Landau levels in graphene:

1. The Hamiltonian is SU(2)-symmetric (independent of the spin σ of the electron) so we drop the index σ for simplicity. The Hamiltonian is

$$\begin{aligned} H &= -t\sum_{\langle ij\rangle}\left[a_i^\dagger b_j + \text{H.c.}\right] = -t\sum_{i\in A}\sum_{j(i)}\left[a_i^\dagger b_j + \text{H.c.}\right] \\ &= -t\frac{1}{N}\sum_{\mathbf{k},\mathbf{k'}}\sum_{j=1}^{3}\sum_{i\in A}\left[e^{i(\mathbf{k'}-\mathbf{k})\cdot\mathbf{r}_i}e^{i\mathbf{k'}\cdot\boldsymbol{\delta}_j}a_\mathbf{k}^\dagger b_\mathbf{k'} + \text{H.c.}\right] \\ &= -t\sum_{\mathbf{k}}\sum_{j=1}^{3}\left[e^{i\mathbf{k}\cdot\boldsymbol{\delta}_j}a_\mathbf{k}^\dagger b_\mathbf{k} + \text{H.c.}\right] = \sum_{\mathbf{k}}\left[\Delta_\mathbf{k}a_\mathbf{k}^\dagger b_\mathbf{k} + \Delta_\mathbf{k}^* b_\mathbf{k}^\dagger a_\mathbf{k}\right], \end{aligned} \tag{1}$$

where $j(i)$ denotes the neighbours of the site i, and we have defined

$$\Delta_\mathbf{k} = -t\sum_{j=1}^{3}e^{i\mathbf{k}\cdot\boldsymbol{\delta}_j} = -te^{-ik_x}\left[1 + 2e^{i\frac{3}{2}k_xa}\cos\left(\frac{\sqrt{3}}{2}k_ya\right)\right]. \tag{2}$$

The last expression in Eq. (1) can be concisely written as

$$H = \sum_\mathbf{k}\begin{pmatrix}a_\mathbf{k}^\dagger & b_\mathbf{k}^\dagger\end{pmatrix}H_\mathbf{k}\begin{pmatrix}a_\mathbf{k}\\ b_\mathbf{k}\end{pmatrix}, \qquad H_\mathbf{k} = \begin{pmatrix}0 & \Delta_\mathbf{k},\\ \Delta_\mathbf{k}^* & 0\end{pmatrix}. \tag{3}$$

2. The last step in the diagonalisation of the Hamiltonian consists of diagonalising $H_\mathbf{k}$ for each $\mathbf{k}$. The energy dispersion is given by its eigenvalues,

$$\begin{aligned} \epsilon_{\mathbf{k}\pm} &= \pm|\Delta_\mathbf{k}| = \pm t\sqrt{3 + 2[\cos(\boldsymbol{\delta}_1-\boldsymbol{\delta}_2)\cdot\mathbf{k} + \cos(\boldsymbol{\delta}_2-\boldsymbol{\delta}_3)\cdot\mathbf{k} + \cos(\boldsymbol{\delta}_3-\boldsymbol{\delta}_1)\cdot\mathbf{k}]} \\ &= \pm t\sqrt{3 + 2\left[\cos\left(\sqrt{3}k_ya\right) + \cos\left(\frac{3}{2}k_xa - \frac{\sqrt{3}}{2}k_ya\right) + \cos\left(\frac{3}{2}k_xa + \frac{\sqrt{3}}{2}k_ya\right)\right]} \\ &= \pm t\sqrt{3 + 2\cos\left(\sqrt{3}k_ya\right) + 4\cos\left(\frac{\sqrt{3}}{2}k_ya\right)\cos\left(\frac{3}{2}k_xa\right)}. \end{aligned} \tag{4}$$

3. We use the expansion $\Delta_{\mathbf{K}+\mathbf{k}} = \Delta_\mathbf{K} + \mathbf{k}\cdot(\boldsymbol{\nabla}_\mathbf{k}\Delta_\mathbf{k})|_{\mathbf{k}=\mathbf{K}} + \mathcal{O}(k^2)$ and we calculate

$$\begin{aligned} (\boldsymbol{\nabla}_\mathbf{k}\Delta_\mathbf{k})|_{\mathbf{k}=\mathbf{K}} &= -tae^{-iK_xa}\left(3ie^{i\frac{3}{2}K_xa}\cos\left(\sqrt{3}K_ya/2\right), -\sqrt{3}e^{i\frac{3}{2}K_x}\sin\left(\sqrt{3}K_ya/2\right)\right) \\ &= -e^{-i2\pi/3}\frac{3ta}{2}(-i,1), \end{aligned} \tag{5}$$

where we have used $\Delta_\mathbf{K} = 0$, $\cos\left(\sqrt{3}K_ya/2\right) = \frac{1}{2}$, $\sin\left(\sqrt{3}K_ya/2\right) = \frac{\sqrt{3}}{2}$, and $3K_xa/2 = \pi$. Similarly,

$$(\boldsymbol{\nabla}_\mathbf{k}\Delta_\mathbf{k})|_{\mathbf{k}=\mathbf{K'}} = -e^{-i2\pi/3}\frac{3ta}{2}(-i,-1). \tag{6}$$

