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Diamagnetic susceptibility of free electrons

Reminder from QM:

Energy spectrum of an electron in the magnetic field

$$E_n = \frac{\hbar^2 k_z^2}{2m} + \hbar \omega_c (n + \frac{1}{2})$$

Each state is degenerate with multiplicity (# of states at the same energy) $N_1 = \frac{L_x L_y}{2\pi e h^2}$, where $l_h = \sqrt{\frac{hc}{eH}}$ is the magnetic length, and $L_x L_y$ is the sample area.

In the Landau gauge $\vec{A} = (-H_y, 0, 0)$, the wavefunction is parameterized by three quantum numbers: n , k_x , and k_z

$$\Psi_{n k_x k_z}(x, y, z) = e^{ik_x x} e^{ik_z z} \Phi_n(y - y_0),$$

where $\Phi_n(y)$ is the n -th eigenstate of the harmonic oscillator, and $y_0 = k_z l_h^2$ is the "guiding center" position.

End of reminder

Grand-canonical ensemble.

Free energy per unit volume (ignoring spin splitting)

$$F = -\frac{k_B T}{L_x L_y l_h^2} \sum_{k_z} \sum_{n=0}^{\infty} \ln \left[1 + e^{\frac{\mu - E_n(k_z)}{k_B T}} \right]$$

$$E_n(k_z) = \frac{\hbar^2 k_z^2}{2m} + \hbar \omega_c (n + \frac{1}{2})$$

Number of k_z values \equiv multiplicity = $\frac{L_x L_y}{2\pi e h^2} \cdot \frac{1}{k_z} \cdot \sum_{k_z} \int_{-\infty}^{\infty} dk_z = \pi L_z \int \frac{dk_z}{2\pi}$

$$F = -\frac{1}{\pi l_h^2} \int_{-\infty}^{\infty} \frac{dk_z}{2\pi} \sum_{n=0}^{\infty} \ln \left[1 + e^{\frac{\mu - E_n(k_z)}{k_B T}} \right].$$

Example: In a "good" metal $\frac{e\omega_c}{k_B} = 10^4 \text{ K}$. (2)

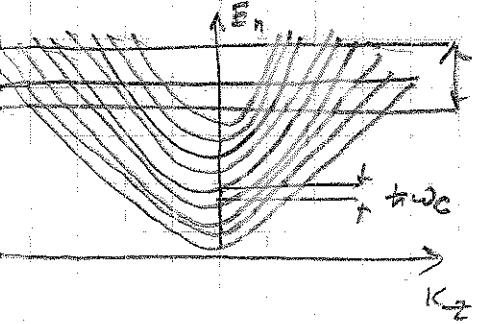
If the effective mass is equal to the bare electron mass,

$$\frac{e\omega_c}{k_B} \sim 1 \text{ K} \times B [T].$$

So, at $T = 300 \text{ K}$ and $B = 1 \text{ T}$

$$\frac{e\omega_c}{k_B T} \sim \frac{1}{300}, \quad \text{and} \quad \frac{e\omega_c}{E_F} \sim 10^{-4}.$$

In other words, there 10^4 Landau levels below the Fermi energy, and 300 out of them are thermally smeared.



In this case, we should expect that many Landau levels contribute to magnetization which, mathematically speaking,

means that the sum almost coincides with the integral. However, if we just replace the sum by integral, we will lose the effect of the magnetic field entirely. To see that, we need to recall the Euler-Maclaurin formula (EM)

$$\sum_{n=0}^{\infty} f(n) = \int dx f(x) + \frac{1}{2} f(0) - \frac{1}{12} f'(0) + \dots$$

valid if $f(\infty) = f'(\infty) \dots = 0$

Since n enters our sum in a combination $n + \frac{1}{2}$, re-write the EM formula as

$$\sum_{n=0}^{\infty} f(n + \frac{1}{2}) = \int_{-\frac{1}{2}}^{\infty} dx f(x) + \frac{1}{2} f(\frac{1}{2}) - \frac{1}{12} f'(\frac{1}{2}) =$$

$$= \int_0^x f(x) - \int_0^x f(x) + \frac{1}{2} f(\frac{x}{2}) - \frac{1}{2} f'(\frac{x}{2}) \quad (3)$$

