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

$\mu(B)$ 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

First we will show that

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

since we will work in the $\mu_B B \ll \epsilon_F$ limit, we will then be able to ignore changes in μ due to the finite B, and just use $\mu(B=0)$.

Proof:

Consider the total density of electrons

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

$$= \frac{1}{2}\int_{-\infty}^{\infty} d\epsilon\, f(\epsilon, \mu(B))\, [\underbrace{g(\epsilon - \mu_B B)}_{\text{shift integration variable } \epsilon - \mu_B B \to \epsilon} + \underbrace{g(\epsilon + \mu_B B)}_{\text{shift integration variable } \epsilon + \mu_B B \to \epsilon}]$$

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

use fact that $f(\epsilon, \mu)$ depends only on $(\epsilon - \mu)$

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

expand f about $\mu(B)$ for small $\mu_B B$

$$n \simeq \frac{1}{2}\int d\epsilon\, g(\epsilon)\Big[f(\epsilon,\mu(B)) - \frac{df}{d\mu}\mu_B B + \frac{1}{2}\frac{d^2f}{d\mu^2}(\mu_B B)^2 + \cdots$$

$$+ f(\epsilon,\mu(B)) + \frac{df}{d\mu}\mu_B B + \frac{1}{2}\frac{d^2f}{d\mu^2}(\mu_B B)^2 + \cdots\Big]$$

where derivatives above are evaluated at $\mu = \mu(B)$. The terms linear in B cancell!

$$n \simeq \int d\epsilon\, g(\epsilon)\Big[f(\epsilon,\mu(B)) + \frac{1}{2}\frac{d^2f}{d\mu^2}(\mu_B B)^2 + \cdots\Big]$$

If we ignored the $(\mu_B B)^2$ term the above would be

$$n = \int d\epsilon\, g(\epsilon)\, f(\epsilon,\mu(B))$$

But this is just the same ~~result~~ formula we use to compute n at $B=0$! The magnetic field B appears nowhere in the above, except via $\mu(B)$. Since the density is physically fixed by the sample and cannot change as one varies B, we would conclude that

$$\mu(B) = \mu(0) \quad \text{is independent of } B!$$

This conclusion depends on our having ignored the $(\mu_B B)^2$ term, so we can expect

$$\mu(B) \simeq \mu(0) + \frac{(\mu_B B)^2}{\epsilon_F}$$

where $\frac{1}{\epsilon_F}$ appears on dimensional grounds.

To see this is so more explicitly, lets include the $(\mu_B B)^2$ term and continue to calculate ...

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

write $\mu(B) = \mu(B=0) + \delta\mu$ and expand in first term

$$n = \int d\epsilon \, g(\epsilon) \left[f(\epsilon, \mu(B=0) + \delta\mu) + \frac{1}{2} \frac{d^2 f}{d\mu^2} (\mu_B B)^2 \right]$$

$$= \int d\epsilon \, g(\epsilon) \, f(\epsilon, \mu(B=0))$$

$$+ \int d\epsilon \, g(\epsilon) \left. \frac{df}{d\mu} \right|_{\mu=\mu(B=0)} \delta\mu$$

$$+ \frac{1}{2} \int d\epsilon \, g(\epsilon) \left. \frac{d^2 f}{d\mu^2} \right|_{\mu=\mu(B)} (\mu_B B)^2$$

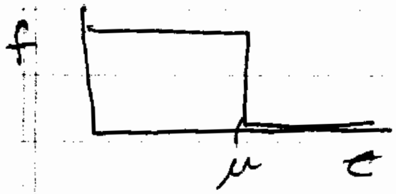
The first term is just the density when $B=0$, ie n. Hence we get

$$0 = \int d\epsilon \, g(\epsilon) \left. \frac{df}{d\mu} \right|_{\mu=\mu(B=0)} \delta\mu + \frac{1}{2} \int d\epsilon \, g(\epsilon) \left. \frac{d^2 f}{d\mu^2} \right|_{\mu=\mu(B)} (\mu_B B)^2$$

