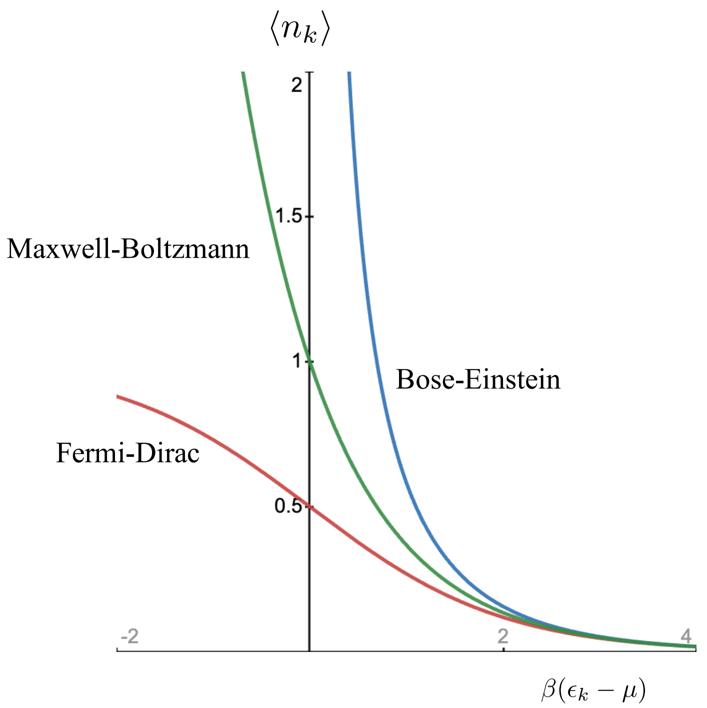
Quantum gases



Fermi - Dirac distribution:

$$\langle n_k \rangle = \frac{1}{e^{\beta(\epsilon_k - \mu)} + 1}$$

Bose - Einstein distribution:

$$\langle n_k \rangle = \frac{1}{e^{\beta(\epsilon_k - \mu)} - 1}$$

Maxwell - Boltzmann distribution:

$$\langle n_k \rangle = e^{-\beta(\epsilon_k - \mu)}$$

Fermi gas (ideal case)

The average number of particles can now be written as

$$\langle N \rangle = \sum_k \frac{1}{\varsigma^{-1} e^{\beta \epsilon_k} + 1}$$

As we approximated for Bosons, $\langle N \rangle$ can be expressed as

$$\langle N \rangle = \frac{4\pi V}{h^3} \int_0^\infty \frac{p^2}{\varsigma^{-1} e^{\beta p^2/(2m)} + 1} dp$$

Choosing a new variable $t = \beta p^2/(2m)$, we get

$$\langle N \rangle = \frac{2V}{\sqrt{\pi}\, h^3} (2\pi\, m\, k_B T)^{3/2} \int_0^\infty \frac{\sqrt{t}}{\varsigma^{-1} e^t + 1} dt$$

Where $\lambda = h/\sqrt{2\pi\, m\, k_B T}$ and the integral is defined as

$$f_\nu(\varsigma) = \frac{1}{\Gamma(\nu)} \int_0^\infty \frac{t^{\nu-1}}{\varsigma^{-1} e^t + 1} dt$$

Here, $\Gamma(\nu)$ is the gamma function. Thus, number of particles per unit volume can be written as

$$\frac{\langle N \rangle}{V} = n = \frac{1}{\lambda^3} f_{3/2}(\varsigma)$$

Where n is particle density.

