Karlsruhe Institute of Technology
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Condensed Matter Theory I WS 2022/2023

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Sheet 7
Tutorial: 15.12.2022

Category A

1. De Haas–van Alphen effect in a 2D system (canonical ensemble) $(5+10=15$ Points)

We consider a 2D electron gas (no spin) with the parabolic dispersion $\varepsilon = \hbar^2 k^2/2m$ in a magnetic field H perpendicular to the plane. In this case, there is no motion in z-direction. The energies of the Landau levels read:

$$E_n = \hbar\omega_c(n+\frac{1}{2}), \qquad \omega_c = \frac{eH}{mc}$$

and the degeneracy of each Landau level is given by

$$N_n = \frac{eH}{hc}L_xL_y = \frac{H\mathcal{A}}{\Phi_0}$$

Here $\mathcal{A} = L_xL_y$ is the total area of the system and $\Phi_0 \equiv \dfrac{hc}{e}$ is the flux quantum. We assume $eH > 0$. Therefore, the density of states is given by:

$$\nu(\varepsilon) = \frac{H}{\Phi_0}\sum_{n=0}^{\infty}\delta(\varepsilon - \hbar\omega_c(n+\frac{1}{2}))$$

(a) In the canonical ensemble the 2D electron density, denoted by n_e, is fixed. Assume $T = 0$. Compute the chemical potential and the free energy per unit of area as functions of H.

Solution: First, we have the inequalities:

$$p\frac{H}{\Phi_0} < n_e < (p+1)\frac{H}{\Phi_0}$$

The free energy of the system at $T = 0$ is the same as internal energy and is given by the sum of energies of occupied single-particle states, yielding (per unit of area):

$$\begin{aligned}\frac{F}{\mathcal{A}} &= \sum_{j=0}^{p-1}\hbar\omega_c(j+\frac{1}{2})\frac{H}{\Phi_0} + (n_e - p\frac{H}{\Phi_0})\hbar\omega_c(p+\frac{1}{2}) \\ &= -(p^2+p)\frac{e^2H^2}{4\pi mc^2} + \left(p+\frac{1}{2}\right)n_e\frac{\hbar eH}{mc}\end{aligned}$$

The chemical potential is:

$$\begin{aligned}\mu &= \frac{\partial F}{\partial N} = \frac{\partial F/\mathcal{A}}{\partial n_e} \\ &= \left(p+\frac{1}{2}\right)\frac{\hbar eH}{mc} = \left(p+\frac{1}{2}\right)\hbar\omega_c\end{aligned}$$

(b) Compute the magnetization $M = -\left(\frac{\partial F/\mathcal{A}}{\partial H}\right)_{T,n_e}$. Express the result by using the Bohr magneton $\mu_B = \frac{e\hbar}{2mc}$. Draw a sketch of the magnetization with respect to the inverse of the magnetic field $1/H$. Find the period of the oscillations of $M(1/H)$.

Hint: It might be useful to introduce an integer p denoting the number of completely filled Landau levels and consider carefully what happens when p changes (jumps).
Solution:

$$\begin{aligned} M &= -\left(\frac{\partial F/\mathcal{A}}{\partial H}\right)_{T,n_e} \\ &= (p^2+p)\frac{e^2 H}{2\pi mc^2} - \left(p+\frac{1}{2}\right) n_e \frac{\hbar e}{mc} \\ &= 2(p^2+p)\frac{\mu_B H}{\Phi_0} - 2(p+\frac{1}{2}) n_e \mu_B \end{aligned} \tag{1}$$

When $n_e = \frac{pH}{\Phi_0} \Rightarrow H = \frac{n_e \Phi_0}{p}$. First, we study the limit when $\lim_{H \to \frac{n_e\Phi_0}{p}^-} H = \lim_{\epsilon \to 0} \frac{n_e \Phi_0}{p} - \epsilon$. Therefore, we are in the case where we approach n_e such that the $p+1$-st level is partly filled and tend to empty:

$$p\frac{H}{\Phi_0} \leq n_e < (p+1)\frac{H}{\Phi_0}$$

This is exactly the same case as when we derived the formula of the magnetization, so we can directly apply the equation (1):

$$\begin{aligned} M(H \to \frac{n_e\Phi_0}{p}^-) &= 2(p^2+p)\frac{\mu_B H}{\Phi_0} - 2(p+\frac{1}{2})\frac{pH}{\Phi_0}\mu_B \\ &= \frac{\mu_B p H}{\Phi_0} = \mu_B n_e \end{aligned}$$

