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Notes on Landau level energy spectrum graphene

Yesterday Nick Read reviewed the basics of Landau quantization for electrons (in 2D) described by the Schrödinger equation.

$$\mathcal{H}_{sch} = \frac{\vec{p}^2}{2m^*} \xrightarrow{\vec{B}\ \text{field}} \mathcal{H}^B_{sch} = \frac{\left(\vec{p} + \frac{|e|}{c}\vec{A}\right)^2}{2m^*}$$

Solution: harmonic oscillator (n: Landau level index)

Energy spectrum: $\epsilon_n = \hbar\omega_c\left(n + \frac{1}{2}\right)$

where $\omega_c = \frac{|e|B}{m^*c} \equiv$ cyclotron frequency

The Hamiltonian for massless Dirac electrons is:

$$\mathcal{H}_D = v_F\,\vec{p}\cdot\vec{\sigma} \xrightarrow{\vec{B}\ \text{field}} \mathcal{H}^B_D = v_F\left[\vec{p} + \frac{|e|}{c}\vec{A}\right]\cdot\vec{\sigma}$$

where $\vec{\sigma} \equiv (\sigma_x, \sigma_y, \sigma_z)$ Pauli matrices

For convenience let's call

$$\vec{\pi} \equiv \vec{p} + \frac{|e|}{c}\vec{A} \quad \text{(kinetic momentum)}$$

Then: $\mathcal{H}^B_D = v_F\,\vec{\pi}\cdot\vec{\sigma}$

Note that, unlike $\vec{p}$, the different components of $\vec{\pi}$ do not commute with each other:

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$$[\Pi_x, \Pi_y] = [p_x + \tfrac{|e|}{c}A_x,\ p_y + \tfrac{|e|}{c}A_y] =$$

$$= \tfrac{|e|}{c}\left([p_x, A_y] - [p_y, A_x]\right) \overset{\text{Landau gauge}}{=} \tfrac{|e|}{c} B\, \underbrace{[p_x, x]}_{-i\hbar} =$$

Landau gauge $\vec{A} = (0, B\cdot x, 0)$

$$= -i\,|e|\hbar B = -i\frac{\hbar^2}{\ell_B^2} \quad ; \quad \ell_B = \frac{\hbar c}{|e|B} \equiv \text{magnetic length}$$

[Note: $[\Pi_x, \Pi_y]$ is gauge invariant (we just chose Landau gauge as a simple example) as expected, since Π_x and Π_y are gauge invariant (this is because $\vec{p}$ also transforms under gauge transformations)]

Now, recall ladder operators for Q.H.O.:

$$\hat{a}_{HO} = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} - i\frac{p}{p_0}\right) ; \quad \hat{a}^+_{HO} = \frac{1}{\sqrt{2}}\left(\frac{x}{x_0} + i\frac{p}{p_0}\right)$$

where $x_0 = \sqrt{\frac{\hbar}{m\omega}}$ and $p_0 = \sqrt{\hbar m\omega}$; $[\hat{a}, \hat{a}^+] = 1$

Similarly we define the following ladder operators:

$$\hat{a} = \frac{\ell_B}{\sqrt{2}\hbar}[\Pi_x - i\Pi_y] \quad ; \quad \hat{a}^+ = \frac{\ell_B}{\sqrt{2}\hbar}[\Pi_x + i\Pi_y]$$

It's easy to see that: $[\hat{a}, \hat{a}^+] = 1$

$$\Pi_x = \frac{\hbar}{\sqrt{2}\ell_B}(\hat{a}^+ + \hat{a}) ; \quad \Pi_y = \frac{\hbar}{i\sqrt{2}\ell_B}(\hat{a}^+ - \hat{a})$$

Note: the components of the gauge invariant momentum $\vec{\pi}$ are mutually conjugate, in the same manner as x and p_x, or y and p_y. That's why this new ladder operators are defined like that. Notice also that one cannot diagonalize at the same time π_x and π_y (since they do not commute).

The Dirac Hamiltonian at finite B can be written in terms of $\hat{a}$ and $\hat{a}^+$:

$$\mathcal{H}_D^B = v_F \vec{\pi}\cdot\vec{\sigma} = v_F \begin{pmatrix} 0 & \pi_x - i\pi_y \\ \pi_x + i\pi_y & 0 \end{pmatrix} =$$

$$= \sqrt{2}\,\frac{\hbar v_F}{l_B}\begin{pmatrix} 0 & \hat{a} \\ \hat{a}^+ & 0 \end{pmatrix} = \hbar\omega' \begin{pmatrix} 0 & \hat{a} \\ \hat{a}^+ & 0 \end{pmatrix}$$

where $\omega' = \sqrt{2}\,\frac{v_F}{l_B} = \sqrt{2}\,v_F\sqrt{\frac{|e|B}{\hbar c}}$ is analogous to the cyclotron frequency. [But note! $\omega' \neq \frac{|e|B}{m^* c}$ because $m^* = \hbar^2 \frac{1}{(\partial^2 E/\partial k^2)} = \infty$ for massless electrons!]

$\mathcal{H}_D^B$ is a 2×2 matrix, so the eigenstates are 2-component spinors:

$$\Psi_n = \begin{pmatrix} u_n \\ v_n \end{pmatrix}; \quad \mathcal{H}_D^B \Psi_n = \epsilon_n \Psi_n$$

This means we must solve the system of eqs:

$$\hbar\omega' \hat{a}\, v_n = \epsilon_n u_n \quad ; \quad \hbar\omega' \hat{a}^+ u_n = \epsilon_n v_n$$
$$(1) \qquad\qquad (2)$$

Multiplying (1) by $\hat{a}^+$ (from left):

$$\hbar\omega' \hat{a}^+\hat{a}\, v_n = \epsilon_n \hat{a}^+ u_n = \frac{(\epsilon_n)^2}{\hbar\omega'} v_n \Rightarrow$$

(using (2))

$$\Rightarrow \hat{a}^+\hat{a}\, v_n = \left(\frac{\epsilon_n}{\hbar\omega'}\right)^2 v_n$$

This means that v_n is an eigenstate of the number operator ($\hat{a}^+\hat{a}|n\rangle = n|n\rangle$), i.e., up to a numerical factor, $v_n \sim |n\rangle$

Notice the spectrum: $\epsilon_n^2 = n(\hbar\omega')^2 \Rightarrow$

$$\Rightarrow \boxed{\epsilon_n = \pm\hbar\omega'\sqrt{n} = \pm\hbar v_F \sqrt{\frac{2|e|}{\hbar c} n \cdot B'}}$$

Note the big difference in the energy spectrum:

$$\epsilon_n^{Sch} = \hbar\omega_c\left(n+\tfrac{1}{2}\right) = \frac{|e|\hbar}{c\cdot m^*} B\left(n+\tfrac{1}{2}\right)$$

$$\epsilon_n^{D} = \pm\hbar v_F \sqrt{\frac{2|e|}{\hbar c}}\sqrt{n}\cdot\sqrt{B}$$

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Consequences / differences:

* ϵ_n^D has a Landau level at zero energy whereas ϵ_n^{Sch} doesn't → most crucial!

* ϵ_n^D has Landau levels both for positive & negative energies, while ϵ_n^{Sch} only for positive energies (although if we would consider valence band, we would also have negative energy LL's for non-relativistic case).

* ϵ_n^D disperses as $\sqrt{nB}$, whereas ϵ_n^{Sch} disperses as $(n \cdot B)$. This means ϵ_n^D is not a harmonic spectrum (LL's are not equidistant in energy).