Equation of state (Fermions)

$$\frac{PV}{k_B T} = \sum_k \ln\left[1 + \varsigma\, e^{-\beta\, \epsilon_k}\right]$$
$$\frac{PV}{k_B T} = \frac{4\,\pi\, V}{h^3} \int_0^\infty p^2 \;\ln\left[1 + \varsigma\, e^{-\beta p^2/(2m)}\right]\, dp$$
$$\frac{PV}{k_B T} = \frac{2\, V}{\sqrt{\pi}\, h^3}\, (2\pi\, m\, k_B T)^{3/2} \int_0^\infty \sqrt{t}\, \ln[1 + \varsigma\, e^{-t}]\; dt$$

The integration can be done by parts to obtain

$$\frac{PV}{k_B T} = \frac{2\, V}{\sqrt{\pi}\, h^3}\, \frac{1}{\lambda^3} \left[\frac{t^{3/2}}{3/2} \ln[1 + \varsigma\, e^{-t}] - \frac{2}{3}\int_0^\infty \frac{t^{3/2}\;\; \varsigma\, e^{-t}}{1 + \varsigma\, e^{-t}}\; dt\right]$$

$$\frac{P}{k_B T} = \frac{1}{\lambda^3} \frac{1}{\Gamma(5/2)} \int_0^\infty \frac{t^{\frac{5}{2}-1}}{\varsigma^{-1}\, e^t + 1}\, dt$$

$$\frac{P}{k_B T} = \frac{1}{\lambda^3}\, f_{5/2}(\varsigma)$$

Alternative expressions for $g_\nu(\varsigma)$ and $f_\nu(\varsigma)$

$$g_\nu(\varsigma) = \sum_{k=1}^\infty \frac{\varsigma^k}{k^\nu}$$
$$f_\nu(\varsigma) = \sum_{k=1}^\infty (-1)^{k+1}\, \frac{\varsigma^k}{k^\nu}$$

Energy density

$$\langle E \rangle = \sum_k \epsilon_k\, \langle n_k \rangle$$

The general expression is

$$\frac{\langle E \rangle}{V} = \frac{1}{V} \sum_k \frac{\epsilon_k}{\varsigma^{-1} e^{\beta \epsilon_k} \pm 1}$$

Where + symbol corresponds to fermions and - symbol corresponds to bosons.

$$\frac{\langle E\rangle}{V}=\frac{4\,\pi}{h^3}\int_0^{\infty}p^2\,\frac{\epsilon(p)}{\varsigma^{-1}e^{\beta\epsilon(p)}\pm 1}\,dp$$

This can be shown as, solving the integrals as above,

$$\frac{\langle E\rangle}{V}=\frac{3}{2}\,P$$

Implies,

$$P=\frac{2}{3}\frac{\langle E\rangle}{V}$$

This expression is true for both fermions and bosons.

Comparison between bosons and fermions

Bosons	Fermions
$\frac{\langle N\rangle}{V}=\frac{1}{\lambda^3}\,g_{3/2}(\varsigma)$	$\frac{\langle N\rangle}{V}=\frac{1}{\lambda^3}\,f_{3/2}(\varsigma)$
$\frac{P}{k_BT}=\frac{1}{\lambda^3}\,g_{5/2}(\varsigma)$	$\frac{P}{k_BT}=\frac{1}{\lambda^3}\,f_{5/2}(\varsigma)$
$\frac{\langle E\rangle}{V}=\frac{3}{2}\,P$	$\frac{\langle E\rangle}{V}=\frac{3}{2}\,P$
$\frac{\langle E\rangle}{\langle N\rangle}=\frac{3}{2}\,k_BT\,\frac{g_{5/2}(\varsigma)}{g_{3/2}(\varsigma)}$	$\frac{\langle E\rangle}{\langle N\rangle}=\frac{3}{2}\,k_BT\,\frac{f_{5/2}(\varsigma)}{f_{3/2}(\varsigma)}$

Equation of state (Virial expansion)

At low densities, i.e., $\varsigma \ll 1$, the equation of state can be expressed as

$$\frac{P}{k_BT}=\frac{1}{\lambda^3}\begin{Bmatrix} f_{\frac{5}{2}}(\varsigma) \\ g_{5/2}(\varsigma)\end{Bmatrix}$$

Where $f_{\frac{5}{2}}(\varsigma)$ corresponds to fermions and $g_{5/2}(\varsigma)$ corresponds to bosons. Using the alternative expressions $g_v(\varsigma)$ and $f_v(\varsigma)$, the equation of state can be written as

$$\frac{P}{k_BT}=\frac{-1}{\lambda^3}\left(-\varsigma\pm\frac{\varsigma^2}{2^{\frac{5}{2}}}\pm\ \dots\dots\right)$$

