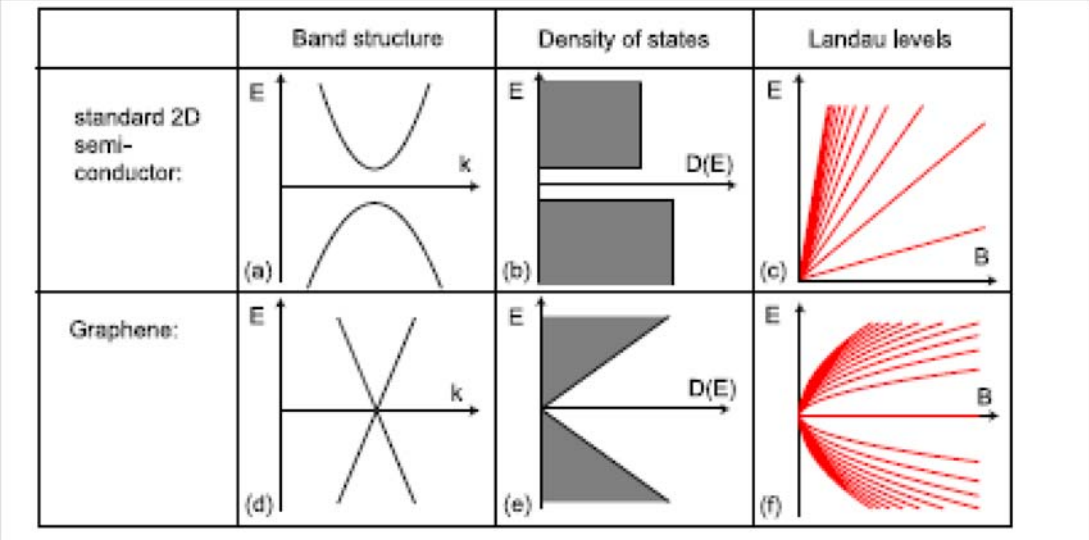


Fig. 6 (Left) Landau levels for Schrödinger electrons with two parabolic bands touching each other at zero energy. (Right) Landau levels for Dirac electrons.




$$s_0^{(K)}(\mathbf{r}) = \begin{pmatrix} 0 \\ h_0(\mathbf{r}) \end{pmatrix} \tag{1.57}$$

and

$$s_n^{(K)}(\mathbf{r}) = \frac{1}{\sqrt{2}} \begin{pmatrix} sgn(n)\, i h_{|n|-1}(\mathbf{r}) \\ h_{|n|}(\mathbf{r}) \end{pmatrix}. \tag{1.58}$$

The functions

$$h_{0,X}(\mathbf{r}) = \frac{1}{\sqrt{L_y}} e^{-iky} \varphi_{0,k}(x), \tag{1.59}$$

and

$$h_{|n|}(\mathbf{r}) = \frac{1}{\sqrt{|n|!}} \left(a^\dagger\right)^{|n|} h_{0,k}(\mathbf{r}) \tag{1.60}$$

are the usual Landau gauge wave functions for an ordinary 2DEG with $\varphi_{n,k}(x) = \varphi_n\left(x - k\ell^2\right)$, the wave functions of the harmonic oscillator in 1D.

For the $K'$ valley

$$E_n^{(K')} = sgn(n) \frac{\sqrt{2}\hbar v_F}{\ell} \sqrt{|n|} \tag{1.61}$$

For $n = 0$

$$s_0^{(K')}(\mathbf{r}) = \begin{pmatrix} h_0(\mathbf{r}) \\ 0 \end{pmatrix} \tag{1.62}$$

and

$$s_n^{(K')}(\mathbf{r}) = \frac{1}{\sqrt{2}} \begin{pmatrix} h_{|n|}(\mathbf{r}) \\ -sgn(n)\, i h_{|n|-1}(\mathbf{r}) \end{pmatrix}. \tag{1.63}$$

For $n = 0$, **valley and sublattice indices are equivalent**.

- **For graphene (monolayer)**

$$H_K = -\frac{\sqrt{2}\hbar v_F}{\ell} \begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix}. \tag{1.64}$$

Note that there is a Landau level $n = 0$ with energy $E = 0$ :

$$-\frac{\sqrt{2}\hbar v_F}{\ell} \begin{pmatrix} 0 & a \\ a^\dagger & 0 \end{pmatrix} \begin{pmatrix} 0 \\ h_0(\mathbf{r}) \end{pmatrix} = 0 \begin{pmatrix} 0 \\ h_0(\mathbf{r}) \end{pmatrix} \tag{1.65}$$

$n = 0$ has degeneracy 2(spin) X 2 (valleys) X $N_\varphi = 4N_\varphi$. The spinor for $K'$ is $\begin{pmatrix} h_0(\mathbf{r}) \\ 0 \end{pmatrix}$, valley and sublattice indices are equivalent.

