<u>Equipartition</u> System of classical (non-interacting) particles at temperature T - the particles have degrees of freedom, e.g.

$$\{x_1, y_1, z_1, p_{x_1}, p_{y_1}, p_{z_1}, x_2, y_2, z_2, p_{x_2}, p_{y_2}, p_{z_2}, \ldots\}.$$

Let the energy per particle be $\varepsilon = ax^2$, $a>0$ then the average energy per degree of freedom is

$$\langle \varepsilon \rangle = \frac{\int_{-\infty}^{\infty} a x^2 e^{-\beta a x^2} dx}{\int_{-\infty}^{\infty} e^{-\beta a x^2} dx} = \frac{a\sqrt{\pi}/2\left(a/k_B T\right)^{3/2}}{\sqrt{\pi}/\left(a/k_B T\right)^{1/2}} = \tfrac{1}{2} k_B T$$

If the particle has n degrees of freedom then energy per particle is

$$\langle \varepsilon \rangle = \tfrac{n}{2} k_B T$$

Equipartition of energy: the energy is, <u>on average</u>, is divided up <u>equally</u> among the n degrees of freedom, each being $\frac{1}{2} k_B T$.

To count degrees of freedom, count the number of quadratic terms.

e.g. $\mathcal{E} = a x^2$ (1 degree) or $\mathcal{E} = a x^2 + b y^2 + c z^2$ (3 degrees)

Note, this is the classical result (MB statistics). You can do a similar analysis on quantum particles, noting in the high T limit both FD and BE tend to MB statistics.

Mathematical Note.

A δ function centred at μ i.e. $\delta(\varepsilon-\mu)$ then the integral

$$\int_{-\infty}^{\infty} \delta(\varepsilon-\mu)\, \delta\varepsilon = 1.$$ then we also have

$$\int_{-\infty}^{\infty} \delta(\varepsilon-\mu)\, F(\varepsilon) = F(\mu).$$

What if instead of δ we had a highly peaked function $\delta_\sigma(\varepsilon-\mu)$

then $$\int_{-\infty}^{\infty} \delta_\sigma(\varepsilon-\mu)\,(\varepsilon-\mu)^2\, d\varepsilon = \sigma^2 \ll 1.$$

In statistical physics the probability $P(\varepsilon)$ is very peaked

(4)

Let's expand some function $F(\varepsilon)$ around $\varepsilon = \mu$.

$$F(\varepsilon) = F(\mu) + (\varepsilon-\mu)F'(\mu) + \tfrac{1}{2}(\varepsilon-\mu)^2 F''(\mu) + \cdots$$

Hence $$\int p(\varepsilon)F(\varepsilon)\,d\varepsilon = F(\mu)\overbrace{\int p(\varepsilon)\,d\varepsilon}^{1} + F'(\mu)\overbrace{\int p(\varepsilon)(\varepsilon-\mu)\,d\varepsilon}^{0}$$
$$+ \tfrac{1}{2}F''(\mu)\underbrace{\int p(\varepsilon)(\varepsilon-\mu)^2\,d\varepsilon}_{\sigma^2} + \cdots$$

i.e $$\int_{-\infty}^{\infty} p(\varepsilon)F(\varepsilon)\,d\varepsilon \simeq F(\mu) + \frac{\sigma^2}{2}F''(\mu)$$

For the variance $\int p(\varepsilon)(\varepsilon-\mu)^2\,d\varepsilon = \sigma^2$ (Book, Appendix C)

$$\int_0^\infty \frac{e^y y^2}{(1+e^y)^2}\,dy = \pi^2/6$$

$$= F(\mu) + \frac{\pi^2 F''(\mu)}{6} k_B^2 T^2, \quad \sigma^2 = \frac{\pi^2 k_B^2 T^2}{3}$$

Fermi - Dirac Gases.

These are quantum objects with ½-integer spin. They can be fundamental (e.g. electrons) or composite, e.g.

- conducting electrons in metals
- liquid He
- white dwarf stars

Any composite object made up of odd number of fermions, e.g. proton with 3 quarks and ^3He not ^4He.