Now, represent $f(x)$ in the interval $0 \leq x \leq \frac{1}{2}$

as $f(x) = f(\frac{1}{2}) - \frac{1}{2} f'(\frac{1}{2})(\frac{1}{2}-x)$

then $\int_0^x f(x) = \int_0^x [f(\frac{1}{2}) - (\frac{1}{2}x)f'(\frac{1}{2})] dx$
 $= \frac{1}{2} f(\frac{1}{2}) - \frac{1}{8} f'(\frac{1}{2})$

and

$$\sum_{n=0}^{\infty} f(n+\frac{1}{2}) = \int_0^{\infty} f(x) + \frac{1}{24} f''(\frac{1}{2}) = \int_0^{\infty} f(x) + \frac{1}{24} f''(0) + O(f''(0))$$

$$\sum_{n=0}^{\infty} \ln \left[1 + e^{-\frac{\mu - \frac{n^2 k_B^2}{2m} - \hbar \omega_c (n+\frac{1}{2})}{k_B T}} \right]$$

$$= \int_0^{\infty} dx \ln \left(1 + e^{-\frac{\mu - \frac{n^2 k_B^2}{2m} - \hbar \omega_c x}{k_B T}} \right) +$$

$$- \frac{1}{24} \frac{\hbar \omega_c}{k_B T} \frac{e^{\frac{\mu - \frac{n^2 k_B^2}{2m}}{k_B T}}}{1 + e^{\frac{\mu - \frac{n^2 k_B^2}{2m}}{k_B T}}}$$

In the integral term, do $y = \frac{\hbar \omega_c}{k_B T} x \Rightarrow \int_0^{\infty} dx = \frac{k_B T}{\hbar \omega_c} dy$

The field dependence of $(\hbar \omega_c)$ cancels with $\frac{1}{k_B^2 T} \Rightarrow$

$$\frac{\hbar \omega_c}{\hbar \omega_c k_B^2 T} = \left(\frac{\hbar \omega_B}{mc} \right)^{-1} \frac{eB}{mc}. \text{ Therefore, the integral}$$

term indeed gives a B -independent constant \Rightarrow no contribution to magnetization.

(4)

Dropping the integral term,

$$F(B) = \frac{1}{24} \frac{1}{\pi l_B^2} \underbrace{\int_{-\infty}^{\infty} \frac{dk_z}{2\pi}}_{\propto B^2} \frac{1}{(\frac{k^2 k_F^2 - \mu}{2m}) K_B T + 1}$$

Fermi function $n(k_z)$
Because $K_B T \ll E_F \Rightarrow \mu \rightarrow E_F$
 $\propto n(k_z)$

$$-k_F \qquad \qquad k_F = \frac{\sqrt{2m E_F}}{\hbar}$$

$$F(B) = \frac{1}{24} \frac{1}{\pi l_B^2} \hbar \omega_c \cdot \frac{2k_F}{2\pi} =$$

$$= \frac{1}{24} \frac{1}{\pi} \frac{eB}{mc} \frac{2eB}{mc} \frac{2k_F}{2\pi}$$

$$M = - \frac{\partial F}{\partial B} = - \frac{1}{12\pi^2} \frac{e^2}{c^2 m} k_F B \Rightarrow$$

\Rightarrow

$$M = - \chi_d B$$

$$\chi_d = \frac{1}{12\pi^2} \frac{e^2}{c^2 m} k_F$$

Recall : Bohr magneton $\mu_B = \frac{e\hbar}{2mc}$

Density of states of 3D electron gas

$$g(E_F) = \frac{m k_F}{\hbar^2 \pi^2}$$

$$\chi_d = \frac{m k_F}{\hbar^2 \pi^2} \cdot \frac{1}{12} \frac{\hbar^2 e^2}{m^2 c^2} = g(E_F) \frac{1}{3} \mu_B^2$$

Recall that $\chi_p = g(E_F) \mu_B^2$.

$$\text{thus: } \mu = \chi_p B - \chi_d B = \frac{2}{3} \chi_p B$$