After multiplying $\Delta_{\mathbf{k}}$ by $-e^{i2\pi/3}$ (which we can because the phase of the Bloch Hamiltonian is arbitrary), we obtain

$$\Delta_{\mathbf{K}+\mathbf{k}} = \hbar v_F(-ik_x + k_y) + \mathcal{O}(k^2), \quad \Delta_{\mathbf{K'}+\mathbf{k}} = \hbar v_F(-ik_x - k_y) + \mathcal{O}(k^2), \tag{7}$$

and thus

$$H^K = \hbar v_F \begin{pmatrix} 0 & -ik_x + k_y, \\ ik_x + k_y & 0 \end{pmatrix} = \hbar v_F(k_x\sigma_y + k_y\sigma_x), \quad H^{K'} = \hbar v_F(k_x\sigma_y - k_y\sigma_x), \tag{8}$$

where $\hbar v_F = 3ta/2$, and σ_x and σ_y are Pauli matrices.

The energy dispersion becomes

$$\epsilon_{\mathbf{K}+\mathbf{k}} = \epsilon_{\mathbf{K'}+\mathbf{k}} = \pm\hbar v_F|\mathbf{k}| = \pm\hbar v_F k, \tag{9}$$

and is linear in k (thus the term "relativistic"). The system has therefore two bands which touch in **K** and **K'**, where the energy dispersion forms "Dirac" cones, as shown in Fig. 1.

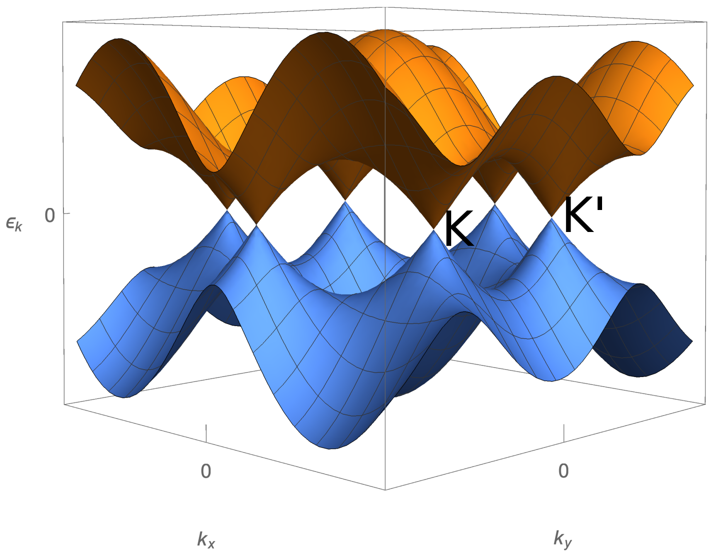

Figure 1: Energy dispersion of graphene.

The density of states $n(E)$ is obtained by counting the number of states in the energy shell $[E, E + dE]$. Near $E = 0$, states exist only in the Dirac cones centered in **K** and **K'**. Let us assume $E \geqslant 0$ and define $E = \hbar v_F k_1$ and $E + dE = \hbar v_F k_2$. The volume in k-space corresponding to states with $\epsilon_{\mathbf{K}+\mathbf{k}} \in [E, E + dE]$ is given by

$$2\pi \int_{k_1}^{k_2} k dk = \pi(k_2^2 - k_1^2) = \frac{2\pi}{\hbar^2 v_F^2} E dE + \mathcal{O}(dE^2). \tag{10}$$

Finally, we have to divide by the elementary volume per point **k** (i.e., the volume in k-space per state): $(2\pi)^2/(L_x L_y)$, and multiply by 2 for the two valleys (**K** and **K'**) and by 2 for the spins. We obtain

$$n(E) = A\frac{2E}{\pi\hbar^2 v_F^2}, \tag{11}$$

where $A = L_x L_y$ is the total area. At half-filling ($E_F = 0$), the density thus vanishes at the Fermi level, $n(E_F) = 0$.

Materials with no band gap and a vanishing density of state at the Fermi levels (such as graphene) are called semimetals.

4. The effect of the perpendicular magnetic field is taken into account through the Peierls substitution (which is only valid as long as the magnetic potential $\mathbf{A}(\hat{\mathbf{r}})$ varies slowly on the scale of the lattice spacing a, or similarly, $l_B \gg a$). It consists of replacing

$$\hbar\mathbf{k} \to \hat{\mathbf{\Pi}} = \hbar\mathbf{k} + \frac{e}{c}\mathbf{A}(\hat{\mathbf{r}}), \tag{12}$$

as for the free electron case (but here $\mathbf{k}$ is the crystal momentum !). Using

$$\hat{\Pi}_x = i\frac{\hbar}{\sqrt{2}l_B}\left(a^\dagger - a\right), \qquad \hat{\Pi}_y = \frac{\hbar}{\sqrt{2}l_B}\left(a^\dagger + a\right), \tag{13}$$