- **For AB-bilayer graphene**

$$H_K \sim \frac{\gamma_0^2}{\gamma_1}\begin{pmatrix} 0 & a^2 \\ \left(a^\dagger\right)^2 & 0 \end{pmatrix}. \tag{1.66}$$

For the $E=0$ Landau level:

$$\begin{pmatrix} 0 & a^2 \\ \left(a^\dagger\right)^2 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ h_0(\mathbf{r}) \end{pmatrix} = 0; \begin{pmatrix} 0 & a^2 \\ \left(a^\dagger\right)^2 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ h_1(\mathbf{r}) \end{pmatrix} = 0 \tag{1.67}$$

The two "orbitals" $h_0$ and $h_1$ are degenerate with $E=0$. The degeneracy is now 2 (spin) X 2 (valleys) X 2 (orbitals) $N_\varphi = 8N_\varphi$. For $K'$, the spinors are $\begin{pmatrix} h_1(\mathbf{r}) \\ 0 \end{pmatrix}, \begin{pmatrix} h_2(\mathbf{r}) \\ 0 \end{pmatrix}$ and so **valley and layer indices** are equivalent.

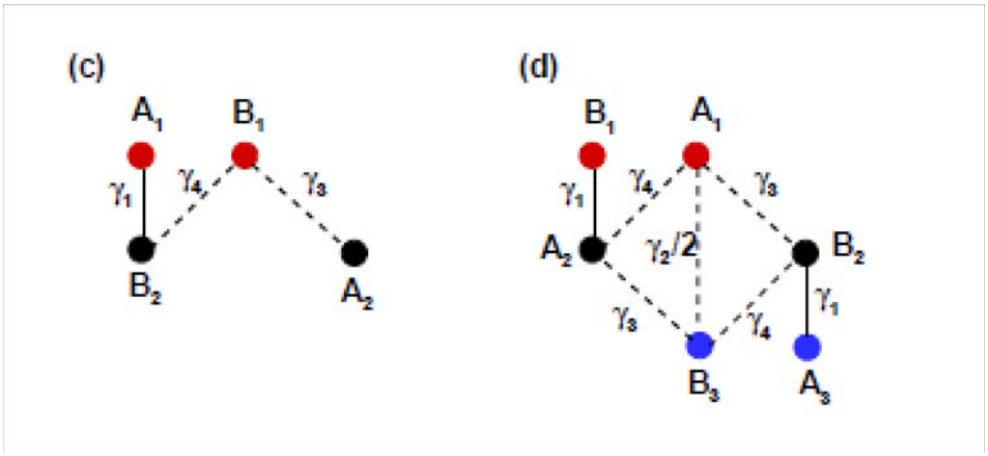
- **For ABC-trilayer graphene**

$$H_K = \frac{\gamma_0^3}{\gamma_1^2}\begin{pmatrix} 0 & a^3 \\ \left(a^\dagger\right)^3 & 0 \end{pmatrix}. \tag{1.68}$$

The $n=0$ spinors are for $K$

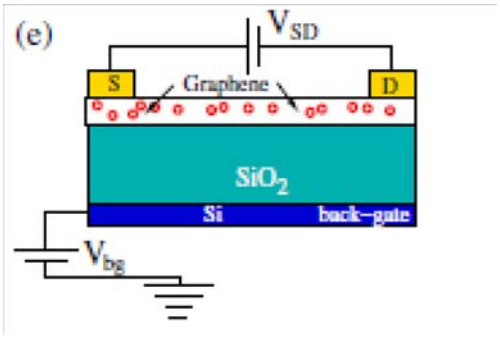
$$\begin{pmatrix} 0 \\ h_0(\mathbf{r}) \end{pmatrix}; \begin{pmatrix} 0 \\ h_1(\mathbf{r}) \end{pmatrix}; \begin{pmatrix} 0 \\ h_2(\mathbf{r}) \end{pmatrix} \tag{1.69}$$

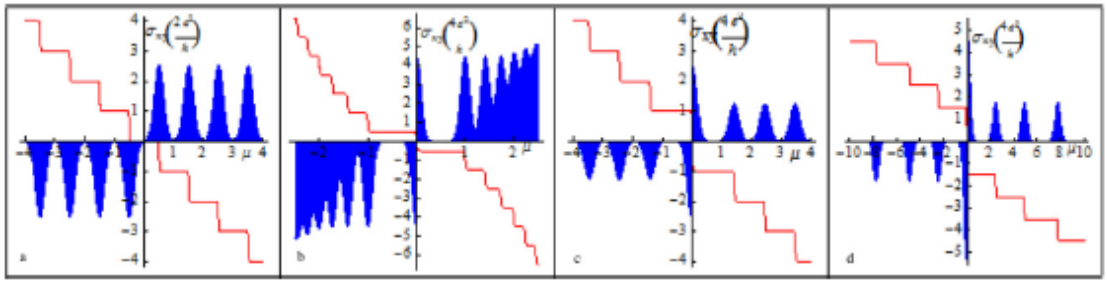
and the reversed for $K'$ so that valley and layer are equivalent. The three "orbitals" $h_0$, $h_1$, and $h_2$ are degenerate with $E=0$. The degeneracy is now 2 (spin) X 2 (valleys) X 3 (orbitals) $N_\varphi = 12N_\varphi$.




