

electron states in a magnetic field

Robert Siebler

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Overview

- ▶ effective Hamiltonian
 - ▶ assumptions
 - ▶ replacing \vec{p} by $\vec{p} - \frac{e}{c}\vec{A}$
- ▶ monolayer graphene
 - ▶ Landau levels (energy spectra)
 - ▶ degeneracy of the eigenstates
- ▶ bilayer graphene
 - ▶ intermediate energies
 - ▶ trigonal warping
 - ▶ unified description

General purpose

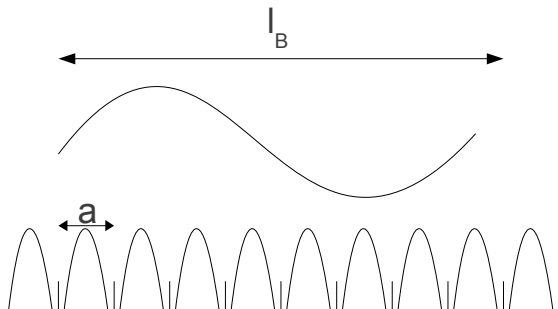
$$\hat{H} = \frac{\vec{p}^2}{2m} + V(\vec{r}) \quad \rightarrow \quad \hat{H} = v\vec{\sigma} \cdot \vec{p}$$

exp. \downarrow verified $\quad \quad \quad \downarrow ?$

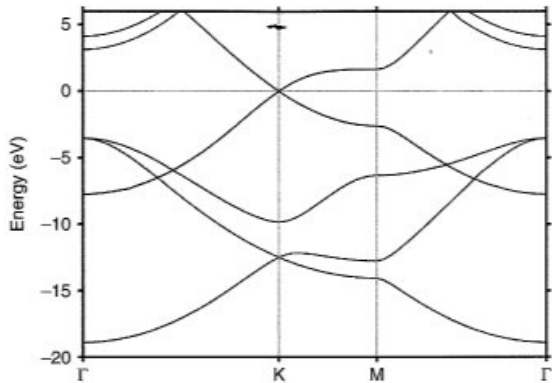
$$\hat{H} = \frac{\vec{\pi}^2}{2m} + V(\vec{r}) \quad \rightarrow \quad \hat{H} = v\vec{\sigma} \cdot \vec{\pi}$$

$$\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A}$$

$$l_B = \sqrt{\frac{\hbar c}{|e|B}} \gg a$$



1.2 π States in graphene



$$\hat{H} = \frac{\vec{\pi}^2}{2m} + V(\vec{r}) \quad (1)$$

$$H\psi = E\psi \quad ; \quad \psi = \sum_i c_i \varphi_i(\vec{r}) \quad (2)$$

$$\varphi_i = \varphi_0(\vec{r} - \vec{R}_i) = \exp\left(-\frac{i}{\hbar} \vec{R}_i \hat{\vec{p}}\right) \varphi_0(\vec{r}) \quad (3)$$

$$\hat{\vec{\Pi}} = \vec{p} + \frac{e}{c} \vec{A} \quad ; \quad \hat{\vec{\pi}} = \vec{p} - \frac{e}{c} \vec{A} \quad (4)$$

$$\rightarrow \tilde{\psi} = \sum_i c_i \tilde{\varphi}_i(\vec{r}) \quad (5)$$

$$\begin{aligned}
 H_{ij} (B \neq 0) &= \\
 &= \int d\vec{r} \varphi_0^* (\vec{r}) \hat{H} (B \neq 0) \exp \left(\frac{i}{\hbar} \vec{R}_i \hat{\Pi} \right) \exp \left(-\frac{i}{\hbar} \vec{R}_j \hat{\Pi} \right) \varphi_0 (\vec{r}) \\
 &= \exp \left(\frac{-ie}{2\hbar c} (\vec{R}_i \times \vec{R}_j) \vec{B} \right) \cdot \\
 &\cdot \underbrace{\int d\vec{r} \varphi_0^* (\vec{r}) \hat{H} (B \neq 0) \exp \left(\frac{i}{\hbar} (\vec{R}_i - \vec{R}_j) \hat{p} \right) \varphi_0 (\vec{r})}_{t_{ij}(\vec{\pi})}
 \end{aligned}$$

$$\begin{aligned}
 H_{ij} (B = 0) &= t_{ij}(\vec{p}) = \\
 &= \int d\vec{r} \varphi_0^* (\vec{r}) \hat{H} (B = 0) \exp \left(\frac{i}{\hbar} (\vec{R}_i - \vec{R}_j) \hat{p} \right) \varphi_0 (\vec{r})
 \end{aligned}$$

