Lecture 24 | Paramagnetism, diamagnetism, de Haas - van Alphen effect

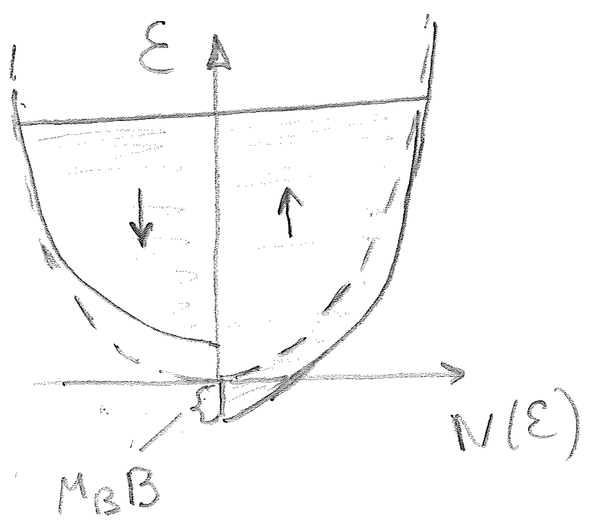
The Hamiltonian of an electron in a magnetic field is

$$\mathcal{H} = -2\mu_B \vec{S}\cdot\vec{B} + \frac{1}{2m}\left(-i\hbar\nabla - \frac{e}{c}A\right)^2$$

$$B = \mathrm{rot}\, A \quad , \quad \mu_B = \frac{e\hbar}{2mc}$$

The first term gives the Pauli spin paramagnetism discussed in the Lecture 17. The second term leads to the Landau diamagnetism.

The spin term changes the balance between spin up and spin down states



$$M = \mu_B (n_+ - n_-) =$$

$$= \frac{1}{2}\mu_B \int_{\varepsilon_F - \mu_B B}^{\varepsilon_F + \mu_B B} N(\varepsilon)\, d\varepsilon =$$

$$= \mu_B^2 B N(\varepsilon_F)$$

and the Pauli susceptibility

$$\chi_p = \mu_B^2 N(\varepsilon_F)$$

Landau levels

Let us choose $\mathbf{B} \parallel z$ and use the Landau gauge $A_y = Bx$, $A_x = A_z = 0$

The Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{2m}\left(-i\hbar\frac{\partial}{\partial y} - \frac{e}{c}\mathbf{B}x\right)^2\psi - \frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial z^2} = \mathcal{E}\psi$$

Looking for the solution in the form

$$\Psi(x,y,z) = e^{\frac{iK_z z}{\hbar}} e^{\frac{iK_y y}{\hbar}} \psi(x)$$

gives equation for $\psi(x)$

$$-\frac{\hbar^2}{2m}\psi''(x) + \frac{e^2B^2}{2mc^2}\left(x - \frac{K_y c}{eB}\right)^2\psi(x) = \left(\mathcal{E} - \frac{K_z^2}{2m}\right)\psi(x)$$

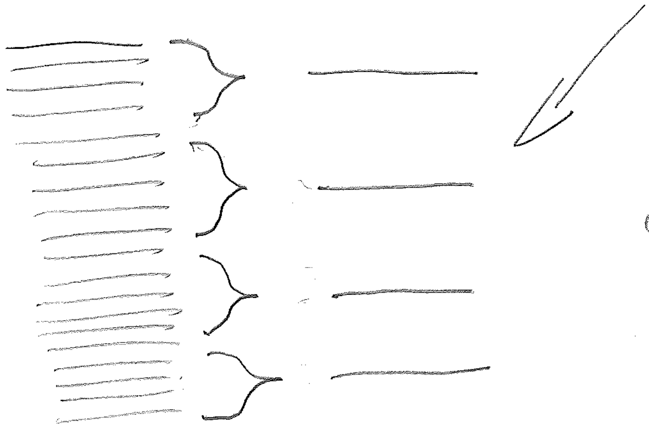
This is the Schrödinger equation for the harmonic oscillator with the energy levels

$$\mathcal{E} = \frac{K_z^2}{2m} + \hbar\omega_c\left(n + \frac{1}{2}\right)$$

with the cyclotron frequency $\omega_c = \frac{|eB|}{mc}$.

Note that $\hbar\omega_c = 2\mu_B B$.

Instead of continuous dependence on k_x and k_y we obtain discrete Landau levels



These levels are highly degenerate. Consider a cube of size L.