- etc. for ABCA, ABCBA,..

## 1.9 Quantum Hall effects



## 1.10 Energies

- In-plane hopping between nearest-neighbors:

$$t = \gamma_0 = 2.8 \text{ eV}, \tag{1.70}$$

- Magnetic length:

$$\ell = \frac{256}{\sqrt{B(\text{Tesla})}}, \tag{1.71}$$

- Gap between $n = 1$ and $n = 0$ :

$$\begin{aligned} E_1 &= 3.2947 \times 10^{-2}\sqrt{B} \text{ eV} \\ &= 382.33\sqrt{B} \text{ K} \end{aligned} \tag{1.72}$$

- Coulomb energy:

$$\begin{aligned} \frac{e^2}{\kappa\ell} &= \frac{5.6249 \times 10^{-2}\sqrt{B}}{\kappa} \text{ eV} \\ &= \frac{652.74}{\kappa}\sqrt{B} \text{ K} \end{aligned} \tag{1.73}$$

- Zeeman energy:

$$\begin{aligned} g\mu_B B &= 1.1577 \times 10^{-4} B \text{ eV} \\ & 1.3434 B \text{ K} \end{aligned} \tag{1.74}$$

## 1.11 Field operators

Here we use the same basis $(A, B)$ for the two valleys:

$$\begin{aligned}\Psi_K(\mathbf{r}) &= \sum_{n,k} e^{-i\mathbf{K}\cdot\mathbf{r}} \langle \mathbf{r}|K;n,k\rangle c_{K,n,k} \\ &= \frac{1}{\sqrt{L_y}}\sum_k e^{-i\mathbf{K}\cdot\mathbf{r}} e^{-iky} \begin{pmatrix} 0 \\ \varphi_0\left(x-k\ell^2\right)\end{pmatrix} c_{K,0,k} \\ &\quad + \sum_{n\neq 0,k} \frac{1}{\sqrt{2L_y}} e^{-i\mathbf{K}\cdot\mathbf{r}} e^{-iky} \begin{pmatrix} isgn(n)\,\varphi_{|n|-1}\left(x-k\ell^2\right) \\ \varphi_{|n|}\left(x-k\ell^2\right)\end{pmatrix} c_{K,n,k}\end{aligned} \tag{1.75}$$

and

$$\begin{aligned}\Psi_{K'}(\mathbf{r}) &= \sum_{n,k} e^{-i\mathbf{K}'\cdot\mathbf{r}} \langle \mathbf{r}|K';n,k\rangle c_{K',n,k} \\ &= \frac{1}{\sqrt{L_y}}\sum_k e^{-i\mathbf{K}'\cdot\mathbf{r}} e^{-iky} \begin{pmatrix} \varphi_0\left(x-k\ell^2\right) \\ 0\end{pmatrix} c_{K',0,k} \\ &\quad + \sum_{n\neq 0,k} \frac{1}{\sqrt{2L_y}} e^{-i\mathbf{K}'\cdot\mathbf{r}} e^{-iky} \begin{pmatrix} \varphi_{|n|}\left(x-k\ell^2\right) \\ -isgn(n)\,\varphi_{|n|-1}\left(x-k\ell^2\right)\end{pmatrix} c_{K',n,k}.\end{aligned} \tag{1.76}$$

## 1.12 Spinor structure and selection rules

The spinor structure plays again an important role in the calculation of the optical conductivity. For example

- Non-chiral 2DEG:

$$\overleftrightarrow{\sigma}_\nu(\omega) = \nu\frac{e^2}{h}\frac{i}{(\omega/\omega_c+i\delta)}\overleftrightarrow{1} - \nu\frac{e^2}{2h}\frac{i}{(\omega/\omega_c+i\delta)}\left[\frac{\begin{pmatrix}1 & i\\ -i & 1\end{pmatrix}}{(\omega/\omega_c+i\delta)+1} - \frac{\begin{pmatrix}1 & -i\\ i & 1\end{pmatrix}}{(\omega/\omega_c+i\delta)-1}\right]. \tag{1.77}$$

  Absorption is at $\omega_c$ only.

- Chiral 2DEG:

$$\sigma^{\alpha,\beta}(\omega) = \frac{2ie^2v_F^2}{\pi\ell^2\hbar(\omega+i\delta)}\sum_{n,m}\Lambda^{(\alpha)}_{n,m}\Lambda^{(\beta)}_{m,n}\frac{\langle\rho_{n,n}(0)\rangle - \langle\rho_{m,m}(0)\rangle}{\omega+i\delta-(E_m-E_n)/\hbar} \tag{1.78}$$

