

**Exercise 8.1 Bohr-van-Leeuwen-Theorem**

The partition function of the system (without external magnetic field) is given by

$$Z_{\mathbf{B}=0} = \int \left( \prod_i d^3 q_i \right) \left( \prod_i d^3 p_i \right) e^{-\beta \mathcal{H}(\mathbf{p}_1, \dots, \mathbf{p}_N; \mathbf{q}_1, \dots, \mathbf{q}_N)}. \quad (1)$$

Since the only consequence of an applied magnetic field  $\mathbf{B}$  is a shift of the momenta  $\mathbf{p}_i \mapsto \mathbf{p}_i - e\mathbf{A}_i/c$  with  $\mathbf{A}_i = A(\mathbf{q}_i)$ , we can write the partition function for the case  $\mathbf{B} \neq 0$  as

$$Z_{\mathbf{B} \neq 0} = \int \left( \prod_i d^3 q_i \right) \left( \prod_i d^3 p_i \right) e^{-\beta \mathcal{H}(\mathbf{p}_1 - e/c\mathbf{A}_1, \dots, \mathbf{p}_N - e/c\mathbf{A}_N; \mathbf{q}_1, \dots, \mathbf{q}_N)}. \quad (2)$$

The integrals over the momenta  $\mathbf{p}_i$  all run from  $-\infty$  to  $\infty$  and hence we can shift every integration variable  $\mathbf{p}_i$  in (2) by an arbitrary constant,  $\mathbf{p}_i \mapsto \mathbf{p}_i + e\mathbf{A}_i/c$ . Finally, we have

$$Z_{\mathbf{B}=0} = Z_{\mathbf{B} \neq 0}, \quad (3)$$

stating that the partition function of a classical system does not depend on the externally applied magnetic field. Thus, the magnetization of a classical system vanishes,

$$M = \frac{1}{\beta} \frac{\partial \log Z}{\partial B} = 0. \quad (4)$$

**Note:** For a discussion on the diamagnetism of electrons and the problem of boundary terms, see *Surprises in Theoretical Physics*, R. Peierls, Princeton University Press (1979).

**Exercise 8.2 Landau Diamagnetism**

In the lecture it was shown that in a two-dimensional system of size  $L \times L$  the number of states in one Landau level is given by  $N_n = L^2/2\pi l^2$  with  $l$  ( $l^2 = \hbar c/|eB|$ ) the Larmor radius. In a three-dimensional system of size  $L \times L \times L = V$  the number of states in the  $n$ -th Landau level with  $z$ -component of the momentum within  $dp_z$  is given by

$$N_n \frac{L dp_z}{2\pi \hbar} = \frac{L^3}{2\pi l^2} \frac{dp_z}{2\pi \hbar} = \frac{V|eB|}{(2\pi \hbar)^2 c} dp_z = \frac{V m^* \omega_c}{(2\pi \hbar)^2} dp_z, \quad (5)$$

where  $m^*$  is the effective mass of the electrons and the cyclotron frequency  $\omega_c$  is given by  $\omega_c = |eB|/m^*c$ .

The density of states in the  $n$ -th Landau level is now given by

$$\rho_n(\epsilon) = 2 \times 2 \times \frac{m^* \omega_c}{(2\pi \hbar)^2} \frac{dp_{z+}(n, \epsilon)}{d\epsilon} = \frac{(2m^*)^{3/2} \omega_c}{4\pi^2 \hbar^2} \frac{1}{\sqrt{\epsilon - \hbar \omega_c (n + 1/2)}}, \quad (6)$$

where the factors  $2 \times 2$  account for the spin degeneracy and for the positive and the negative  $p_z$  values; with

$$p_{z+}(n, \epsilon) = \sqrt{2m^*} \sqrt{\epsilon - \hbar \omega_c (n + 1/2)} \quad (7)$$

according to the energy of a state is given by  $\epsilon = p_z^2/2m^* + \hbar\omega_c(n + 1/2)$ .

