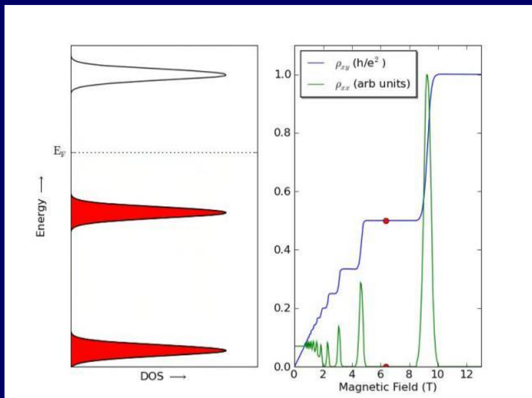
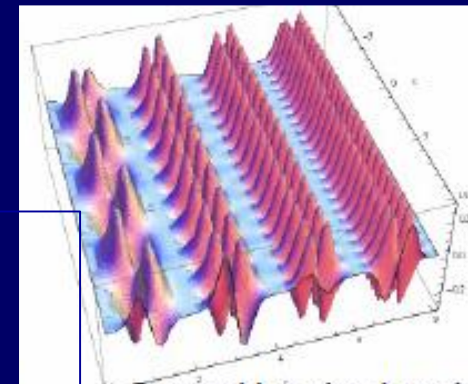
2D Electrons in a magnetic field





- ❖ 2D materials – background
  - Carbon allotropes
  - Graphene Structure and Band structure
  - Electronic properties
- ❖ Electrons in a magnetic field
  - Onsager relation
  - Landau levels
  - Quantum Hall effect
- ❖ Engineering electronic properties
  - Kondo effect
  - Atomic collapse and artificial atom
  - Twisted graphene

Aug 27-29, 2018

Summer School on Collective Behaviour in Quantum Matter

ICTP

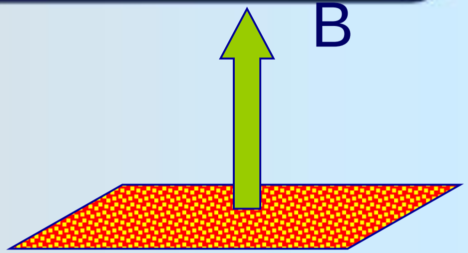
E.Y. Andrei

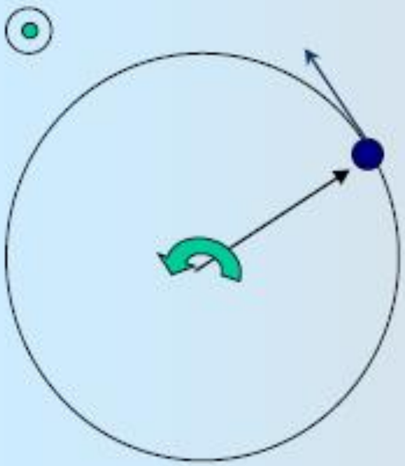
2D electron system in a magnetic field

Classical motion:

Lorentz force: $\mathbf{F} = -e\left(\mathbf{E} + [\mathbf{v} \times \mathbf{B}]\right)$ Perpendicular to the velocity!

Newtonian equation of motion: $\mathbf{E} = 0 \;\rightarrow\; m^*\dot{\mathbf{v}} = -e\,[\mathbf{v} \times \mathbf{B}]$





Cyclotron orbit

Cyclotron frequency, $\omega_c = eB/m^*$

Cyclotron radius, $r_c = v/\omega_c \propto 1/B$

In classical mechanics, any size of the orbit is allowed.

Landau levels

- In the discussion above the radius of the cyclotron orbit could be varied continuously.
- What happens if we add the lattice and quantum mechanics?

- We will start by looking at the effect of the lattice on the electronic motion
- Using a semi-classical approach based on the Onsager relation we will show that the cyclotron orbits are now quantized.
- This will allow us to calculate the Landau level energy sequence

Bloch electrons in external fields

Semiclassical electron dynamics (Kittel, p.192)

Consider a wave packet with average location *r* and wave vector *k*, then

$$\frac{d\vec{r}(\vec{k})}{dt} = \vec{v}_k = \frac{1}{\hbar}\frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}};$$

$$\hbar\frac{d\vec{k}}{dt} = q(\vec{E} + \vec{v}_k \times \vec{B})$$

Derivation neglected here

- Notice that *E* is the external field, which does not include the lattice field. The effect of lattice is hidden in $\varepsilon_n(k)$!

Range of validity

- This looks like the usual Lorentz force eq. But It is valid only when Interband transitions can be neglected. (One band approximation)

In graphene this approximation is valid for all transport experiments.

