Pauli paramagnetism of electron gas

\[ \vec{S} = \frac{1}{2} \vec{\sigma} \]

An electron has intrinsic spin \( \vec{S} \) with intrinsic magnetic moment \( \vec{\mu} = -\mu_B \vec{S} \), where \( \mu_B = \frac{e \hbar}{2mc} \) is Bohr magneton.

In an external magnetic field \( \vec{B} \), there is an interaction energy \( -\vec{\mu} \cdot \vec{B} = \mu_B \sigma \vec{B} \), where \( \sigma = \pm 1 \) for spins parallel and antiparallel to \( \vec{B} \). The energy spectra for up and down electron spins becomes

\[ E_{\pm}(\vec{k}) = E(\vec{k}) \pm \mu_B B \]

where \( E(\vec{k}) \) is spectrum at \( \vec{B} = 0 \).

Since \( \uparrow \) and \( \downarrow \) electrons now have different energy spectra, we should treat them as two different populations of particles. They will be in equilibrium when their chemical potentials are equal, i.e., \( \mu_{\uparrow} = \mu_{\downarrow} \).

This will induce a net magnetization in the system.

To see this, consider free electrons at \( T = 0 \).
When $B \neq 0$, ground state occupations look as shown on the left. Equal numbers of $\uparrow$ and $\downarrow$ electrons $m_{\uparrow} = m_{\downarrow}$.

When $B$ is turned on, if there were no redistribution of electron spins, the situation would look like

Clearly the system can lower its energy by transferring $\uparrow$ electrons to $\downarrow$ electrons.

At equilibrium the system will look like

again the two populations have the same max energy $E_F$. But there are now more $\downarrow$ electrons than $\uparrow$ electrons.

Magnetization $\frac{M}{V} = -\mu_B (m_{\uparrow} - m_{\downarrow}) > 0$

$\frac{M}{V}$ is parallel to $B \Rightarrow$ paramagnetic effect
Let \( g(\epsilon) \) be the density of states when \( B = 0 \).

When \( B > 0 \), the density of states for \( \uparrow \) and \( \downarrow \) electrons are

\[
\begin{align*}
g_\uparrow(\epsilon + \mu(B)) &= \frac{1}{2} g(\epsilon) \\
g_\downarrow(\epsilon - \mu(B)) &= \frac{1}{2} g(\epsilon)
\end{align*}
\]

The density of \( \uparrow \) and \( \downarrow \) electrons is then

\[
m_\pm = \int_{-\infty}^{\infty} d\epsilon \; g_\pm(\epsilon) f(\epsilon, \mu(B))
\]

where \( f(\epsilon, \mu(B)) = \frac{1}{\epsilon - \mu(B)^{\uparrow} + 1} \).

\( \mu(B) \) is the chemical potential — it might depend on \( B \).

\( \mu(B) \) is the same for \( \uparrow \) and \( \downarrow \).

We will consider only the case that \( \mu(B) \ll \mu(B) \approx E_F \).

\( \mu(B) \ll E_F \) means spin interaction is small compared to \( E_F \).
First we will show:

\[ M(B) \approx M(B=0) \left[ 1 + O\left( \frac{\mu B}{E_F} \right)^2 \right] \]

Consider total density of electrons

\[
m = n_+ + n_+ = \int_{-\infty}^{\infty} d\epsilon \ f(\epsilon, \mu(B)) \left[ g_+ (\epsilon) + g_- (\epsilon) \right] \\
= \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon \ f(\epsilon, \mu(B)) \left[ g(\epsilon - \mu B) + g(\epsilon + \mu B) \right] \\
= \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon \ g(\epsilon) \left[ f(\epsilon + \mu B, \mu(B)) + f(\epsilon - \mu B, \mu(B)) \right] \\
= \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon \ g(\epsilon) \left[ f(\epsilon, \mu - \mu B) + f(\epsilon, \mu + \mu B) \right]
\]

Expand for small \( \frac{\mu B}{\mu} \ll 1 \)

\[
m = \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon \ g(\epsilon) \left[ f(\epsilon, \mu) - d f \mu B - f(\epsilon, \mu) + d f \mu B \right] \\
= \int_{-\infty}^{\infty} d\epsilon \ g(\epsilon) \ f(\epsilon, \mu)
\]

Now since \( n \) does not change when one applies \( B > 0 \), and we have:

\[
m = \int_{-\infty}^{\infty} d\epsilon \ g(\epsilon) \ f(\epsilon, \mu(B=0)) \quad \text{when} \quad B = 0,
\]

\[
\Rightarrow \mu(B) = \mu(B=0). \quad \text{Corrections come from next order in the expansion } \frac{d f}{d \mu} \left( \frac{\mu B}{\mu} \right)^2
\]

And at order \( \left( \frac{\mu B}{\mu} \right)^2 \)
Now we compute

2. Magnetization

\[ M = -\mu_B \left( m_+ - m_- \right) = \mu_B \left( m_+ - m_- \right) \]

\[ M = \mu_B \int_{-\infty}^{\infty} d\epsilon f(\epsilon, \mu) \left[ f_+ - f_\pm \right] \]

\[ = \mu_B \int_{-\infty}^{\infty} d\epsilon f(\epsilon, \mu) \left[ \frac{1}{2} g(\epsilon + \mu_B) - \frac{1}{2} g(\epsilon - \mu_B) \right] \]

\[ = \frac{1}{2} \mu_B \int_{-\infty}^{\infty} g(\epsilon) \left[ f(\epsilon, \mu + \mu_B) - f(\epsilon, \mu - \mu_B) \right] \text{ as before} \]

\[ \exp \mu B = f(\epsilon, \mu \pm \mu B) = f(\epsilon, \mu) \pm \frac{df}{d\mu} \mu B \]

\[ M = \frac{1}{2} \mu_B \int_{-\infty}^{\infty} d\epsilon g(\epsilon) \left[ 2 \frac{df}{d\mu} \mu B \right] \]

\[ = \mu_B^2 B \int_{-\infty}^{\infty} d\epsilon g(\epsilon) \left( -\frac{df}{d\epsilon} \right) \text{ since } \frac{df}{d\mu} = -\frac{df}{d\epsilon} \]