$$\hat{H}_{\text{eff}} = t_{ij}(\vec{\pi})$$

while

$$\vec{\pi} = \vec{p} - \frac{e}{c}\vec{A}$$

$$[\pi_x, \pi_y] = \frac{ie\hbar B}{c}$$

$$\pi_- = \pi_x - i\pi_y \quad (6)$$

$$\pi_+ = \pi_x + i\pi_y \quad (7)$$

with

$$[\pi_-, \pi_+] = -\frac{2|e|\hbar B}{c} \quad (8)$$

$$-\frac{c}{2|e|\hbar B} [\pi_-, \pi_+] = 1 \quad (9)$$

$$[b, b^\dagger] = 1 \quad (10)$$

$$\hat{H} = \frac{\vec{p}^2}{2m} + V(\vec{r}) \quad \rightarrow \quad \hat{H} = \vec{\sigma} \cdot \vec{p}$$

exp. \downarrow *verified*

\downarrow ?

$$\hat{H} = \frac{\vec{\pi}^2}{2m} + V(\vec{r}) \quad \rightarrow \quad \hat{H} = \vec{\sigma} \cdot \vec{\pi}$$

In the vicinity of K:

$$\hat{H}_K = \nu \vec{\sigma} \vec{p} \quad (11)$$

$$\hat{H}_{eff} = \nu \begin{pmatrix} 0 & \hat{\pi}_- \\ \hat{\pi}_+ & 0 \end{pmatrix} = \nu \sqrt{\frac{2|e|\hbar B}{c}} \begin{pmatrix} 0 & \hat{b} \\ \hat{b}^\dagger & 0 \end{pmatrix} \quad (12)$$

$$\hat{b}\psi_2 = \epsilon\psi_1 \quad (13)$$

$$\hat{b}^\dagger\psi_1 = \epsilon\psi_2 \quad (14)$$

$$E = \nu \sqrt{\frac{2|e|\hbar B}{c}} \epsilon \equiv \frac{\nu \sqrt{2\hbar}}{l_B} \epsilon \quad (15)$$

There is a zero-energy solution with:

$$\psi_1 = 0 \quad (16)$$

$$\psi_2 = |0\rangle \quad (17)$$

$$b\psi_2 = b|0\rangle = 0 \quad (18)$$

$$b^\dagger 0 = \varepsilon|0\rangle = 0 \rightarrow \varepsilon = 0 \quad (19)$$

applying b^\dagger to $b\psi_2 = \varepsilon\psi_1$ we get

$$b^\dagger b\psi_2 = \varepsilon \underbrace{b^\dagger \psi_1}_{\varepsilon\psi_2} = \varepsilon^2 \psi_2 \quad (20)$$

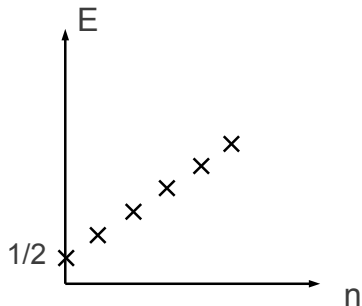
$$\rightarrow \varepsilon_n^2 = n = 0, 1, 2, 3... \quad (21)$$

$$\rightarrow \varepsilon_n^2 = n = 0, 1, 2, 3\dots \quad (22)$$

$$\rightarrow E_n^{(\pm)} = \pm \hbar \omega_c \sqrt{n} \quad (23)$$

$$\hbar \omega_c = \frac{\sqrt{2} \hbar v}{l_B} \quad (24)$$

non-relativistic-electrons

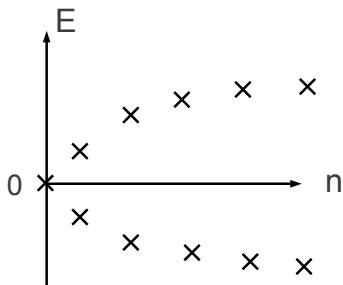


equidistant spectrum

$$\varepsilon = \hbar\omega \left(\frac{1}{2} + n \right)$$

$$t(\vec{\pi}) = \frac{\vec{\pi}^2}{2m^*}$$

electrons in graphene



not equidistant spectrum

$$E_n^{(\pm)} = \pm \hbar\omega_c \sqrt{n}$$

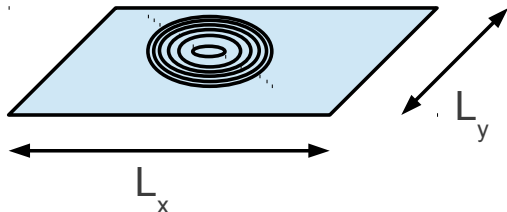
$$t(\vec{\pi}) = \begin{pmatrix} 0 & \hat{\pi}_- \\ \hat{\pi}_+ & 0 \end{pmatrix}$$