Bloch electrons in external fields

Bloch electron in an uniform magnetic field

$$\vec{E} = 0$$

$$\hbar \frac{d\vec{k}}{dt} = -e\vec{v}_k \times \vec{B}, \quad \vec{v}_k = \frac{1}{\hbar}\frac{\partial \varepsilon(\vec{k})}{\partial \vec{k}}$$

$$\Rightarrow \frac{d\vec{k}}{dt} \cdot \vec{B} = 0, \quad \frac{d\vec{k}}{dt} \cdot \vec{v}_k = \frac{1}{\hbar}\frac{\partial \varepsilon(\vec{k})}{\partial t} = 0$$

Therefore, 1. Change of k is perpendicular to the B field,

$k_{||}$ does not change

and 2. $\varepsilon(k)$ is a constant of motion

This determines uniquely the electron orbit on the FS

Bloch electrons in external fields

Cyclotron orbit in real space

The above analysis gives us the orbit in k-space.

What about the orbit in r-space?

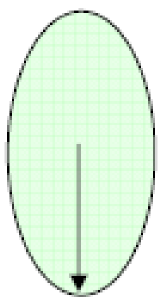
$$\hbar \frac{d\vec{k}}{dt} = -e\vec{v}_k \times \vec{B} \rightarrow \vec{v}_{k_\perp} = -\frac{\hbar}{eB^2}\vec{B} \times \frac{d\vec{k}}{dt}$$

$$\vec{r}_\perp(t) - \vec{r}_\parallel(0) = -\frac{\hbar}{eB}\hat{z} \times (\vec{k}(t) - \vec{k}(0))$$

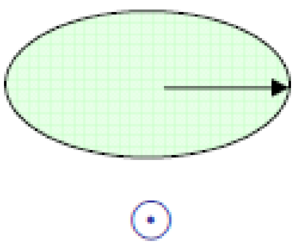
$$\vec{A} \times (\vec{B} \times \vec{C}) = (\vec{A} \cdot \vec{C})\,\vec{B} - (\vec{A} \cdot \vec{B}$$

$$\text{magnetic length} \quad l_B = \sqrt{\frac{\hbar}{eB}}$$

r-orbit



k-orbit



- r-orbit is rotated by 90 degrees from the k-orbit and scaled by $l_B^2 = \frac{\hbar}{eB}$

Flux Quantum

Semiclassical Onsager quantization

Electron wavefunction is single valued. Therefore a closed cyclotron orbit must satisfy:

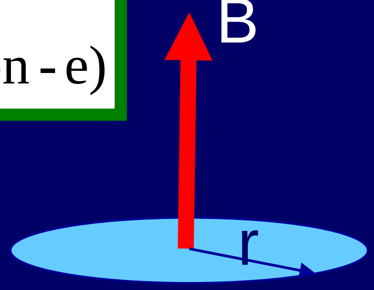
$$\frac{1}{\hbar}\oint \vec{P}\cdot d\vec{r} = 2\pi N;\ \ N\ \textbf{integer}$$

Bohr-Sommerfeld quantization

Electron in a magnetic field

$$\vec{B} = \vec{\nabla}\times\vec{A}$$

$$\vec{P} \rightarrow \vec{p} - e\vec{A} \quad ;\ e\ \text{charge of particle (for electron - e)}$$



$$\frac{1}{\hbar}\oint \vec{P}\cdot d\vec{r} = \frac{1}{\hbar}\oint(\vec{p}-e\vec{A})\cdot d\vec{r} = \theta_{kin} - \theta_{field}$$

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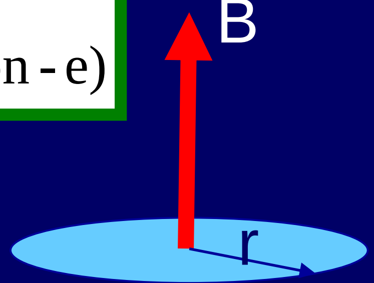

$$\frac{1}{\hbar}\oint \vec{P}\cdot d\vec{r} = \frac{1}{\hbar}\oint (\vec{p} - e\vec{A})\cdot d\vec{r} = \theta_{kin} - \theta_{field}$$

$$\hbar\dot{k} = -e\dot{r}\times B$$

Kinetic energy or de Broglie phase

$$\theta_{kin} = \frac{1}{\hbar}\oint \vec{p}d\vec{r} = \oint \vec{k}\cdot d\vec{r} = -\frac{e}{\hbar}\oint\left(\vec{r}\times\vec{B}\right)\cdot d\vec{r} = \frac{e}{\hbar}2\Phi$$