We now want to calculate the free energy which, for non-interacting electrons, is given by

$$F = N\mu - k_B T \sum_i \ln [1 + e^{-(\epsilon_i - \mu)/k_B T}] . \quad (8)$$

In our case, we can write this as

$$F = N\mu - k_B T V \sum_{n=0}^{\infty} \int_{\hbar\omega_c(n+1/2)}^{+\infty} d\epsilon \rho_n(\epsilon) \ln [1 + e^{-(\epsilon - \mu)/k_B T}] \quad (9)$$

$$= N\mu - V \frac{(2m^*)^{3/2} \omega_c}{2\pi^2 \hbar^2} \sum_{n=0}^{\infty} \int_{\hbar\omega_c(n+1/2)}^{+\infty} d\epsilon \frac{\sqrt{\epsilon - \hbar\omega_c(n+1/2)}}{1 + e^{(\epsilon - \mu)/k_B T}} , \quad (10)$$

where we have used Eq. (6) and integrated by parts in the second step. In the limit  $T \rightarrow 0^+$ , the Fermi function just cuts the integral and the chemical potential  $\mu \rightarrow \epsilon_F$ . Thus, in the limit  $T \rightarrow 0^+$ , we find

$$F = N\epsilon_F - V \frac{(2m^*)^{3/2} \omega_c}{2\pi^2 \hbar^2} \sum_{n=0}^{n_0} \int_{\hbar\omega_c(n+1/2)}^{\epsilon_F} d\epsilon \sqrt{\epsilon - \hbar\omega_c(n+1/2)} \quad (11)$$

$$= N\epsilon_F - V \frac{(2m^*)^{3/2} \omega_c}{3\pi^2 \hbar^2} \sum_{n=0}^{n_0} (\epsilon_F - \hbar\omega_c(n+1/2))^{3/2} \quad (12)$$

$$= N\epsilon_F - V \frac{(2\hbar\omega_c m^*)^{3/2} \omega_c}{3\pi^2 \hbar^2} \sum_{n=0}^{n_0} (x - n - 1/2)^{3/2} . \quad (13)$$

For the last step we introduced  $x = \epsilon_F/\hbar\omega_c$ ;  $n_0$  is defined by the condition  $n_0 + 1/2 \leq x < n_0 + 3/2$ . For small magnetic fields,  $x$  becomes very large and small changes in the magnetic field result in large changes in  $x$ . We can thus virtually tune the magnetic field in a way such that  $n_0 + 1 = x$ .

For large  $n_0$  we can use the Euler-Maclaurin formula from the exercise sheet to perform the approximative summation in Eq. (13)

$$\sum_{n=0}^{n_0} (x - n - 1/2)^{3/2} \approx \left( -\frac{2}{5}(n_0 + 1/2 - n)^{5/2} + \frac{1}{16}(n_0 + 1/2 - n)^{1/2} \right) \Big|_{-1/2}^{n_0+1/2} \quad (14)$$

$$\approx \frac{2}{5}x^{5/2} - \frac{1}{16}x^{1/2} . \quad (15)$$

It is obvious now that  $\mathcal{F}$  would not depend on the magnetic field if we had just replaced the sum by an integral. To find a finite diamagnetic effect, it is important to take into account the correction between the Riemann sum and the integral. The diamagnetism arises thus from the discrete nature of the Landau levels.

The free energy thus yields

$$F = N\epsilon_F - V \frac{2(2m^*)^{3/2} \epsilon_F^{5/2}}{15\pi^2 \hbar^3} + V \frac{(2m^*)^{3/2} \omega_c^2 \epsilon_F^{1/2}}{48\pi^2 \hbar} . \quad (16)$$

Eventually, we find for the magnetization (for  $B \rightarrow 0$ )

$$M = -\frac{1}{V} \frac{\partial F}{\partial B} = \frac{(2m^*)^{3/2} e^2 \epsilon_F^{1/2}}{24\pi^2 \hbar m^{*2} c^2} B = -\frac{1}{3} \left( \frac{m}{m^*} \right)^2 \mu_B^2 \rho(\epsilon_F) B, \quad (17)$$

where we set  $\mu_B = e\hbar/2mc$ . This leads to the susceptibility

$$\chi_L = \left. \frac{\partial M}{\partial B} \right|_{B=0} = -\frac{1}{3} \left( \frac{m}{m^*} \right)^2 \chi_P, \quad (18)$$

the Landau diamagnetism is thus a factor 3 weaker than the Pauli paramagnetism.

**Note:** There are also diamagnetic metals. This has to do with the appearance of the effective mass  $m^*$  from the band structure in (18).