Degeneracy

$$x_0 = l_B^2 k_y$$

$$k_y L_y = 2\pi m$$

$$k_y = \frac{2\pi}{L_y} m$$



$$m = 0, 1, 2, \dots$$

$$0 \leq x_0 = l_B^2 k_y = l_b^2 \frac{2\pi}{L_y} m \leq L_x$$

$$\rightarrow m \leq \frac{L_x L_y}{2\pi l_B^2}$$

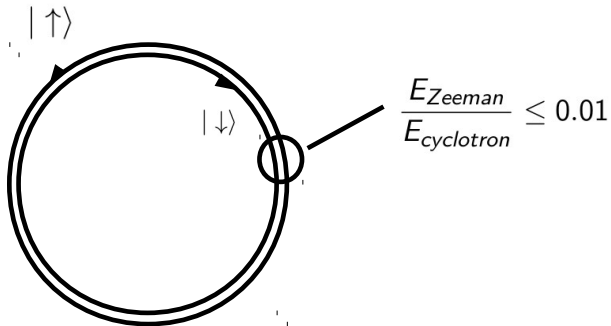
$$\rightarrow m \leq \frac{L_x L_y}{2\pi l_B^2} \quad ; \quad l_B = \sqrt{\frac{\hbar c}{|e|B}}$$

$$m_{\max} = \tilde{g} = \frac{L_x L_y}{2\pi} \frac{|e|B}{\hbar c} = \frac{A}{2\pi} \frac{|e|B}{\hbar c}$$

$$\tilde{g} = \frac{A}{2\pi} \frac{|e|B}{h/(2\pi)c} = \frac{\Phi}{\Phi_0} \quad ; \quad \Phi_0 = \frac{hc}{|e|}$$

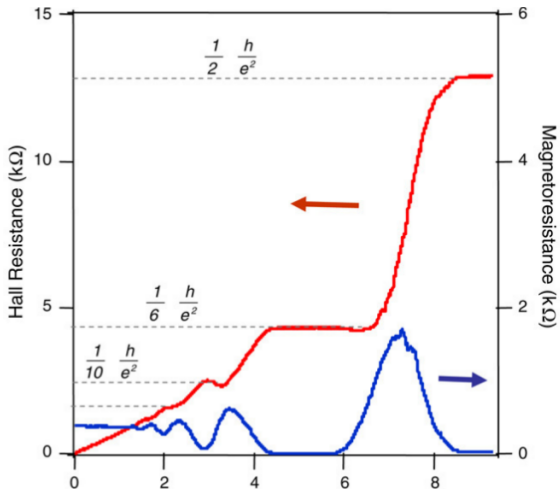
$$g = 2 \cdot 2 \cdot \tilde{g} \quad ; \quad \text{one factor for } K, K'$$

and another factor 2 for the two spin directions:

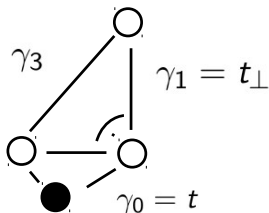
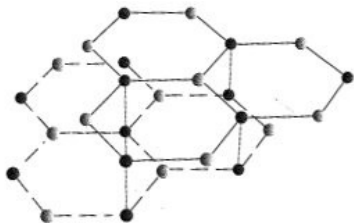


=>almost the same energy

$$R_{xy}^{-1} = \pm 4 \left(|n| + \frac{1}{2} \right) \frac{e^2}{\hbar}$$



Landau levels in bilayer graphene



3 cases:

$$|E| \approx |t_{\perp}|$$

high energies

$$\gamma_3^2 \frac{|t_{\perp}|}{t^2} \ll |E| \ll |t_{\perp}|$$

intermediate energies

$$|E| \approx \gamma_3^2 \frac{|t_{\perp}|}{t^2}$$

low energies

intermediate energies

$$\gamma_3^2 \frac{|t_\perp|}{t^2} \ll |E| \ll |t_\perp| \quad \text{intermediate energies}$$

$$\hat{H} = \frac{1}{2m^*} \begin{pmatrix} 0 & (\hat{p}_x - i\hat{p}_y)^2 \\ (\hat{p}_x + i\hat{p}_y)^2 & 0 \end{pmatrix}$$

