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

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2D electron system in a magnetic field

Classical motion:

Lorentz force: \( \mathbf{F} = -e (\mathbf{E} + [\mathbf{v} \times \mathbf{B}]) \)  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.
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

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

\[
\hbar \frac{dk}{dt} = q(\vec{E} + \vec{v}_k \times \vec{B})
\]

Derivation neglected here

- Notice that \( \vec{E} \) 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.

E.Y. Andrei
Bloch electrons in external fields

Bloch electron in an uniform magnetic field

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

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

Therefore, 1. Change of \( k \) is perpendicular to the \( B \) field, \( k_\parallel \) does not change

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

This determines uniquely the electron orbit on the FS
Cyclotron orbit in real space

The above analysis gives us the orbit in k-space. What about the orbit in r-space?

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

\[ \vec{r}_{\perp}(t) - \vec{r}_{\parallel}(0) = -\frac{\hbar}{eB} \vec{B} \times (\vec{k}(t) - \vec{k}(0)) \]

- r-orbit is rotated by 90 degrees from the k-orbit and scaled by

\[ l_B^2 = \frac{\hbar}{eB} \]

magnetic length \( l_B = \sqrt{\frac{\hbar}{eB}} \)
Semiclassical Onsager quantization

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

\[ \frac{1}{\hbar} \oint \vec{P} \cdot d\vec{r} = 2\pi N; \quad N \text{ integer} \]

Bohr-Sommerfeld quantization

Electron in a magnetic field

\[ \vec{B} = \nabla \times \vec{A} \]
\[ \vec{P} \rightarrow \vec{p} - e\vec{A} ; \quad e \text{ charge of particle (for electron - e)} \]

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

Kinetic energy or de Broglie phase

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

\[\hbar k = -e\hat{r} \times \vec{B}\]

Homework: prove this relationship

\[
\Phi \text{ is the magnetic flux through the orbit}
\]
Semiclassical Onsager quantization

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

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

Bohr-Sommerfeld quantization

Electron in a magnetic field

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

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

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

Kinetic energy or de Broglie phase

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

$$\Phi$$ is the magnetic flux through the orbit

Field phase or Bohr Aharonov Phase:

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

\[ \frac{1}{\hbar} \oint \vec{P} \cdot d\vec{r} = 2\pi N; \ N \text{ integer} \]

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

\[ \Rightarrow 2\pi \frac{e}{\hbar} \Phi = 2\pi N \quad \Rightarrow \Phi = \frac{h}{e} N \equiv \phi_0 N \]

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

\[ \Rightarrow \frac{\Phi}{\phi_0} = N \quad \text{Magnetic flux enclosed by cyclotron orbit is quantized in units of } \phi_0 \]
Onsager quantization condition

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

\[ \Phi = S(r)B = N\varphi_0 \]

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

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

\[ \Rightarrow S(r) = S(k)l_B^4 \]

Area of \( N' \)th cyclotron orbit in \( k \)-space:

\[ \Rightarrow S(k_N)l_B^2 = 2\pi N \]

Generalized Onsager relation

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

\[ \lambda = 1/2 - \gamma/2\pi \]

\( \gamma \) = Berry Phase;

1/2 Maslov phase - (zero-point contribution)
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 \( S(k_N) = \pi k_N^2 \)

\[
\pi k_N^2 l_B^2 = 2\pi \left( N + 1/2 - \gamma/2\pi \right)
\]
\[
\gamma = \text{Berry Phase}
\]

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

Non-relativistic case
\( \gamma = 0 \)

\[
E = \frac{\hbar^2 k^2}{2m}
\]

\[
\Rightarrow E_N = \frac{\hbar^2 k_N^2}{2m} = \frac{\hbar^2}{2m} \frac{2\pi}{\pi l_B^2} (N + \lambda) = \frac{\hbar eB}{m} (N + 1/2)
\]

cyclotron frequency: \( \omega_c = \frac{eB}{m} \)

\[
E_N = \hbar \omega_c (N + 1/2) \quad N = 0,1,2,\ldots
\]
Landau levels

- How does this compare to the full quantum mechanical solution?
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
\[ \vec{A} = \frac{1}{2} \vec{B} \times \vec{r} = \frac{1}{2} B(-y, x, 0) = Br\hat{e}_\phi \]