### Exercise 8.3 Landau Levels in Graphene

We assume we have a magnetic field  $\mathbf{B} = (0, 0, B)$  in  $z$ -direction and use the Landau gauge  $\mathbf{A} = (0, Bx, 0)$ .

a) With the Peierls substitution ( $\mathbf{p} \rightarrow \mathbf{p} - e\mathbf{A}/c$ ) the (relevant) Hamiltonian reads

$$\mathcal{H} = v_F \left[ p_x \sigma_x + \left( p_y - \frac{eBx}{c} \right) \sigma_y \right]. \quad (19)$$

We want to solve  $\mathcal{H}\Psi = E\Psi$ , where  $\Psi$  is a two-component spinor. Instead, we solve the “square” of the Schrödinger equation,<sup>1</sup>  $\mathcal{H}^2\Psi = E^2\Psi$ :

$$\begin{aligned} \mathcal{H}^2 &= v_F^2 \left[ p_x \sigma_x + \left( p_y - \frac{eBx}{c} \right) \sigma_y \right] \left[ p_x \sigma_x + \left( p_y - \frac{eBx}{c} \right) \sigma_y \right] \Psi \\ &= v_F^2 \left[ p_x^2 \mathbb{1}_2 + \left( p_y - \frac{eBx}{c} \right)^2 \mathbb{1}_2 - \frac{\hbar eB}{c} \sigma_z \right] \Psi = E^2 \Psi, \end{aligned} \quad (20)$$

where we have used  $\{\sigma_i, \sigma_j\} = 2\delta_{ij}\mathbb{1}_2$  and  $[x, p_x] = i\hbar$ .

As the problem is translationally invariant in the  $y$ -axis, we make the Ansatz  $\Psi(x, y) = e^{ik_y y} \phi(x)$ , with  $\phi(x)$  a 2-component spinor. Then,

$$\left[ p_x^2 + \frac{e^2 B^2}{c^2} \left( \frac{c\hbar k_y}{eB} - x \right)^2 \right] \mathbb{1}_2 \phi(x) = \left( \frac{E^2}{v_F^2} \mathbb{1}_2 + \frac{\hbar eB}{c} \sigma_z \right) \phi(x). \quad (21)$$

This is the equation(s) of a shifted harmonic oscillator(s),<sup>2</sup> thus we may write the solution(s) of the “squared” Schrödinger equation  $\mathcal{H}^2\Psi = E^2\Psi$  easily

$\Psi$	$E^2/v_F^2$
$e^{ik_y y} \varphi_n(x - x_0) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$	$\frac{2\hbar eB }{c}(n + 1/2) - \frac{\hbar eB}{c}$
$e^{ik_y y} \varphi_n(x - x_0) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$	$\frac{2\hbar eB }{c}(n + 1/2) + \frac{\hbar eB}{c}$

where  $\varphi_n(x - x_0)$  are the harmonic oscillator eigenfunctions shifted by  $x_0 = \frac{c\hbar k_y}{eB}$ . Without loss of generality, let's us now assume  $eB > 0$ . Then we have for  $E_0 = 0$  eigenstates  $e^{ik_y y} \varphi_{n=0}(x - x_0) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ . The subspace corresponding to  $E_1 = \pm v_F \sqrt{\frac{2\hbar eB}{c}}$  is spanned over vectors  $e^{ik_y y} \varphi_{n=1}(x - x_0) \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $e^{ik_y y} \varphi_{n=0}(x - x_0) \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ . In order to get the eigenstates of  $\mathcal{H}$  one should perform diagonalization of  $\mathcal{H}$  in the subspace;

<sup>1</sup>Note that an eigenstate  $\Psi$  of  $\mathcal{H}$  is an eigenstate of  $\mathcal{H}^2$ , but it does not hold the other way round. In general, eigenvectors of  $\mathcal{H}^2$  with eigenvalue  $E^2$  do span the eigensubspaces of  $\mathcal{H}$  corresponding to  $\pm E$ .

<sup>2</sup>And multiplied by  $2m$ .

we need just the eigenvalues and for that we claim,<sup>3</sup> that for each  $k_y$  there will be 1 solution with positive and 1 with negative energy  $E$ , therefore

$$E_m = \text{sign}(m)v_F\sqrt{\frac{2\hbar|eB|}{c}|m|}, \quad m = 0, \pm 1, \dots \quad (27)$$

- b) The degeneracy of the eigenvalues (27) is found in the usual way. From Eq. (21) we see, that the center of the wave function is shifted to  $\frac{ck_y}{eB}$ . In a sample of size  $L \times L$ , we thus have the condition that  $\frac{ck_y}{|eB|} < L$ , with  $k_y = 2\pi n_y/L$ . Hence,

$$N_B = \frac{|eB|}{2\pi\hbar c}L^2 \quad (28)$$

and is independent of  $n$  but dependent on  $B$ . Since we have only considered half of the Hamiltonian (only  $K$ -part), we have to multiply this by 2. Thus, the energies given in Eq. (27) are  $2N_B$ -times degenerate. Special care has to be given to the ( $n = 0$ )-case. There,  $N_B$  states come from one half ( $K$ -part) of the Hamiltonian, thus the degeneracy is also  $2N_B$ .