Then $k_y = \dfrac{2\pi\hbar n}{L}$. The center of orbit is at $\dfrac{k_y c}{eB}$ and should be between 0 and L

Thus $$0 < \frac{k_y c}{eB} < L \iff 0 < k_y < \frac{eBL}{c}$$

And $$0 < n < N_{deg} = \frac{eBL^2}{2\pi\hbar c} = \frac{\Phi}{\Phi_0},$$

where $\Phi = BL^2$ is the flux through the sample and Φ_0 is the (normal) magnetic flux quantum $\Phi_0 = \dfrac{2\pi\hbar c}{e} = \dfrac{hc}{e}$

The degeneracy of every Landau level is equal to the total number of fluxes threading the system.

The number of states is

$$\frac{eB}{c} V \frac{dk_z}{(2\pi\hbar)^2}$$

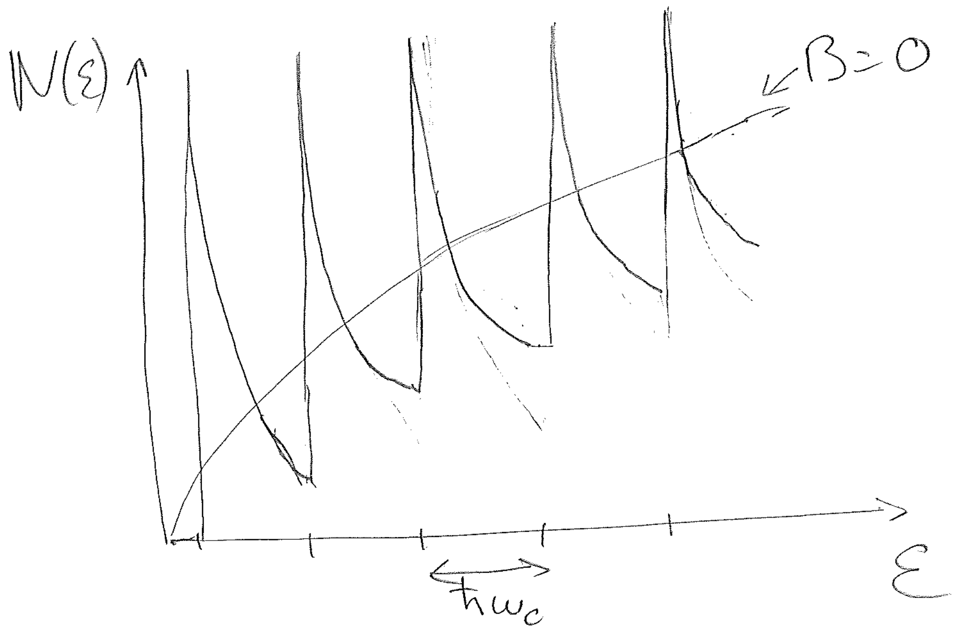
And the density of states (taking spin into account)

$$N(\mathcal{E}, n)\, d\mathcal{E} = \frac{2eB}{c\,(2\pi\hbar)^2} \frac{d|k_z|}{d\mathcal{E}}\, d\mathcal{E}$$

Using $k_z = \left[2m\left(\mathcal{E} - \hbar\omega_c\left(n+\frac{1}{2}\right)\right)\right]^{1/2}$

we obtain

$$N(\mathcal{E}, n) = \frac{(2m)^{3/2}\,\omega_c}{(2\pi\hbar)^2 \sqrt{\mathcal{E} - \hbar\omega_c\left(n+\frac{1}{2}\right)}}$$



Landau diamagnetism

The free energy is given by the sum over all states

$$F = N\mu - T\sum_i \ln\left(1+e^{(\mu-\varepsilon_i)/T}\right) =$$

$$= N\mu - \frac{4VT}{(2\pi\hbar)^2}\frac{eB}{c}\int_0^\infty d\varepsilon \sum_n \frac{d|k_z|}{d\varepsilon}\ln\left(1+e^{\frac{\mu-\varepsilon_n}{T}}\right)$$

Here additional factor 2 comes from

$$\int_{-\infty}^{\infty} dk_z = 2\int_0^\infty d|k_z| = 2\int_0^\infty d\varepsilon\,\frac{d|k_z|}{d\varepsilon}$$

Integrating by parts the field dependent term in F

$$F = -\frac{4VT}{(2\pi\hbar)^2}\frac{eB}{c}\int_0^\infty d\varepsilon \sum_n \frac{\left[2m\left(\varepsilon - \hbar\omega_c\left(n+\frac{1}{2}\right)\right)\right]^{1/2}}{\exp[(\varepsilon-\mu)/T]+1}$$

Summation over n is restricted by $\varepsilon > \hbar\omega_c\left(n+\frac{1}{2}\right)$

For $T << \mu$ we replace

$$\frac{1}{\exp\left[\frac{\varepsilon-\mu}{T}\right]+1} = f_0(\varepsilon) = \text{step function}$$