  with

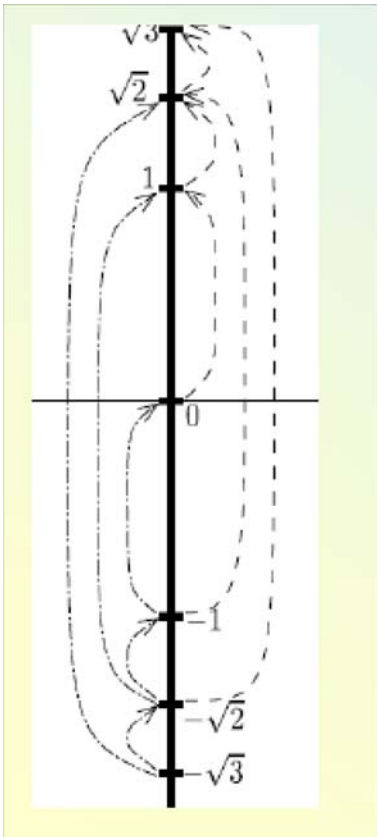
$$\Lambda^{(x)}_{n,m} = i\left[sgn(n)\,\delta_{|n|-1,|m|} - sgn(m)\,\delta_{|m|-1,|n|}\right], \tag{1.79}$$

$$\Lambda^{(y)}_{n,m} = sgn(n)\,\delta_{|n|-1,|m|} + sgn(m)\,\delta_{|m|-1,|n|}. \tag{1.80}$$

  Selection rule is given by:

$$|n|\pm 1 = |m| \tag{1.81}$$

  For ex.: transitions $2\to 3, 2\to 1, -2\to -1, -2\to -3, -2\to 3, -2\to 1$.




## 1.13 Second-quantized Hamiltonian

If we put this expression in the first-quantized hamiltonian, we get the second quantized form

$$\begin{aligned} H_K &= \sum_{\xi} \int d\mathbf{r} \Psi^{\dagger}_{\xi K}(\mathbf{r}) H \Psi^{\dagger}_{\xi K}(\mathbf{r}) \\ &= -\frac{\sqrt{2}\hbar v_F}{\ell} \sum_{n,k} \sum_{n',k'} \left[ \int d\mathbf{r} \langle \mathbf{r}|K;n,k\rangle^{\dagger} \begin{pmatrix} 0 & a \\ a^{\dagger} & 0 \end{pmatrix} \langle \mathbf{r}|K;n',k'\rangle \right] c^{\dagger}_{K,n,k} c_{K,n',k'} + K \rightleftharpoons K' \\ &= \sum_{\xi,n,k} E^{(\xi K)}_n c^{\dagger}_{\xi K,n,k} c_{\xi K,n,k} \end{aligned} \tag{1.82}$$

For the Coulomb interaction

$$U = \frac{1}{2} \sum_{\xi_1 \cdots \xi_4} \sum_{\alpha,\beta} \int d\mathbf{r} \int d\mathbf{r}' \Psi^{\dagger}_{\alpha,\xi_1}(\mathbf{r}) \Psi^{\dagger}_{\beta,\xi_2}(\mathbf{r}') V(\mathbf{r}-\mathbf{r}') \Psi_{\beta,\xi_3}(\mathbf{r}') \Psi_{\alpha,\xi_4}(\mathbf{r}), \tag{1.83}$$

Terms that do not conserve the valley index involves rapidly oscillating integrands $e^{i(\mathbf{K}-\mathbf{K}')\cdot\mathbf{r}}$. These terms are very small and usually neglected. Thus:

$$U = \frac{1}{2} \sum_{\xi_1,\xi_2} \sum_{\alpha,\beta} \int d\mathbf{r} \int d\mathbf{r}' \Psi^{\dagger}_{\alpha,\xi_1}(\mathbf{r}) \Psi^{\dagger}_{\beta,\xi_2}(\mathbf{r}') V(\mathbf{r}-\mathbf{r}') \Psi_{\beta,\xi_2}(\mathbf{r}') \Psi_{\alpha,\xi_1}(\mathbf{r}), \tag{1.84}$$

Now, write

$$V\left(\mathbf{r}-\mathbf{r}'\right)=\frac{1}{S}\sum_{\mathbf{q}}\frac{2\pi e^2}{\kappa q}e^{i\mathbf{q}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}, \tag{1.85}$$

so that with

$$V\left(\mathbf{q}\right)=\frac{2\pi e^2}{\kappa q} \tag{1.86}$$

we have

$$U=\frac{1}{2S}\sum_{\mathbf{q}}V\left(\mathbf{q}\right)\sum_{\xi_1,\xi_2}\int d\mathbf{r}\int d\mathbf{r}'\Psi^{\dagger}_{\alpha,\xi_1}\left(\mathbf{r}\right)\Psi^{\dagger}_{\beta,\xi_2}\left(\mathbf{r}'\right)e^{i\mathbf{q}\cdot\left(\mathbf{r}-\mathbf{r}'\right)}\Psi_{\beta,\xi_2}\left(\mathbf{r}'\right)\Psi_{\alpha,\xi_1}\left(\mathbf{r}\right). \tag{1.87}$$

which gives:

$$\begin{aligned}U &= \frac{1}{2S}\sum_{\mathbf{q}}V\left(\mathbf{q}\right)\sum_{n_1,\ldots,n_4}\sum_{k_1,\ldots,4}\sum_{\xi_1,\xi_2} \\ &\times\int d\mathbf{r}\left\langle\xi_1;n_1,k_1|\mathbf{r}\right\rangle e^{i\mathbf{q}\cdot\mathbf{r}}\left\langle\mathbf{r}|\xi_1;n_4,k_4\right\rangle \\ &\times\int d\mathbf{r}'\left\langle\xi_2;n_2,k_2|\mathbf{r}\right\rangle e^{-i\mathbf{q}\cdot\mathbf{r}'}\left\langle\mathbf{r}|\xi_2;n_3,k_3\right\rangle \\ &\times c^{\dagger}_{\xi_1,n_1,k_1}c^{\dagger}_{\xi_2,n_2,k_2}c_{\xi_2,n_3,k_3}c_{\xi_1,n_4,k_4}\end{aligned} \tag{1.88}$$

The Coulomb interaction will depend on the matrix elements:

$$\int d\mathbf{r}\left\langle\xi;n,k|\mathbf{r}\right\rangle e^{i\mathbf{q}\cdot\mathbf{r}}\left\langle\mathbf{r}|\xi;n',k'\right\rangle\equiv e^{\frac{i}{2}q_x\left(k+k'\right)\ell^2}\Xi_{n,n'}\left(\mathbf{q}\right)\delta_{k,k'-q_y}. \tag{1.89}$$

## 1.14 Hartree-Fock approximation (monolayer graphene)

We approximate the Coulomb interaction by the Hartree-Fock pairings:

$$\begin{aligned}\Psi^{\dagger}_{\xi_1}\left(\mathbf{r}\right)\Psi^{\dagger}_{\xi_2}\left(\mathbf{r}'\right)\Psi_{\xi_2}\left(\mathbf{r}'\right)\Psi_{\xi_1}\left(\mathbf{r}\right) \;\rightarrow\; & 2\left\langle\Psi^{\dagger}_{\xi_1}\left(\mathbf{r}\right)\Psi_{\xi_1}\left(\mathbf{r}\right)\right\rangle\Psi^{\dagger}_{\xi_2}\left(\mathbf{r}'\right)\Psi_{\xi_2}\left(\mathbf{r}'\right) \\ & -2\left\langle\Psi^{\dagger}_{\xi_1}\left(\mathbf{r}\right)\Psi_{\xi_2}\left(\mathbf{r}'\right)\right\rangle\Psi^{\dagger}_{\xi_2}\left(\mathbf{r}'\right)\Psi_{\xi_1}\left(\mathbf{r}\right).\end{aligned} \tag{1.90}$$

After some algebra ... ($N=S/2\pi\ell^2$ is the Landau level degeneracy) and if we ignore Landau level mixing, we get for the electrons in Landau level $n$ :

$$\begin{aligned}H &= N_{\phi}\sum_{n,\xi,\alpha}E_{n,\alpha}\rho^{\alpha,\xi;\alpha,\xi}_{n}\left(\mathbf{q}=0\right) \\ &+N_{\phi}\left(\frac{e^2}{\kappa\ell}\right)\sum_{\alpha,\beta}\sum_{\xi,\xi'}\sum_{\mathbf{q}}H_n\left(\mathbf{q}\right)\left\langle\rho^{\alpha,\xi;\alpha,\xi}_{n}\left(\mathbf{q}\right)\right\rangle\rho^{\beta,\xi';\beta,\xi'}_{n}\left(-\mathbf{q}\right) \\ &-N_{\phi}\left(\frac{e^2}{\kappa\ell}\right)\sum_{\alpha,\beta}\sum_{\xi,\xi'}\sum_{\mathbf{q}}X_n\left(\mathbf{q}\right)\left\langle\rho^{\alpha,\xi;\beta,\xi'}_{n}\left(\mathbf{q}\right)\right\rangle\rho^{\beta,\xi';\alpha,\xi}_{n}\left(-\mathbf{q}\right).\end{aligned} \tag{1.91}$$

where

$$\rho^{\alpha,\xi;\beta,\xi'}_{n}\left(\mathbf{q}\right)\equiv\frac{1}{N_{\phi}}\sum_{k,k'}e^{-\frac{i}{2}q_x\left(k+k'\right)\ell^2}\delta_{k,k'+q_y}c^{\dagger}_{\alpha,\xi,n,k}c_{\beta,\xi',n,k'}. \tag{1.92}$$

The average values of these operators are the order parameters for the different **broken-symmetry** phases of the C2DEG.

$$\left\langle\rho^{a,a}_{n}\left(\mathbf{q}\right)\right\rangle = \text{populations} \tag{1.93}$$

$$\left\langle\rho^{a,b\neq a}_{n}\left(\mathbf{q}\right)\right\rangle = \text{coherences} \tag{1.94}$$

- Exemples of coherence

$$\left\langle \rho_n^{K,K'} \right\rangle = \text{valley coherence,} \tag{1.95}$$

$$\left\langle \rho_n^{\uparrow,\downarrow} \right\rangle = \text{spin coherence,} \tag{1.96}$$

$$\left\langle \rho^{n=0,n=1} \right\rangle = \text{orbital coherence (bilayer and trilayer)} \tag{1.97}$$

The number of possible broken-symmetry states is large (uniform states, CDW states, SDW, PSDW, crystals, etc.)

