Landsau Diamagnetism

Landsau levels

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

In uniform magnetic field $B = \mathbf{\nabla} \times \mathbf{A}$, Hamiltonian becomes:

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

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

$$
= \frac{1}{2m} \left( \frac{\hbar}{c} \mathbf{\hat{A}} + \frac{e}{c} \mathbf{A} \right)^2 \quad \text{as CM operator}
$$

We will choose $\mathbf{A} = -y \mathbf{B} \mathbf{\hat{x}}$ as vector potential.

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

Try solution of the form $\psi(x, y, z) = e^{i k x} e^{i k_z z} \phi(y)$.

Substitute into $\mathcal{H} \psi = E \psi$ to get equation for $\phi(y)$.

$$
\frac{1}{2m} \left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{\hbar^2}{2m} \frac{k_y^2}{k^2} + \left( \frac{\hbar}{c} \frac{\partial}{\partial x} - \frac{e}{c} By \right)^2 \right] \phi(y) = E \phi(y)
$$

$$
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{i}{2m} \left( \frac{\hbar}{c} \frac{\partial}{\partial x} - \frac{e}{c} By \right)^2 \right] \phi(y) = (E - \frac{\hbar^2 k_y^2}{2m}) \phi(y)
$$
Let \( y_0 = \frac{\hbar k_x C}{eB} \). Then

\[
\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{1}{2m} \left( \frac{eB}{C} \right)^2 (y - y_0)^2 \right) \phi = \left( \epsilon - \frac{\hbar^2 k_x^2}{2m} \right) \phi
\]

Define \( W_C = \frac{eB}{mc} \) cyclotron frequency

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

This harmonic oscillator of freq. \( W_C \), centered at \( y_0 \)

\( \Rightarrow \) eigenvalues \( \epsilon = \frac{\hbar^2 k_x^2}{2m} + \hbar W_C(n + \frac{1}{2}) \quad n = 0, 1, \ldots \)

Eigenvalues are indexed by \( k_x \) — momentum \( \parallel \mathbf{B} \)

\( m \) — 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

\[
N_{\phi} = \frac{\hbar k_x C}{eB} \quad \text{and} \quad k_x = \frac{2\pi m_x}{L_x}, \quad m_x = 0, 1, 2, \ldots
\]

\( \Rightarrow \Delta k_x = \frac{2\pi}{L_x} \Rightarrow \Delta y_0 = \frac{2\pi \hbar C}{eB L_x} \)
\[
\frac{L_y}{\Delta y_0} = \frac{L_y L_x e B}{2 \pi \hbar c} = \frac{\Phi}{\Phi_0} \quad \text{(Include electron spin gives extra factor } \frac{1}{2} \text{)}
\]

where \( \Phi = L_x L_y B \) is magnetic flux penetrate the system, and \( \Phi_0 = \frac{2 \pi \hbar c}{e} = \frac{hc}{e} \) is the "flux quantum".

For fixed \( k_3 \), the density of states per unit area looks like:

\[
\mathcal{g}(\epsilon, k_3) \quad \text{\# evenly spaced } \delta \text{-functions} \quad \text{each of weight } \frac{2\Phi}{L_x L_y \Phi_0} = \frac{2B}{\Phi_0}
\]

\[
\text{electron spin degeneracy}
\]

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

\[
\ln \mathcal{Z} = \sum_{k_3} \mathcal{g} \ln \left(1 + 2e^{-\beta E_c}ight) = \frac{1}{2} \mathcal{g} \sum_{k_3} \sum_n \ln \left(1 + 2e^{-\beta E(n, k_3)}\right)
\]

\[
\mathcal{g} = \frac{2B}{\Phi_0} \quad \text{degeneracy per area}
\]

for large \( L_3 \) can approx

\[
\sum_{k_3} \rightarrow \frac{L_3}{2\pi} \int_{-\infty}^{\infty} dk_3
\]
\[ \ln \mathcal{Z} = \frac{4 \pi l \hbar^2}{2 a^2} \sum_{n=0}^{\infty} \int d\mathbf{r} \frac{1}{2} \left[ 1 + \text{e}^{-\beta \left( \frac{n^2}{2m} + \hbar \omega_0 (n + \frac{3}{2}) \right)} \right] \]