So the correction to μ due to finite B is

$$\delta\mu = \frac{-\frac{1}{2} \int d\epsilon \, g(\epsilon) \left. \frac{d^2 f}{d\mu^2} \right|_{\mu=\mu(B)} (\mu_B B)^2}{\int d\epsilon \, g(\epsilon) \left. \frac{df}{d\mu} \right|_{\mu=\mu(B=0)}}$$

To see how big this is, consider the limit $T \to 0$ where $\mu(B=0) = \epsilon_F$, and f is a step function



$$\frac{df}{d\mu} = -\frac{df}{d\epsilon} = \delta(\epsilon - \mu)$$

$$\frac{d^2 f}{d\mu^2} = \frac{d^2 f}{d\epsilon^2} = -\frac{d\,\delta(\epsilon-\mu)}{d\epsilon}$$

so $\displaystyle\int d\epsilon\, g(\epsilon) \frac{df}{d\mu}\bigg|_{\mu = \mu(B=0)} = g(\mu(B=0)) = g(\epsilon_F)$

$$\int d\epsilon\, g(\epsilon) \frac{d^2 f}{d\mu^2}\bigg|_{\mu=\mu(B)} (\mu_B B)^2 = g'(\mu(B))\,(\mu_B B)^2$$

$$\delta\mu = -\frac{1}{2}\,\frac{g'(\mu(B))\,(\mu_B B)^2}{g(\epsilon_F)}$$

to lowest order, evaluate $g'(\mu(B))$ as $g'(\epsilon_F)$
The difference will only give higher order corrections of $O(\mu_B B)^4$

$$\delta\mu = \frac{-g'(\epsilon_F)(\mu_B B)^2}{2g(\epsilon_F)}$$

for free electrons with $g(\epsilon) = c\sqrt{\epsilon}$ so
$g'(\epsilon) = \frac{1}{2}\frac{c}{\sqrt{\epsilon}}$ we get

$$\boxed{\delta\mu = -\frac{(\mu_B B)^2}{4\epsilon_F}} \quad \text{so} \quad \boxed{\mu(B) = \epsilon_F\left(1 - \left(\frac{\mu_B B}{2\epsilon_F}\right)^2\right)}$$

Now we compute

(2) **Magnetization** $\frac{M}{V} = -\mu_B (n_+ - n_-) = \mu_B (n_- - n_+)$

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

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

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

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

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

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

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 free electron gas 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 $(\beta \to 0)$ $\tanh(\beta\mu_B B) \to \beta\mu_B B$

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

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

Ideal Bose Gas

Bose occupation function

Bose Einstein Condensation

$$n(\epsilon) = \frac{1}{z^{-1}e^{\beta\epsilon} - 1}$$

We had for the density of an ideal (non-interacting) bose gas

$$\frac{N}{V} = \frac{1}{V}\sum_k \frac{1}{z^{-1}e^{\beta\epsilon(k)} - 1} = \frac{1}{(2\pi)^3}\int_0^\infty dk\, 4\pi k^2 \frac{1}{z^{-1}e^{\beta\hbar^2k^2/2m} - 1}$$

spin zero bosons $g_s = 1$

recall, we need $z \leq 1$ for the occupation number at $\epsilon(k=0) = 0$ to remain positive $n(0) \geq 0$

$$n(0) = \frac{1}{z^{-1} - 1} = \frac{z}{1-z} \Rightarrow z \leq 1, \quad z = e^{\beta\mu} \Rightarrow \mu \leq 0$$

substitute variables $y = \frac{\beta\hbar^2k^2}{2m} \Rightarrow k = \sqrt{\frac{2my}{\beta\hbar^2}}$

$$dk = \sqrt{\frac{2my}{\beta\hbar^2}}\frac{dy}{2y}$$

$$\Rightarrow \frac{N}{V} = \left(\frac{2m}{\beta\hbar^2}\right)^{3/2}\frac{4\pi}{(2\pi)^3}\frac{1}{2}\int_0^\infty dy \frac{y^{1/2}}{z^{-1}e^y - 1}$$

$$\frac{N}{V} = \frac{1}{\lambda^3} g_{3/2}(z) \quad \text{where } \lambda = \left(\frac{h^2}{2\pi m k_B T}\right)^{1/2} \text{ thermal wavelength}$$

$$g_{3/2}(z) \equiv \frac{2}{\sqrt{\pi}}\int_0^\infty dy \frac{y^{1/2}}{z^{-1}e^y - 1}$$

