Landau Diamagnetism — Landau levels

Preceding discussion ignored the orbital motion of electrons in applied magnetic field. Now we consider this.

In uniform magnetic field $\vec{B} = \vec{\nabla} \times \vec{A}$ single electron Hamiltonian becomes

$$\mathcal{H} = \frac{1}{2m}\left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 \quad \text{for charge } q$$

$$= \frac{1}{2m}\left(\vec{p} + \frac{e}{c}\vec{A}\right)^2 \quad \text{for electron with } q = -e$$

$$= \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla} + \frac{e}{c}\vec{A}\right)^2 \quad \text{as QM operator}$$

We will choose $\vec{A} = -yB\hat{x}$ as vector potential

$$\mathcal{H} = \frac{1}{2m}\left[-\hbar^2\frac{\partial^2}{\partial y^2} - \hbar^2\frac{\partial^2}{\partial z^2} + \left(\frac{\hbar}{i}\frac{\partial}{\partial x} - \frac{e}{c}By\right)^2\right]$$

try solution of the form $\psi(x,y,z) = e^{ik_x x}\, e^{ik_z z}\, \phi(y)$

Substitute into $\mathcal{H}\psi = \epsilon\psi$ to get equ for $\phi(y)$

$$\frac{1}{2m}\left[-\hbar^2\frac{\partial^2}{\partial y^2} + \hbar^2 k_z^2 + \left(\hbar k_x - \frac{e}{c}By\right)^2\right]\phi(y) = \epsilon\,\phi(y)$$

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2m}\left(\hbar k_x - \frac{e}{c}By\right)^2\right]\phi(y) = \left(\epsilon - \frac{\hbar^2 k_z^2}{2m}\right)\phi(y)$$

Let $y_0 \equiv \frac{\hbar k_x c}{eB}$ then

$$\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2m}\left(\frac{eB}{c}\right)^2 (y-y_0)^2\right)\phi = \left(\epsilon - \frac{\hbar^2 k_z^2}{2m}\right)\phi$$

Define $\omega_c = \frac{eB}{mc}$ cyclotron frequency

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial y^2} + \frac{1}{2} m\omega_c^2 (y-y_0)^2\right]\phi(y) = \left(\epsilon - \frac{\hbar^2 k_z^2}{2m}\right)\phi(y)$$

harmonic oscillator of freq ω_c, centered at y_0

$\Rightarrow$ eigenvalues $\epsilon_{n,k_z} = \frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c(n+1/2)$ $\quad n = 0, 1, \ldots$

eigenvalues are indexed by k_z - momentum $\parallel \vec{B}$

n - Landau level for orbital motion in xy plane.

Landau levels are degenerate corresponding to the different possible choices of y_0. We have

$0 < y_0 < L_y$ where L_x, L_y, L_z are system lengths

Now $y_0 = \frac{\hbar k_x c}{eB}$ and $k_x = \frac{2\pi m_x}{L_x}$, $m_x = 0, 1, \ldots$

$\Rightarrow \Delta k_x = \frac{2\pi}{L_x} \Rightarrow \Delta y_0 = \frac{2\pi\hbar c}{eBL_x}$

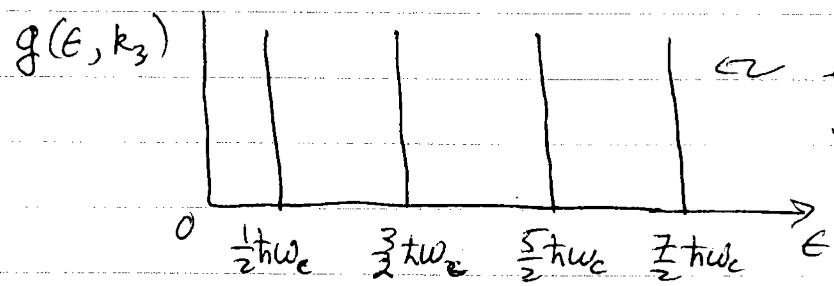
$\Rightarrow$ number of allowed values of y_0 is $L_y / \Delta y_0$

$$\frac{L_y}{\Delta y_0} = \frac{L_y L_x \, eB}{2\pi \hbar c} = \frac{\Phi}{\Phi_0}$$