Here + symbol corresponds to fermions and - symbol corresponds to bosons. Similarly,

$$\frac{\langle N\rangle}{V}=\frac{1}{\lambda^3}\begin{Bmatrix} f_{\frac{3}{2}}(\varsigma) \\ g_{3/2}(\varsigma)\end{Bmatrix}=\frac{-1}{\lambda^3}\left(-\varsigma\pm\frac{\varsigma^2}{2^{\frac{3}{2}}}\pm\ \dots\dots\right)$$

This implies, the ratio of $\frac{P}{k_B T}$ and $\frac{\langle N \rangle}{V}$ will give us

$$\frac{P}{k_B T} = \frac{\langle N \rangle}{V} \frac{\left(-\varsigma \pm \frac{\varsigma^2}{2^{\frac{5}{2}}} \pm \ \ldots\ldots \right)}{\left(-\varsigma \pm \frac{\varsigma^2}{2^{\frac{3}{2}}} \pm \ \ldots\ldots \right)}$$

$$\frac{P}{k_B T} = \frac{\langle N \rangle}{V} \left(-1 \pm \frac{\varsigma}{2^{\frac{5}{2}}} \right) \left(-1 \pm \frac{\varsigma}{2^{\frac{3}{2}}} \right)^{-1}$$

$$\frac{P}{k_B T} = \frac{\langle N \rangle}{V} \left(-1 \pm \frac{\varsigma}{2^{\frac{5}{2}}} \right) \left(-1 \mp \frac{\varsigma}{2^{\frac{3}{2}}} \right)$$

$$\frac{P}{k_B T} = \frac{\langle N \rangle}{V} \left(1 \pm \frac{\varsigma}{2^{\frac{3}{2}}} \mp \frac{\varsigma}{2^{\frac{5}{2}}} \right)$$

$$\frac{P}{k_B T} = \frac{\langle N \rangle}{V} \left(1 \pm \frac{\varsigma}{2^{\frac{5}{2}}} \right)$$

In the above expression, $\pm\, \varsigma/2^{5/2}$ term is the quantum correction to the classical ideal gas. Here, + symbol corresponds to fermions and - symbol corresponds to bosons.

For small ς, we can write $\frac{\langle N \rangle}{V} = \frac{\varsigma}{\lambda^3}$. This implies, $\varsigma = \frac{\langle N \rangle}{V} \lambda^3$. So, in this limit the equation of state reads,

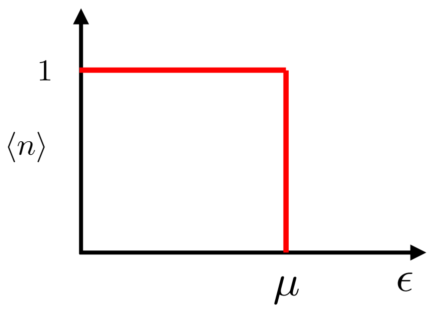
$$P\,V = \langle N \rangle k_B T \left(1 \pm \frac{\langle N \rangle}{V} \frac{\lambda^3}{2^{5/2}} \right)$$

Electrons in a conductor

The average occupation number of fermions, in a particular energy level, is given by the expression

$$\langle n \rangle = \frac{1}{e^{\beta(\epsilon - \mu)} + 1}$$

In the $T \longrightarrow 0$, limit



$$e^{\beta(\epsilon-\mu)} = \begin{cases} \infty & \epsilon > \mu \\ 0 & \epsilon < \mu \end{cases}$$

$$\langle n \rangle = \begin{cases} 0 & \epsilon > \mu \\ 1 & \epsilon < \mu \end{cases}$$

All the states with $\epsilon < \mu$ are filled and all the states $\epsilon > \mu$ are empty. This is the $T = 0$ ground state of the fermi gas. We there see that $\mu\ (T = 0)$ is the highest occupied energy state. One calls this energy the "Fermi - energy" $\epsilon_F = \mu\ (T = 0)$.

