Pauli paramagnetism of electron gas

electron has intrinsic spin $\underbrace{\vec{\sigma}}_{}$ ($\vec{s} = \frac{1}{2}\hbar\vec{\sigma}$) with intrinsic magnetic moment $\vec{\mu} = -\mu_B \vec{\sigma}$ $\quad \mu_B = \frac{|e|\hbar}{2mc}$ is Bohr magneton

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

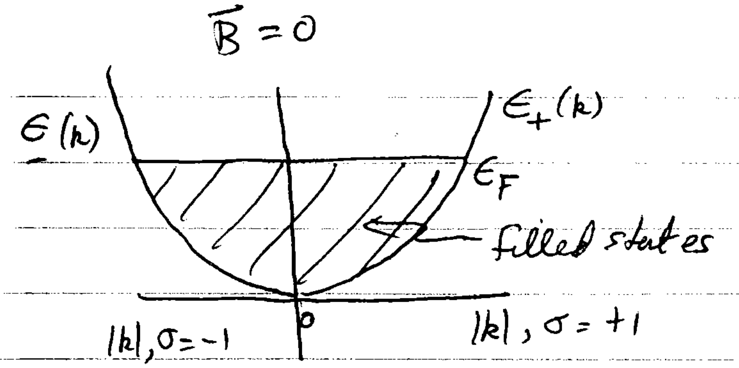
$$\mathcal{E}_{\pm}(\vec{k}) = \epsilon(\vec{k}) \pm \mu_B B$$

where $\epsilon(\vec{k})$ 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 $\Rightarrow$ ~~they~~ they will be in equilibrium when their chemical potentials are equal, ie $\mu_+ = \mu_-$

this will induce a net magnetization in the system.

To see this, consider free electrons at $T = 0$

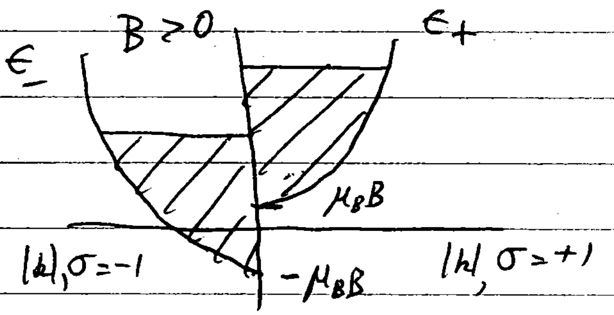


when $\vec{B} = 0$, $\epsilon_+(\vec{k}) = \epsilon_-(\vec{k})$

ground state occupations look as shown on the left. Equal numbers of $\uparrow$ and $\downarrow$ electrons

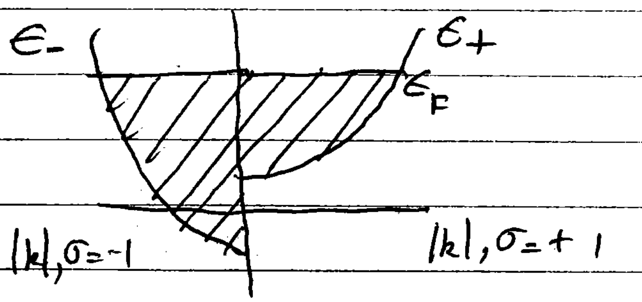
$n_+ = n_-$

when $\vec{B}$ 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 ϵ_F. But there are now more $\downarrow$ electrons than $\uparrow$ electrons

magnetization $\frac{M}{V} = -\mu_B (n_+ - n_-) > 0$

$\frac{\vec{M}}{V}$ is parallel to $\vec{B}$ $\Rightarrow$ <u>paramagnetic effect</u>

The calculation

Let $g(\epsilon)$ be the density of states when $B=0$

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

$$g_+(\epsilon + \mu_B B) = \tfrac{1}{2} g(\epsilon) \Rightarrow g_+(\epsilon) = \tfrac{1}{2} g(\epsilon - \mu_B B)$$
$$g_-(\epsilon - \mu_B B) = \tfrac{1}{2} g(\epsilon) \qquad g_-(\epsilon) = \tfrac{1}{2} g(\epsilon + \mu_B B)$$

The density of $\uparrow$ and $\downarrow$ electrons is then

$$n_\pm = \int_{-\infty}^{\infty} d\epsilon \; g_\pm(\epsilon) \, f(\epsilon, \mu(B))$$

where $f(\epsilon, \mu(B)) = \dfrac{1}{e^{(\epsilon - \mu(B))/k_B T} + 1}$

$\mu(B)$ is the chemical potential – it might depend on B
– it is same for $\uparrow$ and $\downarrow$

We will consider only the case that
$$\mu_B B \ll \mu(B) \approx \varepsilon_F$$
ie spin interaction is small compared to ϵ_F