- c) Usually, the magnetization of a system oscillates with changing the magnetic field, since additional Landau levels are pushed through the chemical potential. In graphene,  $\mu = 0$  and the Landau levels are pushed away from  $\mu$ , but never cross it. Hence the magnetization does not oscillate (this changes for doped graphene).

Let us try to figure out which kind of magnetic response there will be if we apply a magnetic field to graphene. Due to the electronic spins, one expects a paramagnetic response from every partially filled band in general, the so-called Pauli paramagnetism which, at least to lowest order in the magnetic field (linear response), is proportional to the density of states at the Fermi energy. For graphene, the density of states at the Fermi energy vanishes and thus the paramagnetic response due to the electronic spin is zero.

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<sup>3</sup>**Proof:** (assumed  $eB > 0$ ) let us denote

$$|I\rangle = e^{ik_y y} \begin{pmatrix} 1 \\ 0 \end{pmatrix} |n+1\rangle, \quad |II\rangle = e^{ik_y y} \begin{pmatrix} 0 \\ 1 \end{pmatrix} |n\rangle, \quad (22)$$

where  $|n\rangle$  does stand for commonly normalized eigenvector for a harmonic oscillator in  $x$ -direction shifted by  $x_0$ , thus

$$\hat{x} - x_0 = \sqrt{\frac{c\hbar}{2eB}}(\hat{a}^\dagger + \hat{a}), \quad \hat{p}_x = i\sqrt{\frac{\hbar eB}{2c}}(\hat{a}^\dagger - \hat{a}), \quad (23)$$

where  $\hat{a}$  and  $\hat{a}^\dagger$  are the ladder operators,

$$\hat{a}|n\rangle = \sqrt{n}|n-1\rangle, \quad \hat{a}^\dagger|n\rangle = \sqrt{n+1}|n+1\rangle. \quad (24)$$

Then we may rewrite the Hamiltonian  $\mathcal{H}$  using these operators as

$$\mathcal{H} = v_F \left[ i\sqrt{\frac{\hbar eB}{2c}}(\hat{a}^\dagger - \hat{a})\sigma_x + \left( -i\hbar\partial_y - \frac{eB}{c} \left( x_0 + \sqrt{\frac{c\hbar}{2eB}}(\hat{a}^\dagger + \hat{a}) \right) \right) \sigma_y \right]. \quad (25)$$

Further, after an easy calculation, we may find that

$$\mathcal{H}|I\rangle = -iv_F\sqrt{\frac{2\hbar eB}{c}}(n+1)|II\rangle, \quad \mathcal{H}|II\rangle = iv_F\sqrt{\frac{2\hbar eB}{c}}(n+1)|I\rangle, \quad (26)$$

which means that the Hamiltonian  $\mathcal{H}$  is in the corresponding subspace in the basis  $|I\rangle, |II\rangle$  given by the matrix  $-v_F\sqrt{\frac{2\hbar eB}{c}}(n+1)\sigma_y$  and thus the spectrum is  $\pm v_F\sqrt{\frac{2\hbar eB}{c}}(n+1)$ .

The magnetic response of a system is defined as the change of the free energy with respect to a change in the magnetic field

$$M = -\frac{\partial \mathcal{F}(B)}{\partial B} \quad \chi = \left. \frac{\partial M(H)}{\partial H} \right|_{B=0} = -\left. \frac{\partial^2 \mathcal{F}(H)}{\partial B^2} \right|_{B=0} \quad (29)$$

In many cases, it is sufficient to expand the free energy to second order in the magnetic field  $\mathcal{F} \sim \mathcal{O}(B^2)$ , which directly gives a magnetization linear in  $B$  and a susceptibility which is constant. This is known as linear response theory and requires  $\mathcal{F}$  to be analytic for  $B \rightarrow 0$ .

In two dimensions, it is not obvious that this requirement is satisfied, since the spectrum abruptly changes from a continuous spectrum at  $B = 0$  to a discrete spectrum for every  $B \neq 0$ . Therefore one needs to be careful before applying linear response theory. But, since the Eq. (29) holds in general, one can compute  $\mathcal{F}$  exactly and obtain the magnetization and the susceptibility, which then might have a non-trivial structure suggesting the importance of non-linear response.

Instead of going into the quantitative analysis, let us discuss the nature of the response (para- or diamagnetic) by qualitative reasoning. We will for simplicity assume zero temperature, work in the grand canonical ensemble and fix the chemical potential to the band crossing point. To find the magnetization, we would need the free energy as a function of the magnetic field, but for that purpose we may also examine the quantity  $\Delta\mathcal{F}(B) = \mathcal{F}(B) - \mathcal{F}_0$  where  $\mathcal{F}_0 = \mathcal{F}(B = 0)$ .