The total occupation number,

$$\langle N \rangle = \sum_{\substack{States\ with \\ \epsilon < \epsilon_F}} \frac{1}{e^{\beta(\epsilon_F - \mu\ (T=0))} + 1}$$

Here, $\epsilon_F - \mu\ (T = 0) = 0$. So,

$$\langle N \rangle = \sum_{\substack{States\ with \\ \epsilon < \epsilon_F}} 1$$

This can be simplified using the integral

$$\langle N \rangle = \frac{4\,\pi\,V}{h^3} \int_0^{\sqrt{2\,m\,\epsilon_F}} p^2 \ \ dp$$

$$\langle N \rangle = \frac{4\,\pi\,V}{3\,h^3}\ (2\,m\,\epsilon_F)^{3/2}$$

$$\frac{\langle N \rangle}{V} = n = \frac{4\,\pi}{3\,h^3}\ (2\,m\,\epsilon_F)^{3/2}$$

$$n = \frac{4\,\pi}{3} \left(\frac{2\,m\,\epsilon_F}{h^2}\right)^{3/2}$$

Thus, the fermi energy is given by

$$\epsilon_F = \left(\frac{3\,n}{4\,\pi}\right)^{2/3} \frac{h^2}{2\,m}$$

The corresponding fermi temperature is

$$T_F = \frac{\epsilon_F}{k_B}$$

For electrons in a metal $T_F \approx 10{,}000\ K$. So, electrons in a metal always in degenerate limit, i.e. $T < T_F$.

Finite temperature

In the limit, $k_B T \ll \epsilon_F$, we get

$$k_B T \ll \left(\frac{3\,n}{4\,\pi}\right)^{2/3} \frac{h^2}{2\,m}$$

After re-arranging the terms,

$$\frac{2\pi\, m\, k_B T}{h^2} \ll \pi \left(\frac{3\, n}{4\, \pi}\right)^{2/3}$$

$$\left(\frac{2\pi\, m\, k_B T}{h^2}\right)^{3/2} \ll \pi^{3/2} \frac{3\, n}{4\, \pi}$$

$$\left(\frac{\sqrt{2\pi\, m\, k_B T}}{h}\right)^{3} \ll \frac{3\, n\, \sqrt{\pi}}{4}$$

$$\frac{1}{n\, \lambda^3} \ll \frac{3\, \sqrt{\pi}}{4}$$

$$n\, \lambda^3 \gg \frac{4}{3\, \sqrt{\pi}}$$

This implies, $n\, \lambda^3 \gg 1$ is called the low T or high-density limit. Similarly, $n\, \lambda^3 \ll 1$ is called the high T or classical limit.

Energy in the degenerate limit (T = 0)

Consider the expression for the number density,

$$n = \frac{4\, \pi}{3} \left(\frac{2\, m\, \epsilon_F}{h^2}\right)^{3/2} =$$

Using this relation, we can define the density of state, i.e. number of states with energy ε per unit energy per volume $g(\varepsilon)$. The density of states, $g(\varepsilon) = \frac{n}{\varepsilon} = C\, \sqrt{\varepsilon}$. Where the constant

$$C = \frac{2}{\pi} \left(\frac{2\, \pi\, m}{h^2}\right)^{3/2}$$

Now, we will calculate the following quantity,

$$\frac{\langle E \rangle}{V} = \int_0^{\varepsilon_F} d\varepsilon\;\; g(\varepsilon)\, \varepsilon$$

$$= C \int_0^{\varepsilon_F} d\varepsilon\;\; \sqrt{\varepsilon}\;\; \varepsilon$$

$$\frac{\langle E \rangle}{V} = \frac{2\, C}{5}\;\; {\varepsilon_F}^{5/2}$$

In terms of the constant C the density of particles is

$$n = \frac{\langle N \rangle}{V} = \frac{2\, C}{3}\;\; {\varepsilon_F}^{3/2}$$

This implies, the energy per particle is

$$\frac{\langle E \rangle}{\langle N \rangle} = \frac{3}{5}\; \varepsilon_F$$