We have the Fermi-Dirac distribution function.

$$f_{FD}(\varepsilon) = \frac{1}{e^{\alpha} e^{\beta\varepsilon} + 1} = \frac{1}{e^{\beta(\varepsilon - \mu)}} \quad \text{where} \quad \begin{array}{l} \beta = 1/k_B T \\ \alpha = -\beta\mu. \end{array}$$

The constant particle constraint, α, is now appearing as an energy, μ, – this is the Fermi-level, sometimes μ is written as ε_F.

The distribution $f_{FD}(\varepsilon)$ is the average occupation with energy ε, but for single particle states ε_i

$$f_i = n_i / g_i$$

where g_i is the degeneracy of state with energy ε_i, having n_i particles in it. For Fermions $0 \leq f_i \leq 1$.

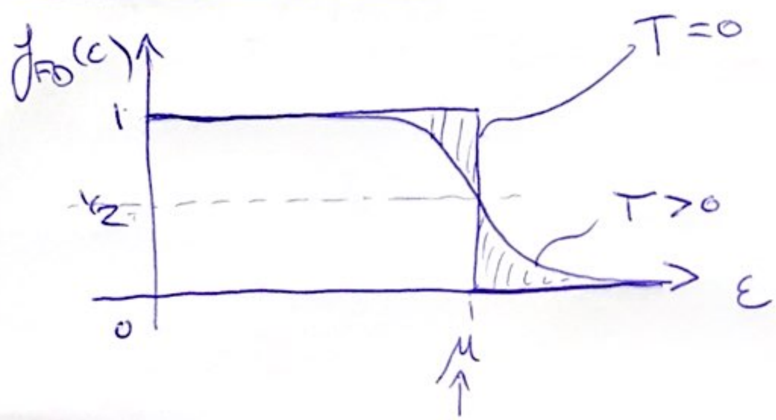
The number of particles in range ε to $\varepsilon + d\varepsilon$ is

$$g(\varepsilon) f_{FD}(\varepsilon)\, d\varepsilon .$$

The total number of particles N is

$$N = \int_0^\infty g(\varepsilon)\, f(\varepsilon)\, d\varepsilon \quad \text{(taking 0 to be lowest energy)}.$$

Properties of $f_{FD}(\varepsilon)$



$$f_{FD}(\mu) = 1/2$$

$$\lim_{T\to 0} f_{FD}(\varepsilon < \mu) = 1$$

$$\lim_{T\to 0} f_{FD}(\varepsilon > \mu) = 0$$

Example. At $T=0$ calculate the Fermi level of a system of N particles contained to the 3D ∞-square well of volume $V = a^3$ (box)

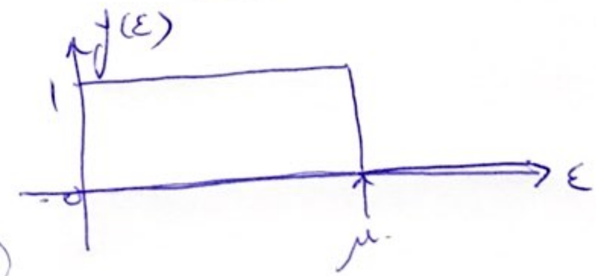
Include spin.

"box" means : $$g(\varepsilon)\, d\varepsilon = 2V \frac{2\pi}{h^3} (2m)^{3/2} \varepsilon^{1/2} d\varepsilon$$

1 up to μ, 0 otherwise.

Note that we need $$N = \int_0^\infty g(\varepsilon) f_{FD}(\varepsilon)\, d\varepsilon.$$

$$N = \int_0^\mu g(\varepsilon)\, d\varepsilon$$ because



$$\Rightarrow N = 2V \cdot \frac{2\pi}{h^3} (2m)^{3/2} \int_0^\mu \varepsilon^{1/2} d\varepsilon$$

Do the above integral and rearrange for μ to get

$$\mu = \frac{h^2}{2M}\left(3N/8\pi V\right)^{2/3}.$$

Recap. if asked for Fermi level we require $g(\varepsilon)$ and $f(\varepsilon)$ then integrate $N = \int_0^{\nu} g\, f \, d\varepsilon$ and rearrange for μ.