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

\[
\text{Total energy in magnetic field} \quad E(B) = E(B=0) - MB
\]

\[ \Rightarrow \quad M = - \frac{\partial E}{\partial B} = - \left\langle \frac{\partial H}{\partial B} \right\rangle \quad \# \text{ Hamiltonian} \]

Now:

\[ \left\langle \frac{\partial H}{\partial B} \right\rangle = - \sum_{\alpha} \frac{e^{-\beta (H(\alpha) - \mu N^a)}}{\sum_{\alpha} e^{-\beta (H(\alpha) - \mu N^a)}} \frac{\partial H}{\partial B} \]

\[ = \frac{1}{\beta} \frac{\partial}{\partial B} \sum_{\alpha} e^{-\beta (H(\alpha) - \mu N^a)} \]

\[ = \frac{1}{\beta} \frac{\partial}{\partial B} \ln \sum_{\alpha} e^{-\beta (H(\alpha) - \mu N^a)} \]

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

or using grand potential

\[ \Sigma = -k_B T \ln \mathcal{Z} \]

\[ \Rightarrow \quad M = - \frac{\partial \Sigma}{\partial B} \]
\[ V = L \times L \times L \]

\[
\ln L = \frac{V}{2\pi} g \sum_{n = 0}^{\infty} \int_{-\infty}^{\infty} dk z^{2} \ln \left[ 1 + z e^{-\beta \left( \frac{\hbar k^{2} z^{2}}{2m} + \frac{\hbar \omega_{c} (n + \frac{1}{2})}{\gamma} \right)} \right]
\]

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

Then

\[
\ln L = \frac{V}{2\pi} g \sum_{n = 0}^{\infty} h \left( \mu - \frac{\hbar \omega_{c} (n + \frac{1}{2})}{\gamma} \right)
\]

Consider the limit of very weak magnetic field \( \hbar \omega_{c} \ll k_B T \)

In this case, many Landau levels are occupied. We might think to replace \( \sum_{n} \) by \( \int dm \), but it turns out that this would remove all dependence on \( B \). To do better, we need to use Euler summation formula (Paffrin 8-2 eq (44))

\[
\sum_{n=0}^{\infty} f(n+\frac{1}{2}) \approx \int f(y)dy + \frac{1}{24} f'(0)
\]

Apply to the above

\[
\ln L = \frac{V}{2\pi} g \int dx \ h(\mu - \frac{\hbar \omega_{c} x}{\gamma}) + \frac{Ve}{2\pi} \frac{1}{24} (-\frac{1}{\hbar \omega_{c}}) \frac{d K}{d \mu}
\]

\[
= \frac{V}{2\pi} \frac{2B}{\gamma \theta_{0}} \left[ \int_{-\infty}^{\infty} dy \ f(y) \left( \frac{1}{\hbar \omega_{c}} \right) - \frac{\gamma \omega_{c}}{24} \frac{d K}{d \mu} \right]
\]

Use \( \theta_{0} = \frac{h \omega_{c}}{e} \)

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

\[ = \frac{V}{2\pi} \frac{z B e}{\hbar c} \frac{mc}{\hbar e B} \left[ \int_{-\infty}^{\infty} dy \, h(y) - \frac{(\hbar \omega_c)^2}{24} \frac{d h(\mu)}{d\mu} \right] \]

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

Grand potential

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

1st term gives

\[ \mathcal{Z}(T, V, \mu, 0) = -k_B T V m \int_{-\infty}^{\infty} dy \, h(y) \]

Now note

\[ -N = \left( \frac{\partial \Sigma}{\partial \mu} \right)_{T, V, B=0} = -k_B T V m \ f(y) \]