Interchanging sum over n and integral over ε

$$F = -\frac{4V}{(2\pi\hbar)^2}\frac{eB}{c}\sum_n \int_{\hbar\omega_c(n+\frac{1}{2})}^{\mu} d\varepsilon \left[2m(\varepsilon - \hbar\omega_c(n+\tfrac{1}{2}))\right]^{1/2} =$$

$$= -\frac{8}{3}\frac{V}{(2\pi\hbar)^2}\frac{eB(2m)^{1/2}}{c}\sum_n \left[\mu - \hbar\omega_c(n+\tfrac{1}{2})\right]^{3/2}$$

$$n < \frac{\mu}{\hbar\omega_c} - \frac{1}{2}$$

For small B and ω_c we can replace the sum by the integral using the Euler-Maclaurin formula

$$\sum_{n=0}^{n_0} f(n+\tfrac{1}{2}) = \int_0^{n_0+1} f(n)\,dn - \frac{1}{24}\left[f'(n_0+1) - f'(0)\right]$$

The integral part gives the field independent contribution. The field dependent part comes from $\frac{f'(0)}{24}$ which gives

$$F(H) = \frac{V}{6}\frac{eB\omega_c(2m)^{1/2}\mu^{1/2}}{(2\pi\hbar)^2 c} = \frac{Ve\mu_B B^2(2m)^{1/2}\mu^{1/2}}{3(2\pi\hbar)^2 c}$$

Using $\mu_B = \frac{e\hbar}{2mc}$, $\mu = \frac{k_F^2}{2m}$ we obtain

$$F(H) = \frac{V \mu_B^2 B^2 \, k_F m}{6 \, \pi^2 \hbar^3}$$

and susceptibility

$$\chi_{dia} = \chi_L = -\frac{1}{3} \mu_B^2 \frac{k_F m}{\pi^2 \hbar^3} = -\frac{\mu_B^2 N(\varepsilon_F)}{3}$$

For free electron gas $\chi_{dia} = -\frac{1}{3} \chi_p$ and the free electron gas will be paramagnetic. In reality there are different masses that appear in the Landau and Pauli term. Without the Fermi liquid corrections paramagnetic term has the free electron mass since it comes from the Bohr magneton $\varepsilon = 2\mu_B \vec{S} \cdot \vec{B}$. But the Landau susceptibility has the band mass then $\frac{|\chi_L|}{\chi_p} = \frac{1}{3} \left(\frac{m}{m^*} \right)^2$. For light carriers it can be bigger than unity.

Expressing density of states $N(\varepsilon_F) = \frac{k_F m}{\pi^2 \hbar^3}$ we can rewrite

$$\chi_p = \frac{e^2 k_F}{4\pi^2 mc^2} \simeq \frac{\varepsilon_F}{mc^2} \simeq 10^{-5}$$

For real metals we should also take into account magnetism of the closed atomic shells. Assuming atoms have even number of electrons. Then only orbital effect is important. For completely filled shell with $L, S = 0$ we have

$$\mathcal{H} = \frac{e^2}{2mc^2} A^2 =$$

Choosing spherically symmetric gauge

$A = \frac{[B \times r]}{2}$ we obtain

$$\mathcal{H} = \frac{e^2}{8mc^2}(x^2+y^2), \quad \delta E = \langle \mathcal{H} \rangle$$

In spherically symmetric system $\langle x^2 \rangle =$ $= \langle y^2 \rangle = \frac{1}{3}\langle r^2 \rangle$

and the change in energy is

$$\delta E = \langle \mathcal{H} \rangle = \frac{e^2 B^2}{12 m c^2} \langle r^2 \rangle$$

and the atom is diamagnetic with the Larmor (Langevin) susceptipility

$$\chi_a = -\frac{e^2}{6mc^2} \frac{N}{V} \langle r^2 \rangle$$

This atomic susceptibility may well exceed the Pauli and the Landau contribution. For partially filled shells one gets additional Van Vleck paramagnetism.