To lowest order in temperature \(-\frac{df}{d\epsilon} \approx \delta(\epsilon - \mu)\) with \(\mu = \epsilon_F\)

\[ \frac{M}{V} = \mu_B^2 B g(\epsilon_F) \]

Could use Sommerfeld expansion to get corrections of order \(\frac{M(V)}{V} \approx \frac{1}{2} \mu_B^2 B \epsilon_F \)

Magnetic susceptibility \(\chi = \frac{\delta M/V}{\delta B}\)

Pauli susceptibility \(\chi_p = \mu_B^2 g(\epsilon_F)\) \(\approx\) density of states at \(\epsilon_F\)

\(\epsilon_F = \hbar^2 k_F^2 / 2m\)

For free electron gas we earlier had \(g(\epsilon_F) = \frac{3}{2} \frac{m}{\epsilon_F} \)

\[ \Rightarrow \chi_p = \mu_B^2 \frac{3}{2} \frac{m}{\epsilon_F} \]

\(\chi_p > 0 \Rightarrow\) paramagnetic
Compare this to classical result. Average magnetization of a single spin: 

\[ \langle m \rangle = \mu_B \tanh(\beta \mu_B B) \]

\[ \frac{M}{V} = \frac{\langle m \rangle N}{V} = \mu_B m \tanh(\beta \mu_B B) \]

\[ \chi = \frac{d(M/V)}{dB} \]

\[ \text{at low } T \to 0, \tanh(\beta \mu_B) \to 1, \quad \frac{M}{V} \to \mu_B m \quad \text{all spins aligned} \]

Compare to quantum case:

\[ \frac{M}{V} = \frac{3}{2} \frac{M}{\varepsilon_F} \mu_B^2 B \]

Smaller than classical result by factor \( \frac{3}{2} \frac{\mu_B^2 B}{\varepsilon_F} \ll 1 \)

\[ \text{at high } T \ (\beta \to 0) \tan(\beta \mu_B B) \to \beta \mu_B B \]

\[ \frac{M}{V} = \frac{\mu_B^2 B m}{k_B T} \quad \chi = \frac{M}{k_B T} \frac{m}{T} \sim \frac{1}{T} \]

\[ \chi_p = \mu_B^2 \frac{3}{2} \frac{m}{\varepsilon_F} \quad \text{indep of } T \]

Smaller than classical by factor \( \frac{3}{2} \left( \frac{k_B T}{\varepsilon_F} \right) \ll 1 \)
Landau Diamagnetism

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

In uniform magnetic field \( \mathbf{B} = \mathbf{V} \times \hat{A} \) a Hamiltonian becomes

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

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

\[
= \frac{1}{2m} \left( \frac{\hbar}{c} \hat{\mathbf{v}} + \frac{e}{c} \hat{A} \right)^2 \quad \text{as \textit{AM} operator}
\]

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

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

The solution of the form \( \psi(x,y,z) = e^{ik_x x} e^{ik_y y} \phi(y) \)

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

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

\[
\left[ -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{1}{2m} \left( \frac{\hbar}{c} k_x - \frac{e}{c} B y \right)^2 \right] \phi(y) = \left( E - \frac{\hbar^2 k_y^2}{2m} \right) \phi(y)
\]
Let $y_0 = \frac{\hbar k_x c}{eB}$ then

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

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

$$\left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial y^2} + \frac{1}{2} m \omega_c^2 (y-y_0)^2\right) \phi(y) = \left(\varepsilon - \frac{\hbar^2 k_y^2}{2m}\right) \phi(y)$$

The harmonic oscillator of freq $\omega_c$, centered at $y_0$

The eigenvalues $\varepsilon = \frac{\hbar^2 k_y^2}{2m} + \hbar \omega_c (n + 1/2)$ $n = 0, 1, \ldots$

Eigenvalues are indexed by $k_y$ - momentum $\vec{k}$

$n$ - 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 $k_x = \frac{2\pi m_x}{L_x}$

$\Rightarrow \Delta k_x = \frac{2\pi}{L_x} \Rightarrow \Delta y_0 = \frac{2\pi \hbar c}{eBL_x}$
Number of allowed values of $y_0 = \frac{L_y}{\Delta y_0}$

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

Include electron spin gives extra factor $\frac{1}{2}$

where $\Phi = L_x L_y B$ is magnetic flux penetrating the system, and $\Phi_0 = \frac{2\pi \hbar c}{e} = \frac{\hbar c}{e}$ is the "flux quantum"

For fixed $k_z$, the density of states per unit area looks like:

- evenly spaced $\delta$-functions
- each of weight $2\Phi = \frac{2\Phi}{L_x L_y \Phi_0} \frac{\Phi}{\Phi_0}$

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

$$\ln \mathcal{Z} = \sum_{k_z} \ln \left( 1 + ze^{-\beta E_c} \right) = \sum_{k_z} \frac{1}{2} \ln \sum_{n} \ln \left( 1 + z e^{-\beta E(n,k_z)} \right)$$

$\Rightarrow$ single particle states $\frac{1}{2}$

$g = \frac{2\Phi}{\Phi_0}$ degeneracy per area

for large $L_z$ can approx

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