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

Consider total density of electrons

$$n = n_+ + n_- = \int_{-\infty}^{\infty} d\epsilon\, f(\epsilon, \mu(B)) \left[g_+(\epsilon) + g_-(\epsilon)\right]$$

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

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

$$= \frac{1}{2}\int d\epsilon\, g(\epsilon) \left[f(\epsilon, \mu - \mu_B B) + f(\epsilon, \mu + \mu_B B)\right]$$

expand for small $\frac{\mu_B B}{\mu} \ll 1$

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

$$= \int_{-\infty}^{\infty} d\epsilon\, g(\epsilon)\, f(\epsilon, \mu)$$

Now since n does not change when one applies $B > 0$, and we know $n = \int_{-\infty}^{\infty} d\epsilon\, g(\epsilon)\, f(\epsilon, \mu(B=0))$ when $B = 0$,

$\Rightarrow \mu(B) = \mu(B=0)$. Corrections come from next order in the expansion $\frac{d^2 f}{d\mu^2}(\mu_B B)^2$ and are order $\left(\frac{\mu_B B}{\mu}\right)^2$

② <u>Magnetization</u> $\frac{M}{V} = -\mu_B(n_+ - n_-) = \mu_B(n_- - n_+)$

$$\frac{M}{V} = \mu_B \int_{-\infty}^{\infty} d\epsilon \; f(\epsilon,\mu)\left[g_-(\epsilon) - g_+(\epsilon)\right]$$

$$= \mu_B \int d\epsilon \; f(\epsilon,\mu)\left[\tfrac{1}{2}g(\epsilon+\mu_B B) - \tfrac{1}{2}g(\epsilon-\mu_B B)\right]$$

$$= \tfrac{1}{2}\mu_B \int d\epsilon \; g(\epsilon)\left[f(\epsilon,\mu+\mu_B B) - f(\epsilon,\mu-\mu_B B)\right] \quad \text{as before}$$

expand $f(\epsilon, \mu \pm \mu_B B) = f(\epsilon,\mu) \pm \frac{df}{d\mu}\mu_B B$

$$\frac{M}{V} = \tfrac{1}{2}\mu_B \int d\epsilon \; g(\epsilon)\left[2\frac{df}{d\mu}\mu_B B\right]$$

$$= \mu_B^2 B \int_{-\infty}^{\infty} d\epsilon \; g(\epsilon)\left(-\frac{\partial f}{\partial \epsilon}\right) \qquad \text{since } \frac{\partial f}{\partial \mu} = -\frac{\partial f}{\partial \epsilon}$$

To lowest order in temperature $-\frac{\partial f}{\partial \epsilon} \approx \delta(\epsilon-\mu)$ with $\mu = \epsilon_F$

$$\boxed{\frac{M}{V} = \mu_B^2 B\, g(\epsilon_F)}$$

could use Sommerfeld expansion to get corrections of order $\left(\frac{k_B T}{\epsilon_F}\right)^2$

magnetic susceptibility $\chi = \frac{\partial(M/V)}{\partial B}$

Pauli susceptibility $\boxed{\chi_p = \mu_B^2 g(\epsilon_F)}$ ~ density of states at ϵ_F

$\epsilon_k = \hbar^2k^2/2m$

For <u>free electron gas</u> we earlier had $g(\epsilon_F) = \frac{3}{2}\frac{n}{\epsilon_F}$

$$\Rightarrow \boxed{\chi_p = \mu_B^2 \frac{3}{2}\frac{n}{\epsilon_F}} \qquad \chi_p > 0 \Rightarrow \text{paramagnetic}$$

Compare this to classical result. Average magnetization of a single spin is

$$\langle m \rangle = (-\mu_B)\left[\frac{e^{-\beta\mu_B B}(+1) + e^{+\beta\mu_B B}(-1)}{e^{\beta\mu_B B} + e^{-\beta\mu_B B}}\right]$$

$$\langle m \rangle = \mu_B \tanh(\beta\mu_B B)$$

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

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

at low $T \to 0$, $\tanh(\beta\mu B) \to 1$, $\frac{M}{V} \to \mu_B n$
all spins alligned!

Compare to quantum cas:

$$\frac{M}{V} = \frac{3}{2}\frac{n}{\epsilon_F}\mu_B^2 B$$

smaller than classical result by factor $\frac{3}{2}\frac{\mu_B B}{\epsilon_F} \ll 1$

at high T $(\beta \to 0)$ $\tanh(\beta\mu_B B) \to \beta\mu_B B$

$$\frac{M}{V} = \frac{\mu_B^2 B n}{k_B T}, \qquad \chi = \frac{\mu_B^2 n}{k_B T} \sim \frac{1}{T}$$

Compare to quantum case - at room temp finite T corrections remain negligible and still

$$\chi_P = \mu_B^2 \frac{3}{2}\frac{n}{\epsilon_F} \quad \text{indep of } T$$

smaller than classical by factor $\frac{3}{2}\left(\frac{k_B T}{\epsilon_F}\right) \ll 1$