$$\hat{H}_K = \frac{1}{2m^*} \begin{pmatrix} 0 & \hat{\pi}_-^2 \\ \hat{\pi}_+^2 & 0 \end{pmatrix}$$

$$\pi_- = \pi_x - i\pi_y = \sqrt{\frac{2|e|\hbar B}{c}} b$$

$$\pi_+ = \pi_x + i\pi_y = \sqrt{\frac{2|e|\hbar B}{c}} b^\dagger$$

$$\hat{H}_K = \frac{1}{2m^*} \sqrt{\frac{2|e|\hbar B}{c}}^2 \begin{pmatrix} 0 & \hat{b}^2 \\ \hat{b}^{\dagger 2} & 0 \end{pmatrix}$$

$$\omega_c^* := \frac{|e|B}{m^*c}$$

$$\hat{H}_K = \frac{2|e|\hbar B}{2m^*c} \begin{pmatrix} 0 & \hat{b}^2 \\ \hat{b}^{\dagger 2} & 0 \end{pmatrix} = \hbar\omega_c^* \begin{pmatrix} 0 & \hat{b}^2 \\ \hat{b}^{\dagger 2} & 0 \end{pmatrix}$$

bilayer

monolayer

$$\begin{aligned} b^2 \psi_2 &= \varepsilon \psi_1 \\ (b^\dagger)^2 \psi_1 &= \varepsilon \psi_2 \end{aligned}$$

$$\begin{aligned} b \psi_2 &= \varepsilon \psi_1 \\ b^\dagger \psi_1 &= \varepsilon \psi_2 \end{aligned}$$

$$b^2 |0\rangle = 0 \quad ; \quad b^2 |1\rangle = 0$$

$$\rightarrow g_0 = 2 \frac{\Phi}{\Phi_0}$$

$$g = \frac{\Phi}{\Phi_0} \quad \text{for } m \geq 2$$

$$\left(\hat{b}\right)^2 \psi_2 = \varepsilon \psi_1$$

$$\left(\hat{b}^\dagger\right)^2 \psi_1 = \varepsilon \psi_2$$

$$\left(b^\dagger\right)^2 b^2 \psi_2 = \varepsilon^2 \psi_2$$

$$b^\dagger b^\dagger b b \psi_2 = \varepsilon^2 \psi_2 \quad ; \quad [b, b^\dagger] = 1$$

$$b^\dagger (bb^\dagger - 1) b = b^\dagger b (b^\dagger b - 1)$$

$$b^\dagger b (b^\dagger b - 1) \psi_2 = \varepsilon^2 \psi_2$$

$$\varepsilon = E_\nu = \pm \hbar \omega_c^* \sqrt{n(n-1)}$$

For large $n \gg 1$:

$$\sqrt{n^2 \left(1 - \frac{1}{n}\right)} = |n| \sqrt{1 - \frac{1}{n}} \approx |n| \left(1 - \frac{1}{2n}\right)$$

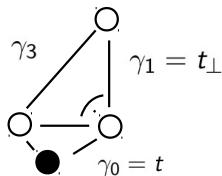
$$\rightarrow E_\nu \approx \pm \hbar \omega_c^* \left(|n| - \frac{1}{2}\right)$$

3 cases:

$$|E| \approx |t_{\perp}| \quad \text{high energies}$$

$$\gamma_3^2 \frac{|t_{\perp}|}{t^2} \ll |E| \ll |t_{\perp}| \quad \text{intermediate energies}$$

$$|E| \approx \gamma_3^2 \frac{|t_{\perp}|}{t^2} \quad \text{low energies}$$



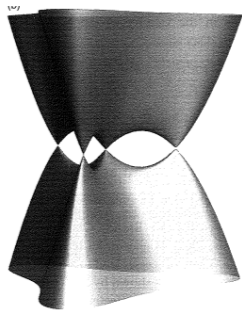
Trigonal warping (low energies)