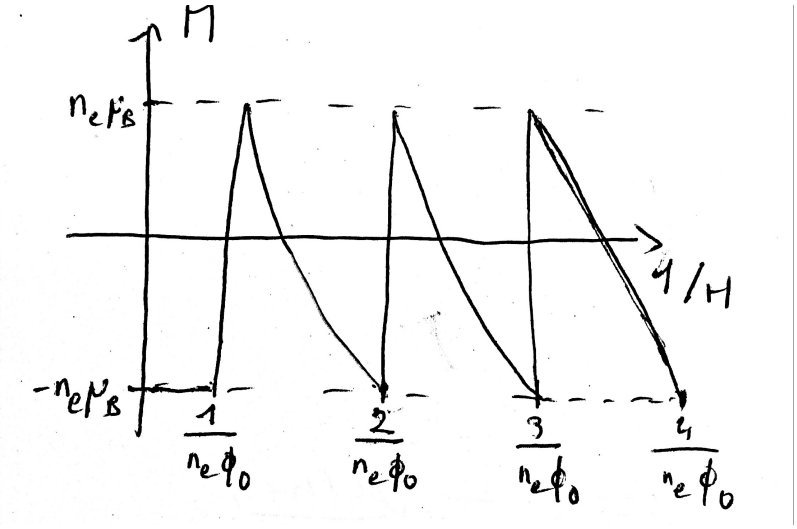
In the other hand, when $\lim_{H \to \frac{n_e\Phi_0}{p}^+} H = \lim_{\epsilon \to 0} \frac{n_e \Phi_0}{p} + \epsilon$, the p-th Landau level is partly filled and tend to be fully occupied:

$$(p-1)\frac{H}{\Phi_0} < n_e \leq p\frac{H}{\Phi_0}$$

We must substitute into equation (1), $p \to p-1$. We obtain:

$$\begin{aligned} M(H \to \frac{n_e\Phi_0}{p}^+) &= 2((p-1)^2+p-1)\frac{\mu_B H}{\Phi_0} - 2(p-\frac{1}{2})\frac{pH}{\Phi_0}\mu_B \\ &= -\frac{\mu_B p H}{\Phi_0} = -\mu_B n_e \end{aligned}$$

Moreover, we have $M(\frac{1}{H} = \frac{p}{n_e\Phi_0}) = M(\frac{1}{H} = \frac{p+1}{n_e\Phi_0})$. The period of the oscillations of the magnetization as a function of $1/H$ is $1/(n_e\Phi_0)$.



2. De Haas–van Alphen effect in a 2D system (grand canonical ensemble) ($5 + 10 = 15$ Points)

Now, let us derive the same effect but in the grand canonical ensemble, still at $T = 0$. The number of particles is not fixed anymore but we fix the chemical potential μ.

(a) Compute the electron density as a function of H. Consider the grand potential $\Omega = U - \mu N$ where U the internal energy and N the number of particles. Compute the density of the grand potential $\Omega/\mathcal{A}$ as a function of H.

Solution: First, let us consider that the chemical potential is between two Landau levels:

$$\hbar\omega_c(n_\mu + \frac{1}{2}) < \mu < \hbar\omega_c(n_\mu + \frac{3}{2})$$

Therefore, the $n_\mu + 1$-st Landau levels are completely filled and the $n_\mu + 2$-nd is emptied. The electron density is $\frac{N}{\mathcal{A}} = (n_\mu + 1)\frac{H}{\Phi_0}$. Moreover, we have:

$$\begin{aligned} \frac{U}{\mathcal{A}} &= \sum_{j=0}^{n_\mu} \hbar\omega_c(j + \frac{1}{2})\frac{H}{\Phi_0} \\ &= \frac{\hbar e H^2}{2\Phi_0 mc}(n_\mu + 1)^2 \end{aligned}$$

Finally we obtain:

$$\frac{\Omega}{\mathcal{A}} = \frac{\hbar e H^2}{2\Phi_0 mc}(n_\mu + 1)^2 - \mu(n_\mu + 1)\frac{H}{\Phi_0}$$

(b) The magnetization is given by $M = -\left(\frac{\partial\Omega/\mathcal{A}}{\partial H}\right)_{T,\mu}$. Compute the magnetization as a function of H. What is the period of the oscillations of the magnetization as a function of $1/H$?