Consider the function

$$g_{3/2}(z) = \frac{2}{\sqrt{\pi}} \int_0^\infty dy \, \frac{y^{1/2}}{z^{-1}e^y - 1} = z + \frac{z^2}{2^{3/2}} + \frac{z^3}{3^{3/2}} + \cdots$$

$g_{3/2}(z)$ is monotonic increasing function of z for $z \leq 1$

as $z \to 1$, $g_{3/2}(z)$ approaches a <u>finite</u> constant

$$g_{3/2}(1) = 1 + \frac{1}{2^{3/2}} + \frac{1}{3^{3/2}} + \cdots \equiv \zeta(3/2) \simeq 2.612$$

Reimann zeta function

We can see that $g_{3/2}(1)$ is finite as follows:

$$g_{3/2}(1) = \frac{2}{\sqrt{\pi}} \int_0^\infty dy \, \frac{y^{1/2}}{e^y - 1}$$

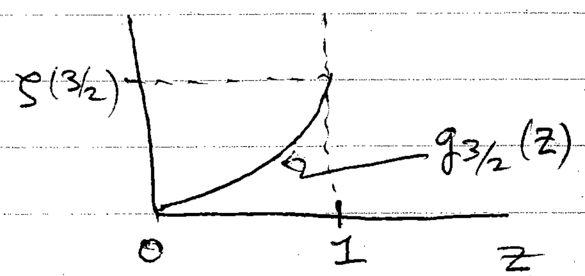
as $y \to \infty$ the integral converges. Integral is <u>largest</u> at small y

(recall small y corresponds to low energy where $n(\epsilon)$ is largest)

For small y we can approx $\frac{1}{e^y - 1} \simeq \frac{1}{y}$

$$\int_0^{y^*} dy \, \frac{y^{1/2}}{e^y - 1} \simeq \int_0^{y^*} dy \, \frac{1}{y^{1/2}} = 2 \, y^{1/2} \Big|_0^{y^*}$$

So we see the integral also converges at its lower limit $y \to 0$.



So we conclude

$$n = \frac{N}{V} = \frac{g_{3/2}(z)}{\lambda^3} \leq \frac{g_{3/2}(1)}{\lambda^3} = \frac{2.612}{\lambda^3} = 2.612\left(\frac{2\pi m k_B T}{h^2}\right)^{3/2}$$

But we now have a contradiction!
For a system with fixed density of bosons n, as T decreases we will eventually get to a temperature below which the above inequality is violated!
This temperature is

$$T_c = \left(\frac{n}{2.16}\right)^{2/3} \frac{h^2}{2\pi m k_B}$$

<u>Solution to the paradox:</u>
when we made the approx $\frac{1}{V}\sum_k \to \frac{1}{(2\pi)^3}\int_0^\infty dk\, 4\pi k^2$

we gave a weight $\frac{4\pi k^2}{(2\pi)^3}$ to states with wavevector $|\vec{k}|$.

This gives <u>zero</u> weight to the state $\vec{k}=0$, ie to the ground state. But as T decreases, more and more bosons will occupy the ground state, as it has the lowest energy. Thus when we approx the sum by an integral, we should treat the ground state separately

$$\frac{1}{V}\sum_k n(\epsilon(k)) \cong \underbrace{\frac{n(0)}{V}} + \frac{1}{(2\pi)^3}\int_0^\infty dk\, 4\pi k^2\, n(\epsilon(k))$$

ground state with occupation $n(0)$.
This term is important when $n(0)/V$ stays finite as $V \to \infty$, ie a macroscopic fraction of bosons occupy the ground state