The spin susceptibility from conduction electrons can be probed by measuring the <u>Knight shift</u>. In nuclear magnetic resonance measurements one looks for the magnetic moments of nuclei $\mu_n = \gamma \hbar S_n$. Usually $\gamma\hbar \sim \mu_B \frac{m}{M_p} \sim 10^{-3} \mu_B$

This magnetic moment interacts with the external field $E = -\vec{\mu}_n \vec{B}$. This leads to typical frequency of precession (absorbtion)

$\omega \sim \gamma h \sim 100\,MHz$ at $B \sim 1T$

Conduction electrons that are usually coming from the s-orbitals which has nonzero wave function at the nucleus interact with nuclear spin via the contact interaction

$$\mathcal{H} = \frac{8}{3}\pi \mu_n \cdot \mu_e \delta(r-R)$$

Since the spins and magnetic moments of conduction electrons are polarized $\propto B$ they produce effective shift of the resonance frequency. (Knight shift). Measuring difference in resonant frequency of the same nuclei for metallic (Na) and nonmetallic (NaCl) state one can extract the Pauli susceptibility

Quantization of orbits

For a general case of band structure we can not solve the problem exactly. But since even for the highest magnetic fields $\mu_B H \ll \varepsilon_F$ we can use the semiclassical approximation. Then for $P = \vec{k} - \frac{e\vec{A}}{c}$ one can use the Bohr-Sommerfeld quantization rule

$$\oint P \cdot dr = 2\pi\hbar(n+\gamma)$$

where $|\gamma| \leq \frac{1}{2}$ is a system specific (but irrelevant for the final result). From the equations of motion

$$\left.\begin{aligned} \dot{r} &= v_k \\ \dot{k} &= -\frac{e}{c} v_k \times B \end{aligned}\right\} \quad k = -\frac{e[r \times B]}{c}$$

Then $\oint P \cdot dr = -\frac{e}{c} \int([r \times B] + A)\, dr =$

$$= -\frac{e}{c}\Phi_n + \underbrace{\frac{eB}{c}\oint r \times dr}_{\frac{2eB_\perp S_n}{c} = \frac{2e\Phi_n}{c}} = 2\pi\hbar(n+\gamma)$$

, thus

$$\Phi_n = (n+\gamma)\Phi_0$$

Consider trajectory in the momentum space A_n. Since $k = -e[r \times B]$ then

$$|dr| = \frac{\Phi_0}{B_\perp}\frac{|dk|}{2\pi\hbar}$$ and

$$S_n = \left(\frac{\Phi_0}{2\pi B_\perp}\right)^2 A_n$$

And we get quantization of the orbit area in k-space

$$A_n = (n+\gamma)\frac{2\pi e B}{c\hbar} \qquad \text{(Onsager)}$$

de Haas - van Alphen effect

As we observed the Landau levels bring oscillatory behavior of the density of states. These oscillation will lead to the oscillation of magnetization

The oscillating part of magnetization is

$$M = \chi_p \frac{\pi T}{\mu_B} \sqrt{\frac{\varepsilon_F}{\mu_B B}} \sum_{\nu=1}^{\infty} \frac{1}{\sqrt{\nu}} \frac{\sin\left(\frac{\pi}{4} - \frac{\pi \nu \varepsilon_F}{\mu_B B}\right)}{\sinh\left(\frac{\pi^2 \nu T}{\mu_B B}\right)}$$

see e.g. Ziman, Abrikosov, Landau & Lifshitz $\underline{V}$

For temperature $T < \mu_B B \simeq \hbar \omega_c$

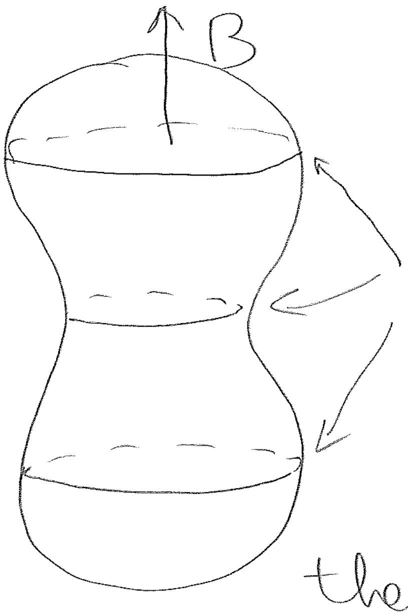
this contribution is bigger then the Pauli / Landau

The period of oscillations is given by

$$\frac{\pi \varepsilon_F}{\mu_B} \Delta \frac{1}{B} = 2\pi$$

or $$\Delta \frac{1}{B} = \frac{2\pi e}{\hbar c \, A(k_F)}$$

where $A(k_F) = \pi k_F^2$ cross section of the Fermi sphere perpendicular to the magnetic field. For a general shape of the Fermi surface the period of oscillations is given by the extremal orbits the orbits with the maximal and minimal cross-section of the Fermi surface normal to the magnetic field. This happens due to the enhancement of the density of states for extremal orbits



By varying direction of the magnetic field the shape of the Fermi surface can be found.

Another manifestation of the similar nature are oscillation of resistivity (Shubnikov - de Haas effect). To observe all these oscillations one needs the well defined Landau levels which means

$$\omega_c \tau \gg 1$$