Solution:

$$\begin{aligned} M &= -\frac{\hbar e H}{\Phi_0 mc}(n_\mu + 1)^2 + \mu(n_\mu + 1)\frac{1}{\Phi_0} \\ &= -\frac{\hbar\omega_c}{\Phi_0}(n_\mu + 1)^2 + \mu(n_\mu + 1)\frac{1}{\Phi_0} \end{aligned} \tag{2}$$

When $\hbar\omega_c(n_\mu + 1/2) = \mu$,

$$n_\mu + \frac{1}{2} = \frac{\mu}{\hbar\omega_c}, \qquad n_\mu + 1 = \frac{\mu}{\hbar\omega_c} + \frac{1}{2}, \qquad n_\mu = \frac{\mu}{\hbar\omega_c} - \frac{1}{2}$$

When the chemical potential is $\hbar\omega_c(n_\mu + \frac{1}{2}) \leq \mu < \hbar\omega_c(n_\mu + \frac{3}{2})$., we increase H so the energy of the Landau level $E_{n_\mu} = \hbar\omega_c(n_\mu + 1/2)$ increases until reaching the value μ. Equation (2) becomes at the crossing:

$$\begin{aligned} M^- &= -\frac{\hbar\omega_c}{\Phi_0}\left(\frac{\mu}{\hbar\omega_c} + \frac{1}{2}\right)^2 + \mu\left(\frac{\mu}{\hbar\omega_c} + \frac{1}{2}\right)\frac{1}{\Phi_0} \\ &= -\frac{\mu}{2\Phi_0} - \frac{\hbar\omega_c}{4\Phi_0} \end{aligned}$$

In the limit when $H \to 0 \Rightarrow \omega_c \to 0$ we have:

$$M^- = -\frac{\mu}{2\Phi_0}$$

When the chemical potential is $\hbar\omega_c(n_\mu - \frac{1}{2}) < \mu \leq \hbar\omega_c(n_\mu + \frac{1}{2})$, we decrease H so the energy of the Landau level $E_{n_\mu} = \hbar\omega_c(n_\mu + 1/2)$ decreases until reaching the value μ. In this case we must substitute in equation (2) $n_\mu \to n_\mu - 1$ and evaluate it at the crossing:

$$\begin{aligned} M^+ &= -\frac{\hbar\omega_c}{\Phi_0}\left(\frac{\mu}{\hbar\omega_c} - \frac{1}{2}\right)^2 + \mu\left(\frac{\mu}{\hbar\omega_c} - \frac{1}{2}\right)\frac{1}{\Phi_0} \\ &= +\frac{\mu}{2\Phi_0} - \frac{\hbar\omega_c}{4\Phi_0} \end{aligned}$$

In the limit when $H \to 0 \Rightarrow \omega_c \to 0$ we have:

$$M^+ = +\frac{\mu}{2\Phi_0}$$

Each time the chemical potential crosses a Landau level there is such a discontinuity. For n_μ, it happens at $\frac{1}{H_{n_\mu}} = \frac{\hbar e(n_\mu + 1/2)}{mc\mu}$ and for $n_\mu - 1$ at $\frac{1}{H_{n_\mu - 1}} = \frac{\hbar e(n_\mu - 1/2)}{mc\mu}$. Period of oscillations of the magnetization is $\frac{1}{H_{n_\mu}} - \frac{1}{H_{n_\mu - 1}} = \frac{\hbar e}{\mu mc}$.

3. 3D electrons in magnetic field (canonical ensemble) $(5 + 5 + 10 = 20$ Points)

(a) Calculate the density of states $\nu_H(\epsilon)$ for free electrons in three dimensions subjected to the magnetic field H:

$$\nu_H(\epsilon) = \frac{1}{L_x L_y L_z}\sum_{k_z,n} N_n \delta(\epsilon - E_n(k_z)).$$

Here, $E_n(k_z) = \hbar\omega_c(n + 1/2) + \frac{\hbar^2 k_z^2}{2m}$ is the spectrum of the system, cyclotron frequency $\omega_c = \frac{eH}{mc}$, $n \geq 0$ is the Landau level number, and k_z is the momentum

along z-direction. The degeneracy factor is $N_n = \dfrac{H}{\Phi_0} L_x L_y$ ($L_{x,y}$ are sizes along x, y-directions, $\Phi_0 = \dfrac{hc}{e}$ is the flux quantum). Use the continuous limit transformation for the sum over k_z, i.e., $\sum\limits_{k_z} = L_z \int \dfrac{dk_z}{2\pi}$.