Φ is the magnetic flux through the orbit

Homework: prove this relationship

Flux Quantum

Semiclassical Onsager quantization

Electron wavefunction is single valued. Therefore a closed cyclotron orbit must satisfy:

$$\frac{1}{\hbar}\oint \vec{P}\cdot d\vec{r} = 2\pi N; \quad N \textbf{ integer}$$

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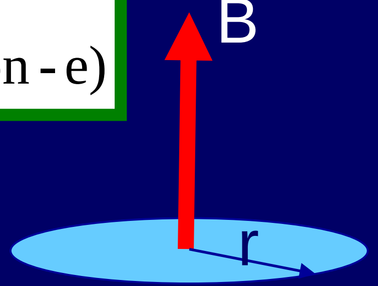


$$\frac{1}{\hbar}\oint \vec{P}\cdot d\vec{r} = \frac{1}{\hbar}\oint (\vec{p} - e\vec{A})\cdot d\vec{r} = \theta_{kin} - \theta_{field}$$

$$\hbar\dot{\mathrm{k}} = \text{-e}\dot{\mathrm{r}}\times\mathrm{B}$$

Kinetic energy or de Broglie phase

$$\theta_{kin} = \frac{1}{\hbar}\oint \vec{p}d\vec{r} = \oint \vec{k}\cdot d\vec{r} = -\frac{e}{\hbar}\oint\left(\vec{r}\times\vec{B}\right)\cdot d\vec{r} = \frac{e}{\hbar}2\Phi$$

Φ is the magnetic flux through the orbit

Field phase or Bohr Aharonov Phase :

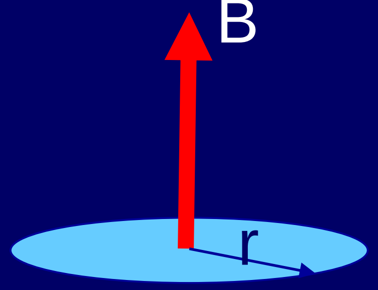
$$\theta_{field} = \frac{e}{\hbar}\oint \vec{A}\cdot dr = \frac{e}{\hbar}\oint\left(\vec{\nabla}\times\vec{B}\right)\cdot dr = \frac{e}{\hbar}\Phi$$

Flux Quantum

$$\frac{1}{\hbar}\oint \vec{P}\cdot d\vec{r} = 2\pi N;\quad N \textbf{ integer}$$

$$\frac{1}{\hbar}\oint \vec{P}\cdot d\vec{r} = \theta_{kin} - \theta_{field} = \frac{e}{\hbar}(2\Phi - \Phi) = 2\pi\frac{e}{h}\Phi$$

$$\Rightarrow 2\pi\frac{e}{h}\Phi = 2\pi N \quad \Rightarrow \Phi = \frac{h}{e}N \equiv \phi_0 N$$



$$\phi_0 = \frac{h}{e} = 4.14\cdot 10^{-7}\,\text{gauss}\cdot\text{cm}^2 \quad \text{Quantum unit of flux}$$

$$\Rightarrow \frac{\Phi}{\phi_0} = N \quad \text{Magnetic flux enclosed by cyclotron orbit is quantized in units of } \phi_0$$

E.Y. Andrei

Onsager quantization condition

→ The area of the cyclotron orbit encloses an integer number of flux lines

$$\Phi = S(r)B = N\varphi_0$$

$$\Rightarrow S(r) = N\frac{h}{eB} = 2\pi N\frac{\hbar}{eB} = 2\pi N l_B^2$$

S(r) =Area of r-orbit

$$\text{If S(k) is the k-orbit, and using}: |\mathrm{k}| = |r|/l_B^2$$

$$\Rightarrow S(r) = S(k) l_B^4$$

$$\text{Area of N'th cyclotron orbit in k-space}:$$

$$\Rightarrow \quad \mathrm{S}(\mathrm{k}_\mathrm{N})\mathrm{l}_\mathrm{B}^2 = 2\pi N$$

Generalized Onsager relation

$$\Rightarrow S(k_N) l_B^2 = 2\pi(N+\lambda)$$

Quantum correction → $\lambda = 1/2 - \gamma/2\pi$

γ = Berry Phase;

1/2 Maslov phase - (zero - point contribution)

The European Physical Journal B 77, 351 (2010)

EXAMPLE:
Landau levels of massive 2D electrons from Onsager relation

For free electrons

In the absence of a scalar potential V(x), orbits are circular and $S(k_N) = \pi k_N^2$

$$\pi k_N^2 l_B^2 = 2\pi(N + 1/2 - \gamma/2\pi)$$

$$\gamma = \text{Berry Phase}$$

Express the area in terms of energy using E(k)