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

Combine to get

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

\[ M_B = \frac{e \hbar}{2mc} \]

\[ \Sigma (T, V, M, B) = \Sigma (T, V, M, 0) + \frac{1}{6} M_B^2 B^2 \left( \frac{\partial^2 N}{\partial M} \right)_{T, V} \]

\[ \text{Nous:} \quad \frac{\partial N}{\partial M} = \frac{2}{\pi} \int \frac{d\varepsilon}{\varepsilon} g(\varepsilon) f(\varepsilon, \mu) \left( \frac{\partial f}{\partial \mu} \right) \]

\[ = V \int d\varepsilon \frac{d\varepsilon}{\varepsilon} \frac{\partial f}{\partial \mu} \]

\[ = V \int d\varepsilon g(\varepsilon) \left( -\frac{\partial f}{\partial \varepsilon} \right) \]

\[ \approx g(\varepsilon_F) \quad \text{to lowest order in Sommerfeld expansion} \]

\[ \text{i.e. to } o \left( \frac{k_B T}{\varepsilon_F} \right) \]

\[ \Sigma (T, V, M, B) = \Sigma (T, V, M, 0) + \frac{V}{6} M_B^2 g(\varepsilon_F) B^2 \]

\[ \text{magnetization} \quad M = -\frac{\partial \Sigma}{\partial B} = -\frac{V}{6} M_B^2 g(\varepsilon_F) B \]

\[ \text{magnetic susceptibility} \]

\[ \chi_L = \frac{\partial (M/V)}{\partial B} = -\frac{1}{3} M_B^2 g(\varepsilon_F) \quad \text{\( < 0 \) \Rightarrow diamagnetic} \]

\[ \chi_L = -\frac{1}{3} \chi_p \]

\[ \text{Compare } \chi_p = M_B g(\varepsilon_F) \]
Total magnetic susceptibility for a free electron gas is:

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

For electrons in metal (as opposed to free electrons)

$$\chi_p = M_B^2 g(\varepsilon_F) \quad \text{(comes from interaction with electron spin)}$$

$$M_B = \frac{\hbar c}{2m} \quad \text{m is rest mass of electron}$$

\(\chi_L\) comes from orbital motion of electrons near Fermi energy.

for such electrons the energy spectrum is

$$\varepsilon(k) \approx \frac{\hbar^2 k^2}{2m^*} \quad \text{where } m^* \text{ is the effective mass of motion in the periodic potential of the ions (take } P521! )$$

The \(M_B\) in \(\chi_L\) should therefore really be \(M_B^* = \frac{\hbar c}{2m^*}$$

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

We derived \(\chi_p\) and \(\chi_L\) 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

$$\chi_L = -\frac{1}{3} M_B^2 g(\varepsilon_F) \quad g(\varepsilon_F) = \frac{3}{2} \frac{m}{\varepsilon_F}$$

$$= -\frac{1}{3} \left( \frac{\hbar c}{2mc} \right)^2 \frac{3}{2} \frac{m}{\varepsilon_F}$$
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

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

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

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

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

same as partition function with $B=0$!

So $Q_1$ is independent of $B$

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

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

Orbital motion gives no magnetization classically.

Bohr-Van Leeuwen Theorem
Amusing aside:

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

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

\[
\begin{array}{c}
\text{Clockwise closed}\hfill \\
\text{orbits in interior}\hfill \\
\end{array}
\]

\[
\begin{array}{c}
\text{Counter clockwise i.e.}\hfill \\
\text{large orbits from}\hfill \\
\text{electrons hitting the surface}\hfill \\
\text{"skipping states"}\hfill \\
\end{array}
\]

Moments from the interior orbits and moments from skipping states exactly cancel! Proof: For any fixed $\theta$ at any point $\mathbf{r}$, 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 $\mathbf{r}$ in the system vanishes! $\Rightarrow$ no magnetic moment.

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