The Hartre and Fock interactions are defined by

$$H_n(\mathbf{q}) = \left(\frac{1}{q\ell}\right) \Xi_n(\mathbf{q}) \Xi_n(-\mathbf{q}),$$

and

$$X_n(\mathbf{q}) = \left(\frac{\kappa\ell}{e^2}\right) \frac{1}{S} \sum_{\mathbf{p}} V(\mathbf{p}) \Xi_n(\mathbf{p}) \Xi_n(-\mathbf{p}) e^{i\mathbf{p}\times\mathbf{q}\ell^2} \tag{1.98}$$

with

$$\Xi_n(\mathbf{q}) = \frac{1}{2}\Theta(|n|) e^{\frac{-q^2\ell^2}{4}} \left[ L_{|n|}^0\left(\frac{q^2\ell^2}{2}\right) + L_{|n|-1}^0\left(\frac{q^2\ell^2}{2}\right)\right] + \delta_{n,0} e^{\frac{-q^2\ell^2}{4}} \tag{1.99}$$

The Hartree-Fock energy of the C2DEG in a magnetic field is:

$$\begin{aligned} \frac{E}{N} &= \frac{1}{\nu} \sum_{\xi,\alpha} E_\alpha \nu_{n,\sigma,\alpha} \\ &+ \frac{1}{2\nu} \left(\frac{e^2}{\kappa\ell}\right) \sum_{\alpha,\beta} \sum_{\xi,\xi'} \sum_{\mathbf{q}} H_n(\mathbf{q}) \left\langle \rho_n^{\alpha,\xi;\alpha,\xi}(\mathbf{q}) \right\rangle \left\langle \rho_n^{\beta,\xi';\beta,\xi'}(-\mathbf{q}) \right\rangle \\ &- \frac{1}{2\nu} \left(\frac{e^2}{\kappa\ell}\right) \sum_{\alpha,\beta} \sum_{\xi,\xi'} \sum_{\mathbf{q}} X_n(\mathbf{q}) \left| \left\langle \rho_n^{\alpha,\xi;\beta,\xi'}(\mathbf{q}) \right\rangle \right|^2. \end{aligned} \tag{1.100}$$

Interactions $H_n(q) - X_n(q)$ for $n = 1, 2, 3, 4$ (blue: normal 2DEG, violet C2DEG)

- $H$ and $X$ in $n = 0$ are identical to the normal 2DEG interactions
- The Fock and Hartree interactions are indepenent of spin and valley indices
- In this form, we can study uniform and well as non-uniform states of the C2DEG.
- For a **uniform state,**

$$\left\langle \rho_n^{\alpha,\xi;\alpha,\xi}(\mathbf{q}=\mathbf{0}) \right\rangle \neq 0 \tag{1.101}$$

and

$$H_n(\mathbf{0}) = 0 \tag{1.102}$$

(infinite terms are cancelled by the positive background). Also

$$\sum_{\alpha,\beta} \sum_{\xi,\xi'} \left| \left\langle \rho_n^{\alpha,\xi;\beta,\xi'}(0) \right\rangle \right|^2 = \nu. \tag{1.103}$$

Thus

$$\frac{E}{N} = \frac{1}{\nu} \sum_{\xi,\alpha} E_\alpha \nu_{n,\xi,\alpha} - \frac{1}{2} \left(\frac{e^2}{\kappa\ell}\right) X_n(0). \tag{1.104}$$

The Fock term is constant. It follows that the ground states for $\nu = 1, 3$ are spin polarized while the ground states for $\nu = 2, 4$ are spin unpolarized.

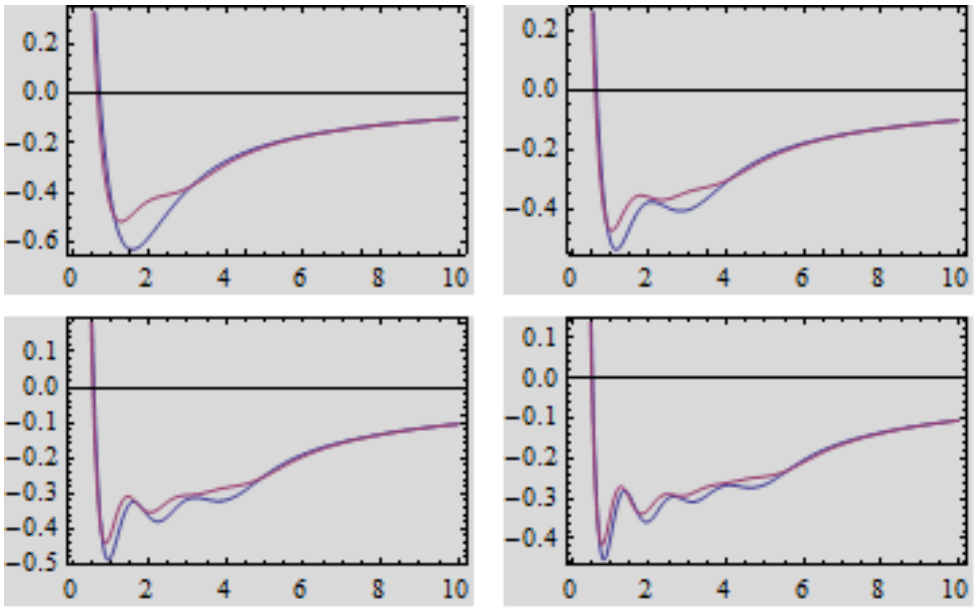



FIGURE 1.1.

