

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

$$\begin{aligned} g_+(\epsilon + \mu_B B) &= \frac{1}{2} g(\epsilon) \Rightarrow g_+(\epsilon) = \frac{1}{2} g(\epsilon - \mu_B B) \\ g_-(\epsilon - \mu_B B) &= \frac{1}{2} g(\epsilon) \quad g_-(\epsilon) = \frac{1}{2} g(\epsilon + \mu_B B) \end{aligned}$$

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

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

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

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

We will consider only the case that

$$\mu_B B \ll \mu(B) \approx \epsilon_F$$

i.e. spin interaction is small compared to ϵ_F

First we will show:

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

Consider total density of electrons

$$\begin{aligned} n &= n_+ + n_- = \int_{-\infty}^{\infty} d\epsilon f(\epsilon, \mu(B)) [g_+(\epsilon) + g_-(\epsilon)] \\ &= \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon f(\epsilon, \mu(B)) [g(\epsilon - \mu_B B) + g(\epsilon + \mu_B B)] \\ &= \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon g(\epsilon) [f(\epsilon + \mu_B B, \mu(B)) + f(\epsilon - \mu_B B, \mu(B))] \\ &= \frac{1}{2} \int_{-\infty}^{\infty} d\epsilon g(\epsilon) [f(\epsilon, \mu - \mu_B B) + f(\epsilon, \mu + \mu_B B)] \end{aligned}$$

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

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

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 $\frac{d^2 f}{d\mu^2} (\mu_B B)$

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

Now we compute

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

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

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

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

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

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

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

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 $\boxed{\chi_P = \mu_B^2 g(\epsilon_F)}$

$\sim$ density of states at ϵ_F

$\epsilon_F = \hbar^2 k_F^2 / 2m$

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

$$\Rightarrow \boxed{\chi_P = \mu_B^2 \frac{3}{2} \frac{m}{\epsilon_F}}$$

$\chi_P > 0 \Rightarrow$ paramagnetic

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

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

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

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

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

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

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 ($\beta \rightarrow 0$) $\tanh(\beta \mu_B B) \rightarrow \beta \mu_B B$

$$\frac{M}{V} = \frac{\mu_B^2 B n}{k_B T}$$

$$\chi = \frac{\mu_B^2 n}{k_B T} \sim \frac{1}{T}$$

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 Einstein Condensation

Bose occupation function

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

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

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

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

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

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

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

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

Consider the function

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

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

As $z \rightarrow 1$, $g_{3/2}(z)$ approaches a finite constant

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

↑ Riemann zeta function

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

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

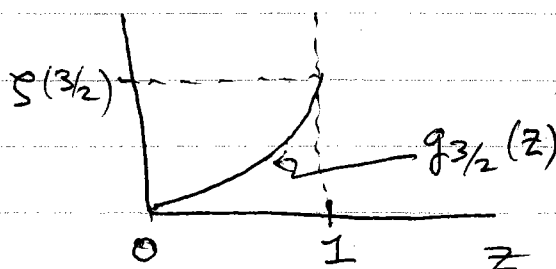
as $y \rightarrow \infty$ the integral converges. Integral is largest at small y

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

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

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

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



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

$$T_c = \left(\frac{n}{2.612} \right)^{2/3} \frac{h^2}{2\pi m k_B}$$

Solution to the paradox:

When we made the approx $\frac{1}{V} \sum_k \rightarrow \frac{1}{(2\pi)^3} \int_0^\infty dk \, 4\pi k^2$

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

This gives zero weight to the state $\vec{k}=0$, i.e. 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

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

ground state with occupation $n(0)$.