Non-relativistic case

γ=0

$$\mathrm{E} = \frac{\hbar^2 k^2}{2\mathrm{m}}$$

$$\Rightarrow E_N = \frac{\hbar^2 k_N^2}{2\mathrm{m}} = \frac{\hbar^2}{2\mathrm{m}} \frac{2\pi}{\pi l_\mathrm{B}^2}(N+\lambda) = \hbar \frac{eB}{\mathrm{m}}(N+1/2)$$

$$\text{cyclotron frequency}: \quad \omega_c = \frac{eB}{m}$$

$$E_N = \hbar\omega_c(N + 1/2) \qquad N = 0,1,2\ldots$$

Landau levels

- How does this compare to the full quantum mechanical solution?

2D electron system in a magnetic field

$$\vec{B} = \vec{\nabla} \times \vec{A}$$

$$\vec{P} \to \vec{p} + e\vec{A} \quad \text{for electrons}$$

$$\vec{A} \Rightarrow \vec{A} + \vec{\nabla} \cdot \vec{\lambda}$$

The magnetic field is independent of the choice of gauge

Example:

Landau gauge:

$$\vec{A} = (0, Bx, 0) \Rightarrow \vec{B} \parallel \hat{z}$$

Symmetric gauge

$$\vec{A} = \frac{1}{2}\vec{B} \times \vec{r} = \frac{1}{2}B(-y, x, 0) = Br\widehat{e}_{\phi}$$

- All gauges give the same energy spectrum.
- The wavefunctions will be different they will have the symmetry of the gauge.

2D electron system in a magnetic field

Non-relativistic - 2D in semiconductors

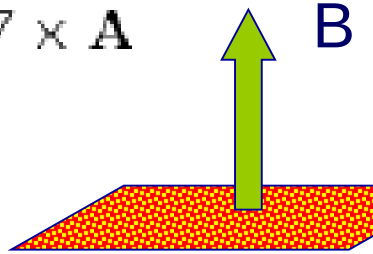
$$\hat{H} = \frac{\hat{p}^2}{2m} \Rightarrow \frac{1}{2m}\left(\hat{\boldsymbol{p}} - e\hat{\boldsymbol{A}}\right)^2 = \frac{\hat{\boldsymbol{P}}^2}{2m}$$

Canonical momentum $\hat{\boldsymbol{p}}$

Covariant momentum $\hat{\boldsymbol{P}} \equiv \hat{\boldsymbol{p}} - e\hat{\boldsymbol{A}}$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\hat{\mathbf{A}} = \begin{pmatrix} 0 \\ B\hat{x} \\ 0 \end{pmatrix}$$



Landau gauge

Contains p^2 and x^2 : Resembles Harmonic oscillator

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega^2\hat{x}^2$$

→ Quantized levels

Plan : transform Hamiltonian to HO

Solve in energy base .

2D electron system in a magnetic field

1. Landau levels

$$\hat{H} = \frac{\hat{P}^2}{2m}$$

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2m}\left(\hat{p}_y - eB\hat{x}\right)^2$$

Note: $\left[\hat{H}, \hat{p}_y\right] = 0$

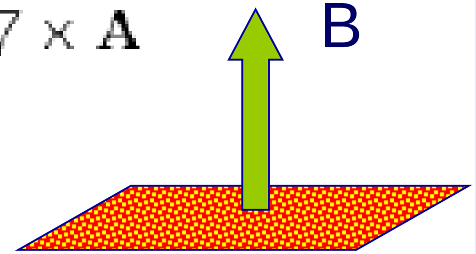
$\Rightarrow$ replace $\hat{p}_y$ with eigenvalue $\hbar k_y$

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}\omega_c^2\left(\hat{x} - \frac{\hbar k_y}{m\omega_c}\right)^2$$

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2}m\omega_c^2(\hat{x} - x_0)^2$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\hat{\mathbf{A}} = \begin{pmatrix} 0 \\ B\hat{x} \\ 0 \end{pmatrix}$$



Landau gauge

cyclotron frequency: $\omega_c = \frac{eB}{m}$

magnetic length $l_B = \sqrt{\frac{\hbar}{eB}}$

$$x_0 = \frac{\hbar k_y}{m\omega_c} = l_B^2 k_y$$

- 1D Harmonic oscillator
- Shifted origin to x_0 does not affect energy

$$E_N = \hbar\omega_c(N + 1/2) \quad N = 0,1,\ldots$$

Landau levels

$$E_N = \hbar\omega_c(N + 1/2) \quad N = 0,1,\ldots$$

- Same as the semiclassical result!!
- But now we can also calculate the wavefunctions