- **For the spin polarized state**, the energy is independent of how the electrons are distributed in the two valleys. If we define a valley pseudospin, then at $\nu = 1$ :

$$\begin{aligned} \frac{E}{N} &= E_{n,K} \\ &+\frac{1}{4\nu_n}\left(\frac{e^2}{\kappa\ell}\right)\sum_{\mathbf{q}} \Upsilon_n(\mathbf{q})\langle\rho_n(-\mathbf{q})\rangle\langle\rho_n(\mathbf{q})\rangle \\ &+\frac{1}{\nu_n}\left(\frac{e^2}{\kappa\ell}\right)\sum_{\mathbf{q}} J_n(\mathbf{q})\left[\langle\mathbf{S}_n(-\mathbf{q})\rangle\cdot\langle\mathbf{S}_n(\mathbf{q})\rangle\right]. \end{aligned} \tag{1.105}$$

with

$$J_n(\mathbf{q}) = -X_n(\mathbf{q}), \tag{1.106}$$

and

$$\Upsilon_n(\mathbf{q}) = 2H_n(\mathbf{q}) - X_n(\mathbf{q}). \tag{1.107}$$

For the liquid state

$$\frac{E}{N} = E_{n,K} - \frac{1}{4}\left(\frac{e^2}{\kappa\ell}\right)X_n(0) + J_n(0)\left(\frac{e^2}{\kappa\ell}\right)|\langle\mathbf{S}_n(0)\rangle|^2 \tag{1.108}$$

and so, because $J_n(0) < 0$, the minimal energy is obtained when $|\mathbf{S}_n(0)|$ is maximized in any direction. The ground state is pseudo-ferromagnetic. We then expect a Goldstone mode with a quadratic dispersion relation.

- (From R. Côté, J. -F. Jobidon, and H. A. Fertig, PRB 78, 085309 (2008).):

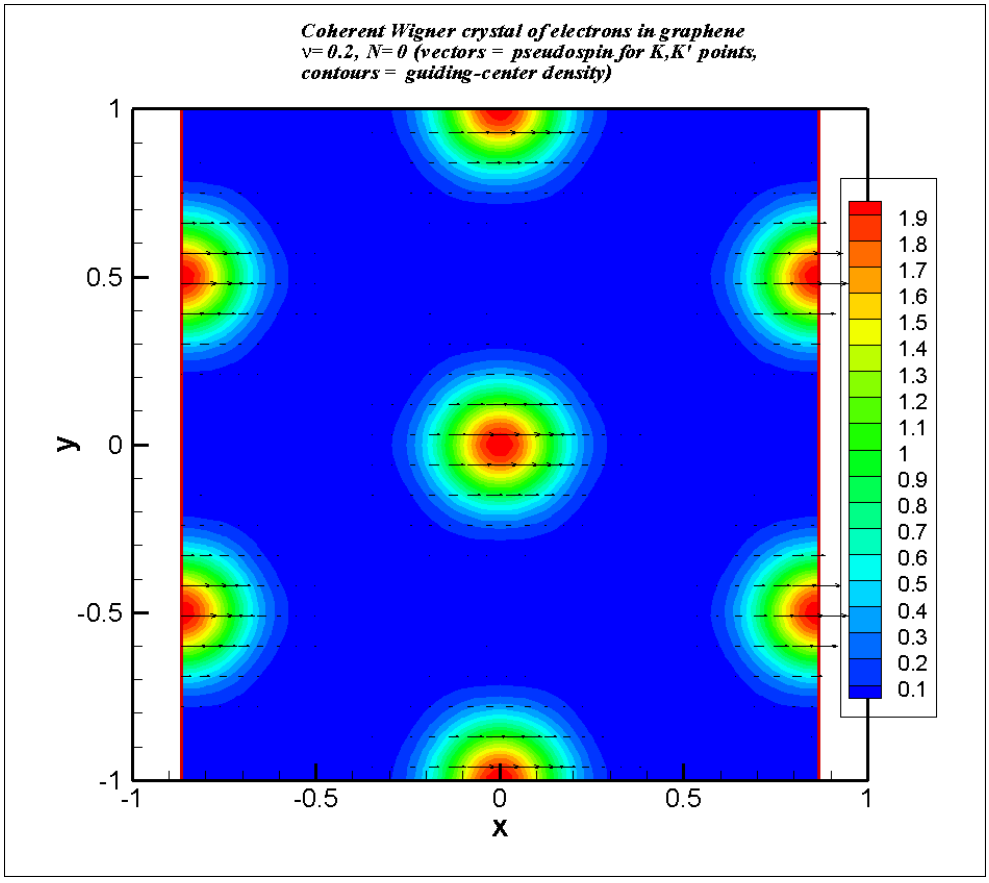

Coherent Wigner crystal of electrons in graphene
ν= 0.2, N= 0 (vectors = pseudospin for K,K' points,
contours = guiding-center density)
1
0.5
0
-0.5
-1
y
-1
-0.5
0
0.5
1
x
1.9
1.8
1.7
1.6
1.5
1.4
1.3
1.2
1.1
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1

FIGURE 1.2.