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

Then we get

$$n = \frac{N}{V} = \frac{n(0)}{V} + \frac{g_{3/2}(z)}{\lambda^3}$$

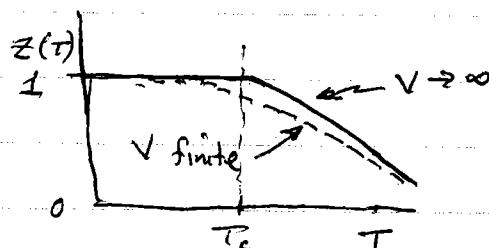
$$n = n_0 + \frac{g_{3/2}(z)}{\lambda^3} \quad \text{where } n_0 = \frac{n(0)}{V} \text{ density of bosons in ground state}$$

For a system with fixed n , at higher T one can always choose z so that $n = \frac{g_{3/2}(z)}{\lambda^3}$ and $n_0 = 0$.

But when $T < T_c$ it is necessary to have $n_0 > 0$.

Using $n(0) = \frac{z}{1-z}$ we can write above as

$$n = \frac{z}{1-z} \frac{1}{V} + \frac{g_{3/2}(z)}{\lambda^3}$$



For $T > T_c$ we will have a solution to the above for some fixed $z < 1$. In thermodynamic limit $V \rightarrow \infty$, the first term will then vanish, i.e. the density of bosons in the ground state vanishes.

As $T \rightarrow T_c$, $z \rightarrow 1$ and ^{as $V \rightarrow \infty$} the first term $\left(\frac{z}{1-z}\right)\left(\frac{1}{V}\right)$ stays finite to give the additional needed density at $T < T_c$:

$$\frac{z}{1-z} \frac{1}{V} = n_0 = n - \frac{g_{3/2}(1)}{\lambda^3}$$

↑ diverges as $z \rightarrow 1$ ↑ vanishes as $V \rightarrow \infty$

T_c defines the Bose-Einstein transition temperature below which the system develops a finite density of particles in the ground state n_0 .

n_0 is also called the condensate density.

The particles in the ground state are called the condensate.

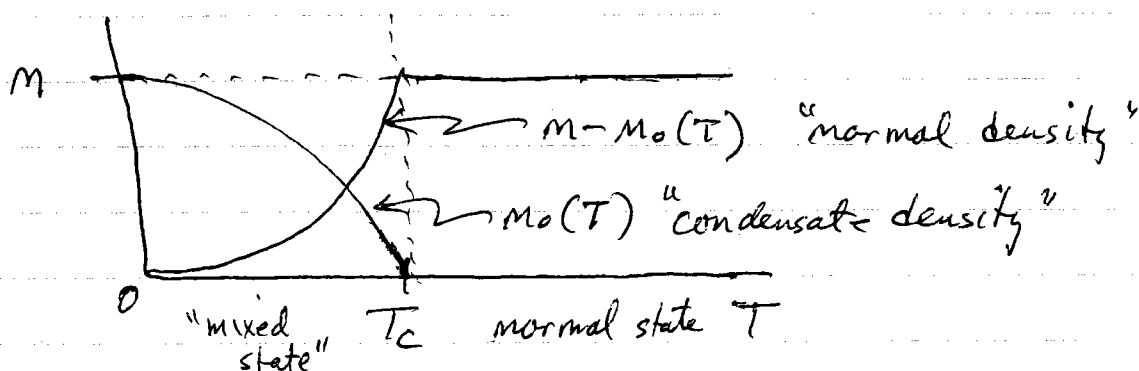
$$\left. \begin{array}{l} z(T) \rightarrow 1 \\ \mu(T) \rightarrow 0 \end{array} \right\} \text{ as } T \rightarrow T_c, \quad \left. \begin{array}{l} z(T) = 1 \\ \mu(T) = 0 \end{array} \right\} \text{ for } T \leq T_c$$

For $T \leq T_c$

$$n_0(T) = n - \frac{g_{3/2}(1)}{\lambda^3} = n - 2.612 \left(\frac{2\pi m k_B T}{h^2} \right)^{3/2}$$

$$n_0(T) = n \left(1 - \left(\frac{T}{T_c} \right)^{3/2} \right)$$

condensate density vanishes continuously as $T \rightarrow T_c$ from below



At $T=0$, all bosons are in condensate

At $T > T_c$, all bosons are in the "normal state"

At $0 < T < T_c$, a macroscopic fraction of bosons are in the condensate, while the remaining fraction are in the normal state — call it the "mixed state"