- All gauges give the same energy spectrum.
- The wavefunctions will be different they will have the symmetry of the gauge.
Contains $p^2$ and $x^2$: Resembles Harmonic oscillator

\[ \hat{H} = \frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2 \]

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: \([\hat{H}, \hat{p}_y] = 0\)

⇒ replace \(\hat{p}_y\) with eigenvalue \(\hbar k_y\)

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

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

1D Harmonic oscillator

Shifted origin to \(x_0\) does not affect energy

\[ B = \nabla \times A \]

\[ \hat{A} = \begin{pmatrix} 0 \\ B\hat{x} \\ 0 \end{pmatrix} \]

Landau gauge

Cyclotron frequency: \(\omega_c = \frac{eB}{m}\)

Magnetic length \(l_B = \sqrt{\frac{\hbar}{eB}}\)

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

\[ E_N = \hbar \omega_c (N + 1/2) \quad N = 0, 1, \ldots \]
Landau levels

\[ E_N = \hbar \omega_c (N + 1/2) \quad N = 0, 1, ... \]

- 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

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

cyclotron frequency: \( \omega_c = \frac{eB}{m} \)
magnetic length \( l_c = \sqrt{\frac{\hbar}{eB}} \)

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

\[
E_N = \hbar \omega_c (N + 1/2) \quad N = 0, 1, \ldots
\]
2D electron system in a magnetic field: wave function

2. Wavefunctions – Landau gauge

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

- 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 Landau level \( N=1 \)
2D electron system in a magnetic field: wave function

2. Wavefunctions – symmetric gauge

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

Symmetric gauge

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

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

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

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

\[ k_y = \frac{2\pi}{L_y} N; \quad N = 0, 1, 2, \ldots \]

\[ 0 \leq x_0 = l_B^2 \frac{2\pi}{L_y} N < L_x \]

\[ \Rightarrow 0 \leq N < \frac{L_x L_y}{2\pi l_B^2} = L_x L_y \frac{eB}{\hbar} \]

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

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: \( \gamma = \pi \)

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

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 \( E(k) \)

\[ E(k) = \hbar v_F k \]

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

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

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

\[ \omega_c = \frac{v_F}{l_B} \]

Berry’s phase “swallowed” the zero point energy
Landau levels in graphene from Dirac-Weyl equation

Band structure

Density of states

H = \nu_F \begin{pmatrix} 0 & \vec{\sigma} \cdot \vec{p} \\ -\vec{\sigma}^* \cdot \vec{p} & 0 \end{pmatrix}

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

Finite B \rightarrow Landau Levels

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

\hbar \omega_c = \hbar \nu_F / l_B \approx 35\sqrt{B} \text{ meV}

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

Degeneracy: g = 4g_0; \quad \phi_0 = \hbar / e

Orbital Degeneracy g_0 = B / \phi_0 = 2.5 \times 10^{14} m^{-2} B[T]
Graphene and conventional 2d electron systems

Low energy excitations

Conventional semiconductor

Graphene

Density of states

Landau levels

\[ E = \pm v |p| \]

\[ E = \frac{m^*_h}{\pi \hbar^2} \]

\[ E = \frac{m^*_e}{\pi \hbar^2} \]

\[ D(E) \]

\[ E_N = \frac{eB}{m} (N + 1/2) \]

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

\[ E \]

\[ D(E) \]

\[ \frac{N_B}{v_F} E \]

\[ \frac{N_{BeF}}{m^*_e} \]
Summary of part II

Quantum unit of flux

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

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

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

<table>
<thead>
<tr>
<th>Non-relativistic</th>
<th>Ultra-relativistic (graphene)</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ E_N = \frac{\hbar eB}{m} (N + 1/2) ]</td>
<td>[ E_N = \pm v_F \sqrt{2e\hbar B</td>
</tr>
</tbody>
</table>

2 \[ \frac{B}{\phi_0} \]

degeneracy: \( g_l g_o \)

4 \[ \frac{B}{\phi_0} \]