Include electron spin gives extra factor of $\underline{\underline{2}}$

where $\Phi = L_x L_y B$ is magnetic flux ~~pentor~~ penetrating the system, and $\Phi_0 = \dfrac{2\pi\hbar c}{e} = \dfrac{hc}{e}$ is the "<u>flux quantum</u>"

For fixed k_z, the density of states <u>per unit area</u> looks like



$\leftarrow$ evenly spaced δ-functions each of weight $\dfrac{2\Phi}{L_x L_y \Phi_0} = \underset{\uparrow}{\dfrac{2B}{\Phi_0}} \equiv g$

electron spin degeneracy

We should use this Landau level energy spectrum when computing the partition function.

$$\ln \mathcal{L} = \sum_i \ln\left(1 + z e^{-\beta\epsilon_i}\right) = L_x L_y \, g \sum_{k_z} \sum_n \ln\left(1 + z e^{-\beta\epsilon(n, k_z)}\right)$$

$\uparrow$ single particle states i

$g = \dfrac{2B}{\Phi_0}$ degeneracy per area

for large L_z can approx

$$\sum_{k_z} \rightarrow \frac{L_z}{2\pi} \int_{-\infty}^{\infty} dk_z$$

$$\ln \mathcal{Z} = \frac{L_x L_y L_z}{2\pi} g \sum_{n=0}^{\infty} \int dk_z \ln \left[1 + z e^{-\beta\left(\frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c (n+1/2)\right)} \right]$$

Once we find $\ln \mathcal{Z}$, we can compute M, the total dipole moment, as follows:

Total energy in magnetic field is $E(B) = E(B=0) - MB$

$$\Rightarrow \quad M = -\frac{\partial E}{\partial B} = -\left\langle \frac{\partial \mathcal{H}}{\partial B} \right\rangle \qquad \mathcal{H} \text{ is Hamiltonian}$$

Now $$-\left\langle \frac{\partial \mathcal{H}}{\partial B} \right\rangle = \frac{-\sum_\alpha e^{-\beta(\mathcal{H}(\alpha) - \mu N_\alpha)} \frac{\partial \mathcal{H}}{\partial B}}{\sum_\alpha e^{-\beta(\mathcal{H}(\alpha) - \mu N_\alpha)}}$$

all many particle states α

$\mathcal{H}(\alpha)$ is total energy in state α

$$= \frac{\frac{1}{\beta} \frac{\partial}{\partial B} \sum_\alpha e^{-\beta(\mathcal{H}(\alpha) - \mu N_\alpha)}}{\sum_\alpha e^{-\beta(\mathcal{H}(\alpha) - \mu N_\alpha)}}$$

$$= \frac{1}{\beta} \frac{\partial}{\partial B} \ln \sum_\alpha e^{-\beta(\mathcal{H}(\alpha) - \mu N_\alpha)}$$

$$\boxed{M = \frac{1}{\beta} \frac{\partial}{\partial B} \ln \mathcal{Z}}$$

or using grand potential $\Sigma = -k_B T \ln \mathcal{Z}$

$$\Rightarrow \quad M = -\frac{\partial \Sigma}{\partial B}$$

(Landau + Lifshitz Part I § 59)

$V = L_x L_y L_z$

$$\ln \mathcal{Z} = \frac{V}{2\pi} g \sum_{n=0}^{\infty} \int_{-\infty}^{\infty} dk_z \ln \left[1 + z e^{-\beta\left(\frac{\hbar^2 k_z^2}{2m} + \hbar\omega_c (n+1/2)\right)} \right]$$

Define function $h(x) = \int_{-\infty}^{\infty} dk_z \ln \left[1 + e^{-\beta\left(\frac{\hbar^2 k_z^2}{2m} - x\right)} \right]$

Then using $z = e^{-\beta\mu}$

$$\ln \mathcal{Z} = \frac{V}{2\pi} g \sum_{n=0}^{\infty} h\left(\mu - \hbar\omega_c (n+1/2)\right)$$

Consider the limit of very weak magnetic field $\hbar\omega_c \ll k_B T$. In this case many Landau levels occupied. We might think to replace $\sum_n$ by $\int dn$, but it turns out that this would remove all dependence on B. To do better we need to use Euler summation formula (Pathria 8-2 Eq (44))

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

Apply to the above

$$\ln \mathcal{Z} = \frac{V}{2\pi} g \int_0^{\infty} dx\, h(\mu - \hbar\omega_c x) + \frac{Vg}{2\pi}\frac{1}{24}(-\hbar\omega_c)\frac{dh}{d\mu}(\mu)$$