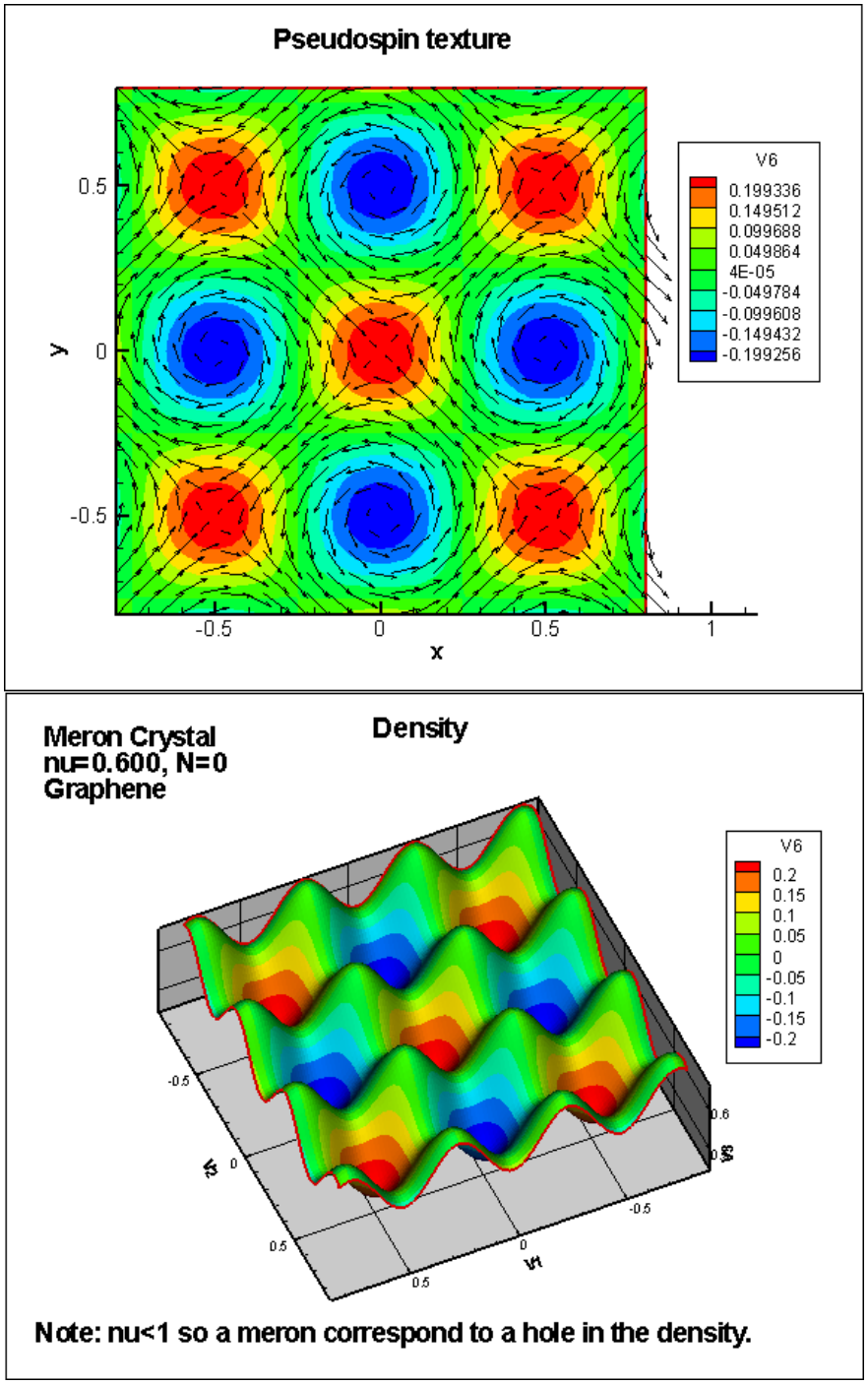

Pseudospin texture
V6
0.199336
0.149512
0.099688
0.049864
4E-05
-0.049784
-0.099608
-0.149432
-0.199256
0.5
0
-0.5
y
-0.5
0
0.5
1
x
Meron Crystal
nu=0.600, N=0
Graphene
Density
V6
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
-0.2
Note: nu<1 so a meron correspond to a hole in the density.

FIGURE 1.3.