We know that the density of states per spin in graphene at zero field is linear,

$$\rho(E) = \frac{L^2}{\pi} \left| k \frac{dk}{dE} \right| = \frac{L^2}{\pi} \frac{|E|}{(\hbar v_F)^2}, \quad (30)$$

and we know the degeneracy of each Landau level is  $2N_B = 2L^2|eB|/(2\pi\hbar c)$  at positions  $E_m = \text{sign}(m)v_F\sqrt{2\hbar|meB|}/c$  as found in the first part of this exercise. As a consequence, there are exactly as much states in between the position of two Landau levels as the degeneracy of one Landau level. At zero temperature, the 0<sup>th</sup> Landau level will be exactly half filled<sup>4</sup> and hence all the states from zero energy to  $-E_1/\sqrt{2}$  will be lifted to the energy  $E_0$ . For the  $m$ -th Landau level ( $m < 0$ ), states from energy range  $-\sqrt{|m|}E_1$  to  $-\sqrt{|m|-1/2}E_1$  will be pushed down and the states from  $-\sqrt{|m|+1/2}E_1$  to  $-\sqrt{|m|}E_1$  will be pushed up; look at Fig. (1) The energy changes corresponding to the levels are thus

$$\begin{aligned} \Delta E_0 &= 2N_B E_1 \left[ \frac{2}{3} \left( \frac{1}{2} \right)^{3/2} \right], \\ \Delta E_{-1} &= 2N_B E_1 \left[ -\sqrt{1} + \frac{2}{3} \left( \frac{3}{2} \right)^{3/2} - \frac{2}{3} \left( \frac{1}{2} \right)^{3/2} \right], \\ &\vdots \\ \Delta E_{-m} &= 2N_B E_1 \left[ -\sqrt{m} + \frac{2}{3} (m+1/2)^{3/2} - \frac{2}{3} (m-1/2)^{3/2} \right], \quad (m > 0) \\ \Rightarrow \Delta E &\equiv \sum_{m=0}^{\infty} E_{-m} = 2N_B E_1 \lim_{M \rightarrow \infty} \left( \frac{2}{3} (M+1/2)^{3/2} - \sum_{m=1}^M \sqrt{m} \right) \approx 0.416 N_B E_1, \end{aligned}$$

<sup>4</sup>This can be understood as the  $T \rightarrow 0$  limit of the finite temperature occupation numbers.

where the last limit including the summation might be performed either using the approximative Euler–MacLaurin formula from the exercise sheet (which does give a numerical prefactor  $\frac{7}{12\sqrt{2}} \approx 0.412$ ) or analytically by use of special functions. At  $T = 0$  we have  $\mathcal{F} = E_{\text{total}}$ . For the magnetization we get

$$\Delta\mathcal{F} = \Delta E \propto |B|^{3/2}, \quad \Delta\mathcal{F} > 0 \quad \Rightarrow \quad M = -\frac{\partial \Delta\mathcal{F}}{\partial B} = -c \operatorname{sign}(B)|B|^{1/2}, \quad (31)$$

with a positive constant  $c$ . From this we immediately conclude that the magnetization is finite and has the opposite sign as  $B$ ; thus the response is diamagnetic.

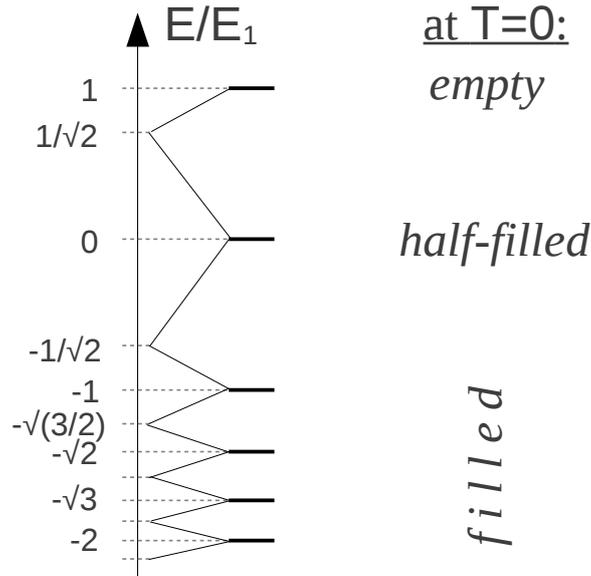


Figure 1: To the c) part: the change of the total energy at  $T = 0$  might be easily calculated looking at figure above.