$y = \mu - \hbar\omega_c x$

$$= \frac{V}{2\pi}\frac{2B}{\Phi_0}\left[\int_{-\infty}^{\mu} dy\, h(y)\left(\frac{1}{\hbar\omega_c}\right) - \frac{\hbar\omega_c}{24}\frac{dh}{d\mu}(\mu)\right]$$

use $\Phi_0 = \frac{hc}{e}$ $\omega_c = \frac{eB}{mc}$

$$\ln \mathcal{Z} = \frac{V}{2\pi} \frac{2B}{\Phi_0} \frac{1}{\hbar\omega_c} \left[\int_{-\infty}^{\mu} dy\, h(y) - \frac{(\hbar\omega_c)^2}{24} \frac{dh(\mu)}{d\mu} \right]$$

$$= \frac{V}{2\pi} \frac{2Be}{hc} \frac{mc}{\hbar eB} \left[\int_{-\infty}^{\mu} dy\, h(y) - \frac{(\hbar\omega_c)^2}{24} \frac{dh(\mu)}{d\mu} \right]$$

$$= \frac{Vm}{h^2} \left[\int_{-\infty}^{\mu} dy\, h(y) - \frac{(\hbar\omega_c)^2}{24} \frac{dh(\mu)}{d\mu} \right]$$

grand potential

$$\Sigma(T,V,\mu,B) = -k_B T \ln \mathcal{Z} = \frac{-k_B T V m}{h^2} \left[\int_{-\infty}^{\mu} dy\, h(y) - \frac{(\hbar\omega_c)^2}{24} \frac{dh(\mu)}{d\mu} \right]$$

indep of B

1st term gives

$$\Sigma(T,V,\mu,0) = \frac{-k_B T V m}{h^2} \int_{-\infty}^{\mu} dy\, h(y)$$

Now note

$$-N = \left(\frac{\partial \Sigma}{\partial \mu}\right)_{T,V,B=0} = \frac{-k_B T V m}{h^2} h(y)$$

$$-\left(\frac{\partial N}{\partial \mu}\right)_{T,V} = \left(\frac{\partial^2 \Sigma}{\partial \mu^2}\right)_{T,V} = \frac{-k_B T V m}{h^2} \frac{dh(\mu)}{d\mu}$$

Combine to get

$$\Sigma(T,V,\mu,B) = \Sigma(T,V,\mu,0) + \frac{(\hbar\omega_c)^2}{24} \left(\frac{\partial N}{\partial \mu}\right)_{T,V}$$

$$\Sigma(T,V,\mu,B) = \Sigma(T,V,\mu,0) + \left(\frac{\hbar e B}{mc}\right)^2 \frac{1}{24}\left(\frac{\partial N}{\partial \mu}\right)_{T,V}$$

$$\mu_B = \frac{e\hbar}{2mc}$$

$$\Sigma(T,V,\mu,B) = \Sigma(T,V,\mu,0) + \frac{1}{6}\mu_B^2 B^2 \left(\frac{\partial N}{\partial \mu}\right|_{T,V}$$

Now $\dfrac{\partial N}{\partial \mu} = \dfrac{\partial}{\partial \mu}\left\{ V\int d\epsilon\, g(\epsilon) f(\epsilon,\mu) \right\}$ $\qquad f(\epsilon,\mu) = \dfrac{1}{e^{\beta(\epsilon-\mu)}+1}$

$$= V\int d\epsilon\, g(\epsilon)\,\frac{\partial f}{\partial \mu}$$

$$= V\int d\epsilon\, g(\epsilon)\left(-\frac{\partial f}{\partial \epsilon}\right)$$

$\approx g(\epsilon_F)$ to lowest order in Sommerfeld expansion
ie to $o\left(\frac{k_B T}{\epsilon_F}\right)$

$$\Sigma(T,V,\mu,B) = \Sigma(T,V,\mu,0) + \frac{V}{6}\mu_B^2\, g(\epsilon_F)\, B^2$$

magnetization

$$M = -\frac{\partial \Sigma}{\partial B} = -\frac{V}{3}\mu_B^2\, g(\epsilon_F)\, B$$

magnetic susceptibility

$$\chi_L = \frac{\partial (M/V)}{\partial B} = -\frac{1}{3}\mu_B^2\, g(\epsilon_F)$$ $< 0 \Rightarrow$ <u>diamagnetic</u>