we obtain

$$H^K = \hbar v_F\left(\hat{\Pi}_x\sigma_y + \hat{\Pi}_y\sigma_x\right) = \frac{\hbar v_F}{\sqrt{2}l_B}\left(i(a^\dagger - a)\sigma_y + (a^\dagger + a)\sigma_x\right) = \hbar\omega_0\begin{pmatrix}0 & a^\dagger\\ a & 0\end{pmatrix}, \tag{14}$$

where $\hbar\omega_0 = \frac{\sqrt{2}\hbar v_F}{l_B}$. Similarly,

$$H^{K'} = \hbar v_F\left(\hat{\Pi}_x\sigma_y - \hat{\Pi}_y\sigma_x\right) = \frac{\hbar v_F}{\sqrt{2}l_B}\left(i(a^\dagger - a)\sigma_y - (a^\dagger + a)\sigma_x\right) = -\hbar\omega_0\begin{pmatrix}0 & a\\ a^\dagger & 0\end{pmatrix}, \tag{15}$$

5. Let us first consider the eigenvalue equation at $\mathbf{K}$ (the equation at $\mathbf{K'}$ is obtained by swapping u_n and v_n and the sign of the energy):

$$\begin{cases}\hbar\omega_0 a^\dagger v_n = \epsilon_n u_n\\ \hbar\omega_0 a u_n = \epsilon_n v_n\end{cases} \Rightarrow v_n = \frac{\hbar\omega_0}{\epsilon_n}a u_n \Rightarrow a^\dagger a u_n = \frac{\epsilon_n^2}{(\hbar\omega_0)^2}u_n. \tag{16}$$

Thus u_n must be an eigenstate of $a^\dagger a$ (say $|n\rangle$, so that now n labels the corresponding eigenvalue of $a^\dagger a$) and we have

$$u_n = |n\rangle \quad \Rightarrow \quad n = \frac{\epsilon_n^2}{(\hbar\omega_0)^2} \quad \Rightarrow \quad \epsilon_{\lambda,n} = \lambda\hbar\omega_0\sqrt{n} = \lambda\frac{\hbar v_F}{l_B}\sqrt{2n}, \tag{17}$$

where $\lambda = \pm 1$ is a band index. Furthermore, we have

$$v_n = \frac{\hbar\omega_0}{\epsilon_n}a u_n = \lambda\,|n-1\rangle\,, \tag{18}$$

for $n \neq 0$ and $v_0 = 0$. Therefore, the eigenvectors are

$$\psi^K_{\lambda,n=0} = \begin{pmatrix}|n\rangle\\ 0\end{pmatrix}, \qquad \psi^{K'}_{\lambda,n=0} = \begin{pmatrix}0\\ |n\rangle\end{pmatrix}, \tag{19}$$

$$\psi^K_{\lambda,n\neq 0} = \begin{pmatrix}|n\rangle\\ \lambda\,|n-1\rangle\end{pmatrix}, \qquad \psi^{K'}_{\lambda,n\neq 0} = \begin{pmatrix}|n-1\rangle\\ \lambda\,|n\rangle\end{pmatrix}. \tag{20}$$

The energy levels are $\epsilon_{\lambda,n} \propto \lambda\sqrt{nB}$ for $n \neq 0$ and $\epsilon_{n=0} = 0$ for $n = 0$ (there is no band index in this case). As for $B = 0$, for all n and λ the levels are twofold valley degenerate ($\mathbf{K}$ and $\mathbf{K'}$). The energy levels disperse as $\sqrt{B}$, whereas in the non-relativistic case, the relation is linear ($\epsilon_n = \hbar\omega_c(n + 1/2)$, $\omega_c \propto B$).

6. The zero-energy Landau levels ($n = 0$) are peculiar. Only one of the spinor components is nonzero. Remember that the first and second components of the spinor correspond to the A and B sublattices, respectively. Hence, $\psi^K_{\lambda,n=0}$ is entirely localized on the A sublattice and $\psi^{K'}_{\lambda,n=0}$ on the B sublattice. The two sublattices are decoupled at zero energy.

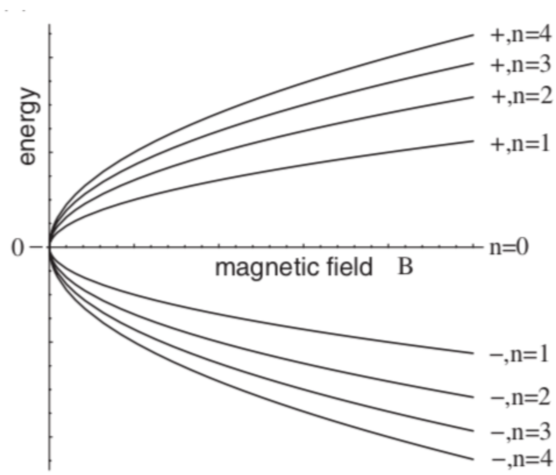

Figure 2: Relativistic Landau levels energy as a function of the magnetic field.