2D electron system in a magnetic field

2. Wavefunctions – Landau gauge

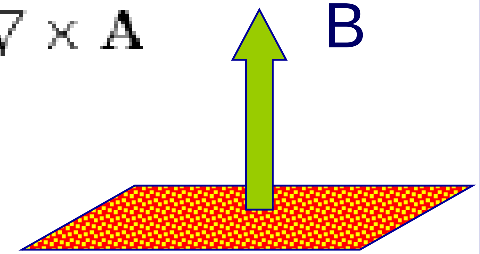
$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{1}{2} m\omega_c^2 (\hat{x} - x_0)^2$$

X and Y motion decoupled:
X: Harmonic oscillator Y: Free

$$\Psi(x,y) = e^{ik_y y} \phi_n(x - x_0) \; .$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\hat{\mathbf{A}} = \begin{pmatrix} 0 \\ B\hat{x} \\ 0 \end{pmatrix}$$



Landau gauge

$\hat{x}$

$$\text{cyclotron frequency:} \quad \omega_c = \frac{eB}{m}$$

$$\text{magnetic length} \quad l_c = \sqrt{\frac{\hbar}{eB}}$$

$$x_0 = \frac{\hbar k_y}{m\omega_c} = l_c^2 k_y$$

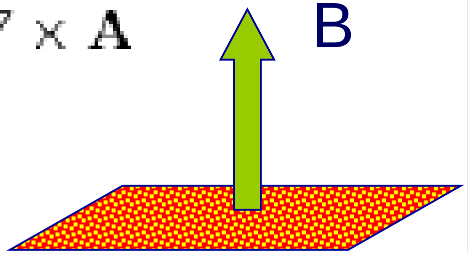
$$E_N = \hbar\omega_c (N + 1/2) \quad N = 0,1,\ldots$$

2D electron system in a magnetic field: wave function

2. Wavefunctions – Landau gauge

$$\mathbf{B} = \nabla \times \mathbf{A}$$

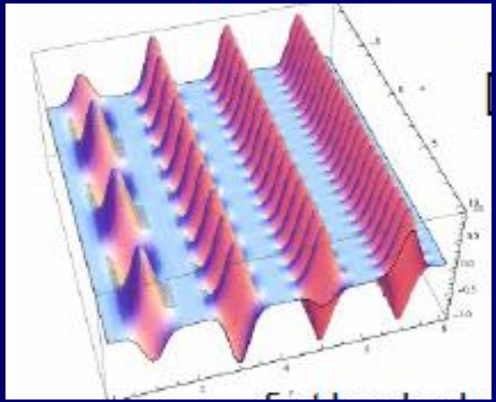
$$\hat{\mathbf{A}} = \begin{pmatrix} 0 \\ B\hat{x} \\ 0 \end{pmatrix}$$



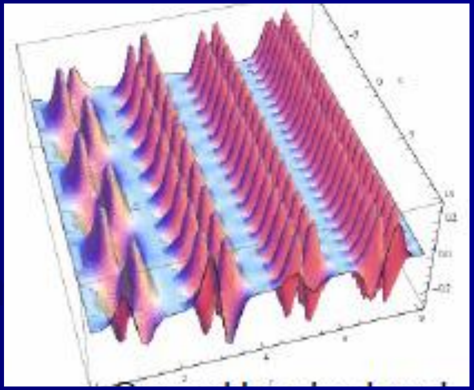
Landau gauge

$$\Psi(x,y) = e^{ik_y y}\phi_n(x - x_0) \ .$$

- Y direction- Plane wave
- X direction - Gaussian around x_0 (k_y) of width l_B $(2N)^{1/2}$



1’st Landau level N=0



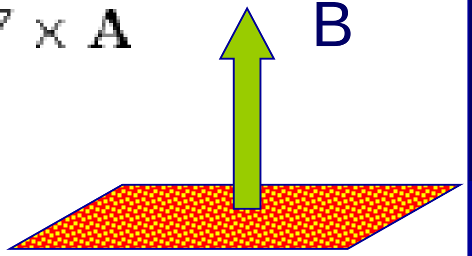
2’nd Landu level N=1

2D electron system in a magnetic field: wave function

2. Wavefunctions – symmetric gauge

$$\psi_N(r,\theta) = \left(N!(2l_B)^{N+1}\right)^{-1/2} r^N e^{iN\theta} e^{-(r/2l_B)^2}$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$