Compare $\chi_P = \mu_B^2\, g(\epsilon_F)$

$$\chi_L = -\frac{1}{3}\chi_P$$

Total magnetic susceptibility for a free electron gas is

$$\chi_{tot} = \chi_p + \chi_L = \frac{2}{3}\chi_p$$

For electrons in metal (as opposed to free electrons)

$\chi_p = \mu_B^2 g(\epsilon_F)$ comes from interaction with electron spin

$\mu_B = \frac{\hbar e}{2mc}$ m is rest mass of electron

χ_L comes from orbital motion of electrons near fermi energy.
for such electrons the energy spectrum is
$\epsilon(k) \approx \frac{\hbar^2 k^2}{2m^*}$ where m^* is the effective mass of motion in the periodic potential of the ions (take P521!)

The μ_B in χ_L should therefore really be $\mu_B^* = \frac{\hbar e}{2m^* c}$

Then $\chi_L = -\frac{1}{3}\left(\frac{m}{m^*}\right)\chi_p$

We derived χ_p and χ_L by separately considering effects of spin and orbital motion. One could get the same results by combining the derivations into a single one that includes both effects

Note that $\chi_L = -\frac{1}{3}\mu_B^2\, g(\epsilon_F)$ $\qquad g(\epsilon_F) = \frac{3}{2}\frac{n}{\epsilon_F}$

$$= -\frac{1}{3}\left(\frac{\hbar e}{2mc}\right)^2 \frac{3}{2}\frac{n}{\epsilon_F}$$

Note: Landau diamagnetism is a purely quantum mechanical effect - does not exist classically

Classical N particle partition function

$$Q_N = \frac{Q_1^N}{N!}$$

where

$$Q_1 = \int \frac{d^3r \int d^3p}{h^3} \, e^{-\beta H}$$

$$= \int \frac{d^3r \int d^3p}{h^3} \, e^{-\beta \left[\frac{1}{2m} \left(\vec{p} + \frac{e}{c} \vec{A}(\vec{r}) \right)^2 \right]}$$

just substitute $\vec{p}\,' = \vec{p} + \frac{e}{c}\vec{A}(\vec{r})$ to get

$$Q_1 = \int \frac{d^3r \int d^3p'}{h^3} \, e^{-\beta \frac{p'^2}{2m}}$$

same as partition function with $B = 0$!

So Q_1 is independent of B

$$\Rightarrow \quad \chi = -\frac{1}{V} \frac{\partial^2 \Sigma}{\partial B^2} = 0$$

$$M = -\frac{\partial \Sigma}{\partial B} = 0$$

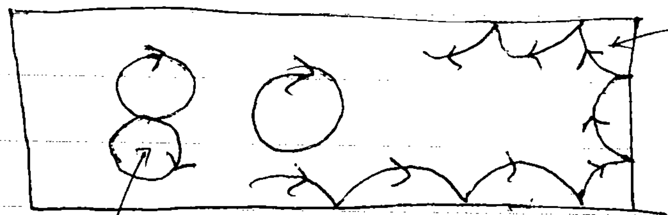
$\Big\}$ orbital motion gives <u>no</u> magnetization <u>classically</u>

Bohr - Van Leeuwen theorem

Amusing aside:

The classical result $\chi = 0$ may seem confusing if one considers that the classical electron in a uniform $\vec{B}$ undergoes a circular motion $\Rightarrow$ electron is effectively a current loop $\Rightarrow$ should have an orbital magnetic moment from classical $\vec{r} \times \vec{j}$ (where $\vec{j}$ is electric current). Each electron goes around in a circular orbit and so the contributions from all electrons should add and give $M \neq 0$!

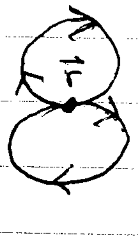
Arguement fails when one considers electrons traveling close to the finite boundaries of the system.



Counter clockwise i.e. large orbits from electrons hitting the surface "skipping states"

Clockwise closed orbits in interior

Moments from the interior orbits and moments from skipping states exactly cancel! Proof: For any fixed $|\vec{p}|$ at any point $\vec{r}$, we get contributions to current from electrons going in opposite directions. These always cancel,



True even near boundary.
When we average over all electron orbits the resulting average current at any point $\vec{r}$ in the system vanishes!
$\Rightarrow$ no magnetic moment.

Sometimes it is important to consider in detail what happens at the boundaries!