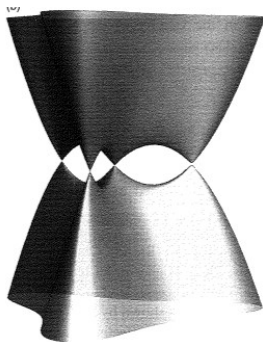
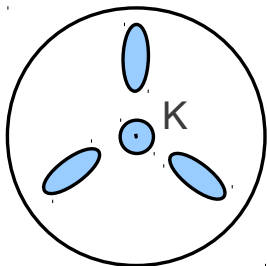
$$|E| \approx \gamma_3^2 \frac{\gamma_1}{\gamma_0^2} = \gamma_3^2 \frac{|t_\perp|}{t^2}$$

$$\hat{H} = \hbar\omega_c \begin{pmatrix} 0 & b^2 + \alpha b^\dagger \\ (b^\dagger)^2 + \alpha b & 0 \end{pmatrix}$$

$$\alpha = \frac{\gamma_3 a m^*}{\hbar^2} \sqrt{\frac{2\hbar c}{|e|B}}$$

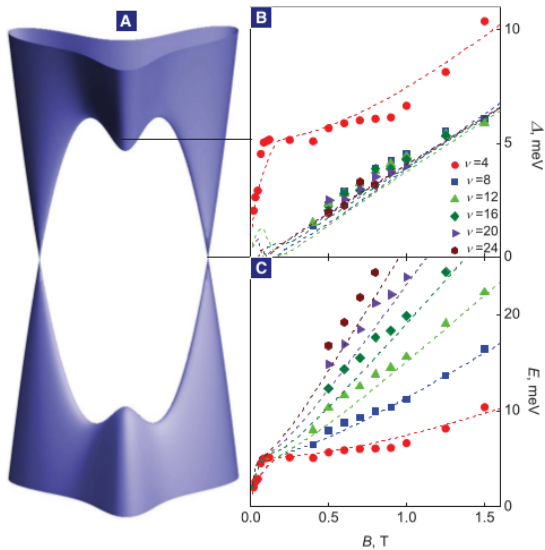
$$\tilde{g} = 2 \cdot 2 \cdot 4 \cdot g \quad \text{for low enough energies}$$





$$\begin{aligned}\sigma_z &= 16 \cdot g = 16 \cdot \frac{\Phi}{\Phi_0} && \text{theoretically} \\ \sigma_z &= 8 \cdot g && \text{experimentally}\end{aligned}$$

ν : "filling factor"



3 cases:

$$|E| \approx |t_{\perp}| \quad \text{high energies}$$

$$\gamma_3^2 \frac{|t_{\perp}|}{t^2} \ll |E| \ll |t_{\perp}| \quad \text{intermediate energies}$$

$$|E| \approx \gamma_3^2 \frac{|t_{\perp}|}{t^2} \quad \text{low energies}$$

Unified description (higher energies)

$$|E| \geq |t_{\perp}|$$

$$\hat{H} = \begin{pmatrix} 0 & \nu\vec{\pi}_+ & t_{\perp} & 0 \\ & 0 & 0 & 0 \\ & & 0 & \nu\vec{\pi}_- \\ (\dots)^{\dagger} & & & 0 \end{pmatrix}$$

$$t_{\perp} = \Gamma \sqrt{\frac{2|e|B\nu^2}{c}}$$

$$\varepsilon_n^2 = \frac{\Gamma^2 + 2n + 1}{2} \pm \sqrt{\left(\frac{\Gamma^2 + 2n + 1}{2}\right)^2 - n(n + 1)}$$

For $\Gamma = 0$:

$$\varepsilon_n^2 = n + \frac{1}{2} \pm \frac{1}{2}$$

For $\Gamma \gg 1$:

$$\varepsilon_{n1}^2 = \frac{n(n + 1)}{\Gamma^2}$$

$$\varepsilon_{n2}^2 = \Gamma^2 + 2n + 1$$

$$\varepsilon_{n2} \approx \pm \left[\Gamma + \frac{1}{\Gamma} \left(n + \frac{1}{2} \right) \right]$$

For $\Gamma \approx 1$

$$B_c \approx \frac{2}{9} \left(\frac{t_{\perp}}{t} \right)^2 \frac{\hbar c}{|e|a^2} \approx 70 T$$

conclusion

- ▶ effective Hamiltonian
 - ▶ assumptions
 - ▶ replacing \vec{p} by $\vec{p} - \frac{e}{c}\vec{A}$
- ▶ monolayer graphene
 - ▶ Landau levels (energy spectra)
 - ▶ degeneracy of the eigenstates
- ▶ bilayer graphene
 - ▶ intermediate energies
 - ▶ trigonal warping
 - ▶ unified description

References:



Graphene

Book over Graphene, M.Katsnelson, 2012, Cambridge University Press



Interaction-Driven Spectrum Reconstruction In bilayer Graphene

A. S. Mayorov et al. Science 333, 860 (2011);



Quantum Hall effect in graphene

Z. Jiang et al., Solid State Commun.143, 14 (2007)