Solution: Using the expression for N_n, assuming the continuous limit and introducing $\xi = \dfrac{\hbar^2 k_z^2}{2m}$ with $\xi > 0$, the density of states is reduced to

$$\nu_H(\epsilon) = \frac{H}{\Phi_0} \sum_{n=0}^{\infty} \int \frac{dk_z}{2\pi} \delta(\epsilon - E_n(k_z)) =$$

$$= \frac{H}{\Phi_0} \sum_{n=0}^{\infty} 2 \int_0^{\infty} \delta\left(\epsilon - \hbar\omega_c(n + 1/2) - \xi\right) \frac{1}{2\pi} \frac{\sqrt{2m}}{\hbar} \frac{d\xi}{2\sqrt{\xi}} =$$

$$= \frac{\sqrt{m} H}{\sqrt{2}\pi\hbar\Phi_0} \sum_{n=0}^{\infty} \frac{\theta\left(\epsilon - \hbar\omega_c(n + \frac{1}{2})\right)}{\sqrt{\epsilon - \hbar\omega_c(n + \frac{1}{2})}} \, .$$

Note that at $H \to 0$, when $\omega_c \to 0$, the density of states becomes the same as in 3D case with $\nu(\epsilon) \propto \sqrt{\epsilon}$.

(b) Without explicit calculations of a magnetization M, estimate the period of oscillations of M as a function of $\dfrac{1}{H}$. To do that, use $\nu_H(\epsilon)$ found above, assuming that a large number $n \gg 1$ of Landau levels is occupied and the Fermi-energy ϵ_F does not depend on H.

Solution: The singularities in $\nu_H(\epsilon)$ are located at the energies $\epsilon_n = \hbar\omega_c(n+1/2)$. Physical quantities, such as magnetization, have peaks at the corresponding values of the field H_n when the condition, $\epsilon_n = e_F(H)$, holds. Assuming that n is large, we conclude that the Fermi energy for the canonical ensemble depends slightly on H. Namely, $\epsilon_F(H)$ has oscillations as a function of H because particle number is fixed. But these oscillations are relatively small at $n \gg 1$, consequently, we approximate $\epsilon_F = \text{const}$. Take two equations for H_n and H_{n+1} that are related to neighbouring singularities, i.e., $\epsilon_F = \hbar\dfrac{eH_n}{mc}(n + 1/2)$ and $\epsilon_F = \hbar\dfrac{eH_{n+1}}{mc}(n + 1 + 1/2)$. We then find the osillations period $\Delta\left(\dfrac{1}{H}\right) = \dfrac{\hbar e}{mc\epsilon_F}$.

(c) Assuming a constant electron density, n_e, obtain the chemical potential μ as a function of H at $T = 0$. Use the following identity:

$$n_e = \int_0^{\mu} \nu_H(\epsilon) d\epsilon.$$

Solution: Integration by ϵ yields:

$$n_e = 2\frac{\sqrt{m} H}{\sqrt{2}\pi\hbar\Phi_0} \sum_{n=0}^{m} \sqrt{\mu - \hbar\omega_c(n + 1/2)}$$

where m is a total number of sub-bands that are crossed by an unknown chemical potential $\mu(n_e, H)$. The chemical potential is such that it provides the given particle density, n_e. It is difficult to resolve μ as a function of H and n_e in a general case. However, a solution can be found at very high fields, when only one Landau level is occupied, i.e. $m = 0$, and we have only one term into the sum. The chemical potential in this case reads

$$\mu = \frac{\pi^2\hbar^2\Phi_0^2 n_e^2}{2mH} + \frac{\hbar eH}{2mc} \ .$$

Another limit is $n \gg 1$, when one can replace the sum by the integral because $\dfrac{\hbar\omega_c}{\mu} \ll 1$. Having introduced $x = \dfrac{\hbar\omega_c(n+1/2)}{\mu}$ and $dx = \dfrac{\hbar\omega_c}{\mu}$ we have

$$n_e = 2\frac{\sqrt{m}H}{\sqrt{2}\pi\hbar\Phi_0}\frac{\mu^{3/2}}{\hbar\omega_c}\int\limits_0^1 \sqrt{1-x}dx \ .$$

The field H drops from this equation and we recover the result for μ which coincides with the expression for 3D electron gas at $H = 0$:

$$\mu = \frac{\sqrt[3]{9\pi^4}\hbar^2}{\sqrt[3]{2}m} n_e^{2/3} \ .$$