$$\hat{A} = \frac{B}{2}\begin{pmatrix} -\hat{y} \\ \hat{x} \\ 0 \end{pmatrix}$$

Symmetric gauge

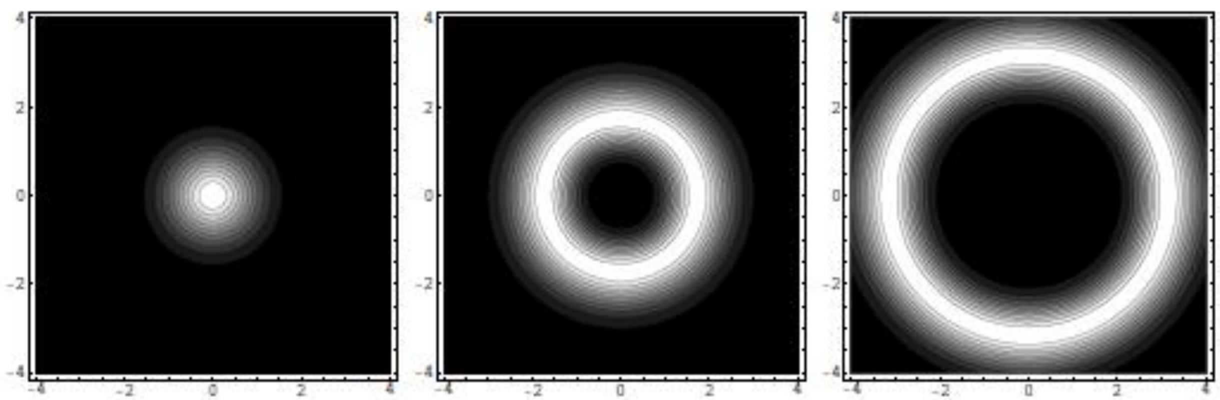


Figure 3: The ground state wave functions with $n = 0, 3,$ and 10.

Landau levels in non-relativistic 2D electron system

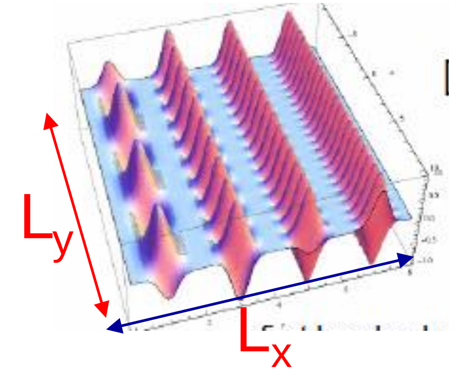
3. Landau level degeneracy

$$E_N = \hbar\omega_c (N + 1/2) \quad N = 0,1,\ldots$$

$$\Psi(x, y) = e^{ik_y y}\phi_n(x - x_0)\ .$$

$$\mathbf{B} = \nabla \times \mathbf{A}$$

$$\hat{\mathbf{A}} = \begin{pmatrix} 0 \\ B\hat{x} \\ 0 \end{pmatrix}$$



$$k_y = \frac{2\pi}{L_y} N; \quad N = 0,1,2..$$

$$0 \le x_0 = l_B^2 \frac{2\pi}{L_y} N < L_x$$

$$\Rightarrow 0 \le N < \frac{L_x L_y}{2\pi l_B^2} = L_x L_y \frac{eB}{h}$$

$$\Rightarrow \text{Degeneracy per area} = \frac{B}{\phi_o}; \quad \phi_o \equiv \frac{h}{e}$$

$$\text{Orbital Degeneracy } g_o = \frac{B}{\phi_o} = \frac{1}{2\pi l_B^2}$$

One orbital state per flux line

Total degeneracy

$$\text{Degeneracy} = g_i g_o$$

g_i degeneracy from internal degrees of freedom: spin, valley ..

Landau levels in graphene from Onsager relation

Onsager relation

$$S(k)l_B^2 = 2\pi(N + 1/2 - \gamma/2\pi)$$

$$\gamma = \text{Berry Phase}$$

Graphene: $\gamma=\pi$

$$S(k)l_B^2 = 2\pi(N + 1/2 - \gamma/2\pi) = 2\pi N$$

$$\text{no electric field: } S(k)l_B^2 = \pi k_N^2 l_B^2 = 2\pi N$$

Express the area S(k) in terms of energy using E(k)

$$\mathrm{E(k)} = \hbar v_F k$$

$$k_N = \pm\frac{1}{l_B}\sqrt{2|N|}$$

$$\Rightarrow E_N = \hbar v_F k_N = \pm\hbar\frac{v_F}{\mathrm{l_B}}(2|N|)^{1/2}$$

