Pauli paramagnetism of electron gas

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

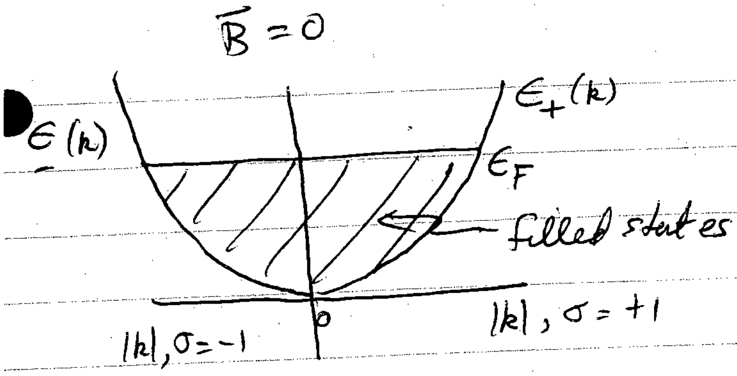
In an external magnetic field $\vec{B}$, there is an interaction energy $-\vec{\mu}\cdot\vec{B} = \mu_B \sigma B$ where $\sigma = \pm 1$ for spins parallel and antiparallel to $\vec{B}$. The energy spectra for up and down electron spins becomes

$$\epsilon_\pm(\vec{k}) = \epsilon(\vec{k}) \pm \mu_B B$$ where $\epsilon(\vec{k})$ is spectrum at $\vec{B} = 0$

Since ↑ and ↓ 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 $T=0$

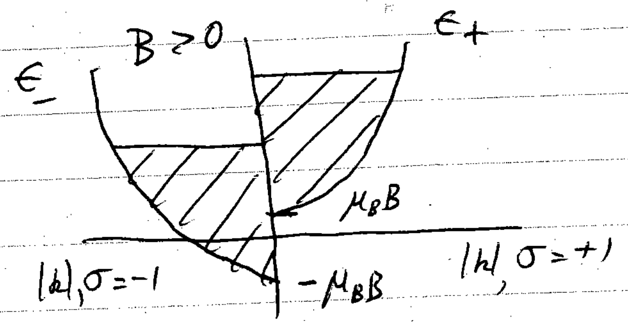


when $\vec{B} = 0$, $\epsilon_+(\vec{k}) = \epsilon_-(\vec{k})$

ground state occupations look as shown on the left. Equal numbers of ↑ and ↓ electrons

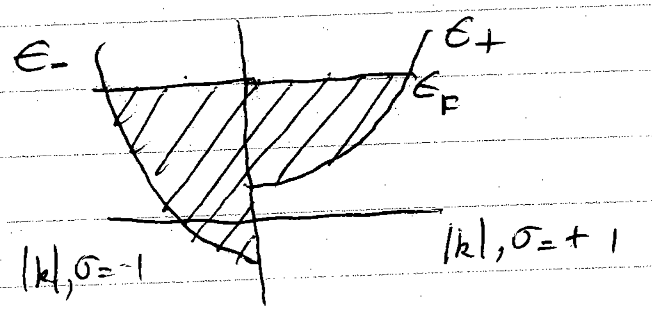
$n_+ = n_-$

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 ↑ electrons to ↓ electrons.

At equilibrium the system will look like



again the two populations have the same max energy ϵ_F. But there are now more ↓ electrons than ↑ electrons

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

$\dfrac{\vec{M}}{V}$ is parallel to $\vec{B}$ $\Rightarrow$ paramagnetic effect

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

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

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

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

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

$\mu(B)$ 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

First we will show:

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

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 $\left(\frac{\mu_B B}{\mu}\right)^2$

Now we compute

(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 $f(\epsilon,\mu \pm \mu_B B) = f(\epsilon,\mu) \pm \frac{\partial f}{\partial \mu}\mu_B B$

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

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

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

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

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 case:

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

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

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

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

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 $\frac{3}{2}\left(\frac{k_B T}{\epsilon_F}\right) \ll 1$

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 eqn 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 $y_0 \equiv \dfrac{\hbar k_x c}{eB}$ 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 $\omega_c = \dfrac{eB}{mc}$ 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 $\epsilon_{n,k_z} = \dfrac{\hbar^2 k_z^2}{2m} + \hbar\omega_c (n + 1/2) \qquad n = 0, 1, \ldots$

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

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

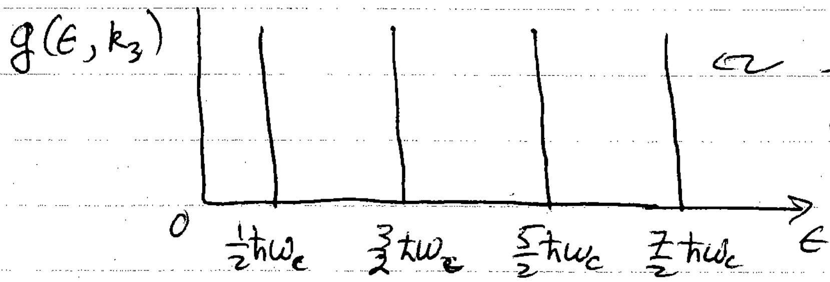
$\Rightarrow$ number of allowed values of y_0 is $L_y/\Delta y_0$

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

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

where $\Phi = L_x L_y B$ is magnetic flux ~~[illegible]~~ penetrating the system, and $\phi_0 = \frac{2\pi\hbar c}{e} = \frac{hc}{e}$ is the "<u>flux quantum</u>"

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



or evenly spaced δ-functions each of weight $\frac{2\Phi}{L_x L_y \Phi_0} = \frac{2B}{\Phi_0} \equiv g$

$\uparrow$ electron spin degeneracy

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

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

$\nwarrow$ single particle states i

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

for large L_z can approx

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