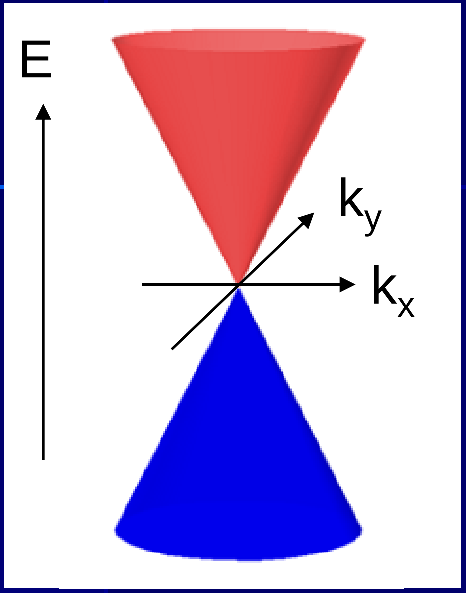
$$E_N = \pm v_F\sqrt{2e\hbar B|N|} = \hbar\omega_c\sqrt{2N}; \qquad N = 0, \pm 1, ..$$

$$\omega_c = v_F / l_B$$

Berry’s phase “swallowed” the zero point energy

Landau levels in graphene from Dirac-Weyl equation

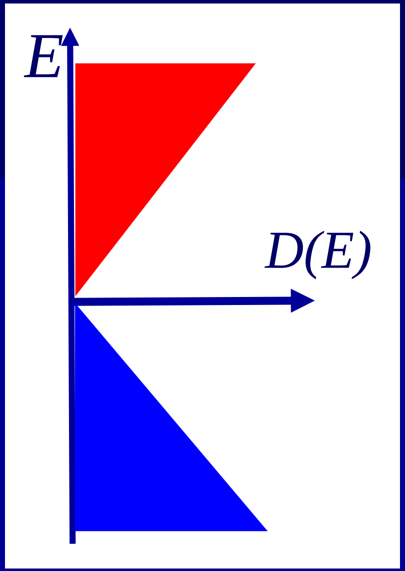
Band structure

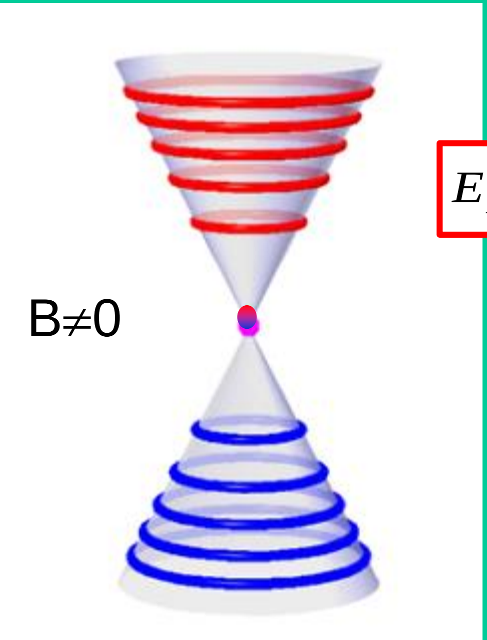


$$H = v_F \begin{pmatrix} 0 & \vec{\sigma}.\vec{p} \\ -\vec{\sigma}^*.\vec{p} & 0 \end{pmatrix}$$

$$H = v_F \begin{pmatrix} 0 & \vec{\sigma}.(\vec{p}-e\vec{A}) \\ -\vec{\sigma}^*.(\vec{p}-e\vec{A}) & 0 \end{pmatrix}$$

Density of states





Finite B → Landau Levels

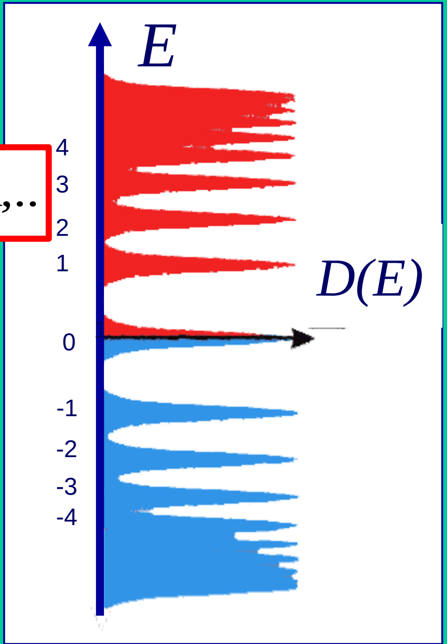
$$E_N = \pm v_F \sqrt{2e\hbar B|N|} = \pm\hbar\omega_c\sqrt{2N}; \quad N = 0, \pm 1, ..$$

$$\hbar\omega_c = \hbar v_F / l_B \approx 35\sqrt{\mathrm{B}}\ \mathrm{meV}$$

$$l_B = \sqrt{\hbar / eB} = 25/\sqrt{\mathrm{B}}\ \mathrm{nm}$$

$$Degeneracy: g = 4g_0; \qquad \phi_0 = h/e$$

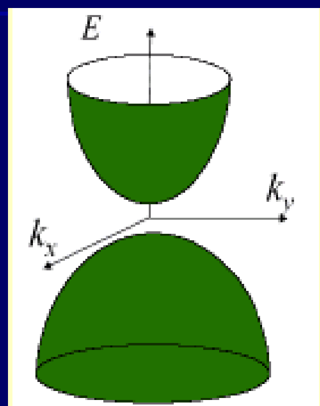
$$Orbital\ \ Degeneracy\ \ \boldsymbol{g_0} = B/\phi_0 = 2.5\times10^{14}\ m^{-2}B[T]$$

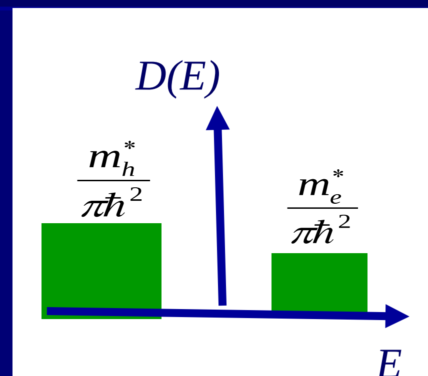


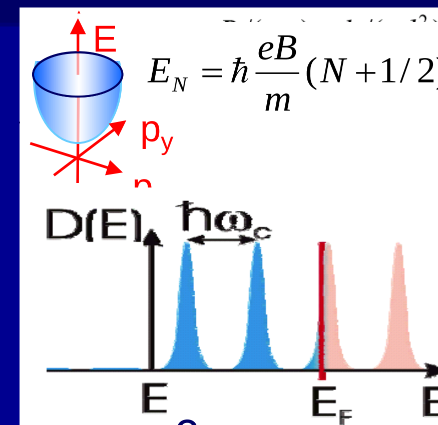
Graphene and conventional 2d electron systems

Low energy excitations | Density of states | Landau levels

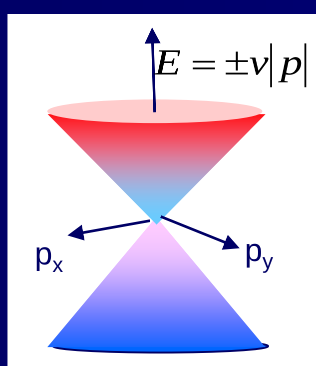
Conventional semiconductor

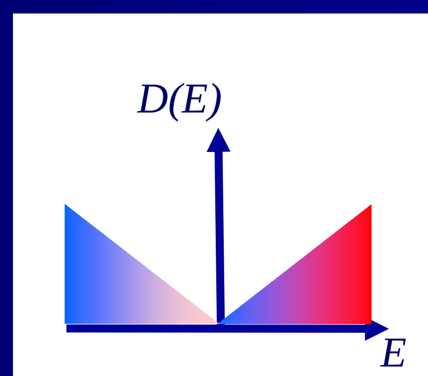


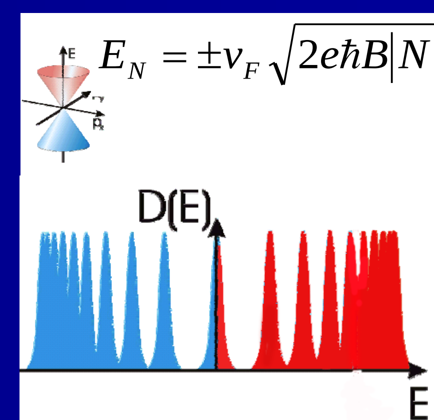




Graphene







Summary of part II

Quantum unit of flux

$$\phi_0 = \frac{h}{e} = 4.14\cdot 10^{-7}\,\text{gauss}\cdot\text{cm}^2 \quad [\text{Tesla}\cdot\text{m}^2]$$

$$\Rightarrow \frac{\Phi}{\phi_0} = N \quad \text{flux enclosed by cyclotron orbit}$$

Onsager relation :k-space area of cyclotron orbit

$$S(k_N)l_B^2 = 2\pi(N + 1/2 - \gamma/2\pi)$$

$$\gamma = \text{Berry Phase}$$

Landau level energy

Non-relativistic

$$E_N = \hbar\frac{eB}{m}(N+1/2)$$

Ultra-relativistic (graphene)

$$E_N = \pm v_F\sqrt{2e\hbar B|N|}$$

$$2\frac{B}{\phi_0}$$

degeneracy: $g_i g_o$

$$4\frac{B}{\phi_0}$$