

## Particle distribution function

Last time we calculated the number of possible ways to spread  $N$  particles b/w different energy states  $E_n$  (each with degeneracy  $d_n$ ) such that  $N_n$  particles are in  $n$ -th state.

Distinguishable particles:  $W(N_1, N_2, \dots, N_n, \dots) = N! \prod_{n=1}^{\infty} \frac{d_n^{N_n}}{N_n!}$

Fermions:  $W(N_1, N_2, \dots) = \prod_{n=1}^{\infty} \frac{d_n!}{N_n!(d_n - N_n)!}$

Bosons:  $W(N_1, N_2, \dots) = \prod_{n=1}^{\infty} \frac{(d_n + N_n - 1)!}{N_n!(d_n - 1)!}$

Suppose that we now need to determine the most probable configuration  $(N_1, N_2, \dots)$  if we know the total energy of the system. Essentially, we need to determine for what combination of  $(N_1, N_2, \dots)$   $W(N_1, N_2, \dots)$  is maximum, with constraints  $\sum_{n=1}^{\infty} N_n = N$  and  $\sum_{n=1}^{\infty} E_n N_n = E$

To find such configuration we can use a mathematical trick using Lagrange multipliers:

To maximize  $F(x_1, x_2, \dots)$  subject of constraints  $f_1(x_1, x_2, \dots) = 0$  and  $f_2(x_1, x_2, \dots) = 0$ , we need to construct a function  $G(x_1, x_2, \dots) = F + \alpha f_1 + \beta f_2$  and set all partial derivatives equal to zero

$$\frac{\partial G}{\partial x_1} = 0 \quad \frac{\partial G}{\partial x_2} = 0$$

Since it is inconvenient to work with products  $\Pi$ , we are going to maximize  $\ln W(N_1, N_2, \dots)$  so that our  $G(N_1, N_2, \dots)$  is

$$G(N_1, N_2, \dots) = \ln W + \alpha \left[ N - \sum_{n=1}^{\infty} N_n \right] + \beta \left[ E - \sum_{n=1}^{\infty} E_n N_n \right]$$

By calculating  $\frac{\partial G}{\partial N_n}$  for each type of particle and setting the derivative to zero, we obtain the following functional dependence for the most probable number of particles in the  $n^{\text{th}}$  state

Distinguishable particles :  $N_n = d_n e^{-(\alpha + \beta E_n)}$

Fermions :  $N_n = \frac{d_n}{e^{(\alpha + \beta E_n)} + 1}$       Bosons :  $N_n = \frac{d_n - 1}{e^{(\alpha + \beta E_n)} - 1}$

How do we know what are  $\alpha$  and  $\beta$ ?  
From our constraints:

$$N = \sum_{n=1}^{\infty} N_n = \sum_{n=1}^{\infty} \frac{d_n}{e^{(\alpha + \beta E_n)} \begin{pmatrix} +0 \\ +1 \\ +1 \end{pmatrix}} \begin{matrix} \text{DP} \\ \text{Fermions} \\ \text{Bosons} \end{matrix}$$

$$E = \sum_{n=1}^{\infty} E_n N_n = \sum_{n=1}^{\infty} \frac{d_n E_n}{e^{(\alpha + \beta E_n)} \begin{pmatrix} +0 \\ +1 \\ -1 \end{pmatrix}} \begin{matrix} \text{Disting. part} \\ \text{Fermions} \\ \text{Bosons} \end{matrix}$$

However, this calculation will require more specific information about energy states.

Ideal gas: a collection of non-interacting non-relativistic massive particles

Continuous spectrum, momentum  $\vec{p} = (\hbar k_x, \hbar k_y, \hbar k_z)$

Energy  $\rightarrow$  kinetic energy  $E_k = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$

Each state with wave-vector  $\vec{k}$  occupies unique "Volume" in  $k$  space  $-\frac{V}{\pi^3}$  (here  $V$  is a physical volume of the whole system)

Degeneracy  $d_k = \frac{1}{8} \frac{4\pi k^2 dk}{(\pi^3/V)} = \frac{V}{2\pi^2} k^2 dk$  (if not include spin)

For distinguishable particles:  $N_n = \frac{d_n}{e^{\alpha + \beta E_n}} = e^{-\alpha} d_n e^{-\beta E_n}$

$$N = \sum_{n=1}^{\infty} N_n \rightarrow e^{-\alpha} \int_0^{\infty} \frac{V}{2\pi^2} k^2 dk \cdot e^{-\beta \frac{\hbar^2 k^2}{2m}}$$

$$N = V e^{-\alpha} \left( \frac{m}{2\pi\beta\hbar^2} \right)^{3/2}$$

$$E = \sum_{n=1}^{\infty} E_n N_n \rightarrow e^{-\alpha} \int_0^{\infty} \frac{V}{2\pi^2} k^2 dk \cdot \frac{\hbar^2 k^2}{2m} e^{-\beta \frac{\hbar^2 k^2}{2m}} = \frac{3V}{2\beta} e^{-\alpha} \left( \frac{m}{2\pi\beta\hbar^2} \right)^{3/2}$$

$$\frac{E}{N} = \frac{3}{2\beta} = \frac{3}{2} k_B T \quad \text{from kinetic theory of an ideal monatomic gas}$$

Thus, it looks like  $\beta = 1/k_B T$

Since we have  $e^{\alpha + \beta E_n}$ , it is traditional to write  $\alpha = -\mu(T)/k_B T$ , so that  $e^{\alpha + \beta E_n} \rightarrow e^{E_n - \mu(T)/k_B T}$

$\mu(T)$  - chemical potential, the energy "price" for adding an extra particle to the system

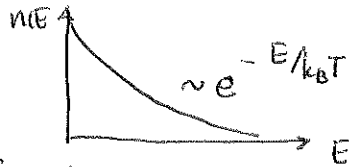
$$\text{Since } N/V = e^{-\alpha} \left( \frac{m}{2\pi\beta\hbar^2} \right)^{3/2},$$

$$\mu(T) = k_B T \left[ \ln\left(\frac{N}{V}\right) + \frac{3}{2} \ln\left(\frac{2\pi\hbar^2}{mk_B T}\right) \right] \quad \text{for the distinguishable particles}$$

Thus, depending on statistics, we can describe an ideal gas of mass  $m$  using following distributions for the number of particles in each state  $n = N/d$

Distinguishable particles!

① Maxwell-Boltzmann distribution



$$n(E_k) = e^{-(E_k - \mu)/k_B T}$$

more familiar form

$$E_k = mv^2/2, \text{ for all } E_k$$

$$n(E_k) = e^{-mv^2/2k_B T} \cdot \frac{N}{V} \left( \frac{2\pi\hbar^2}{k_B T m} \right)^{3/2}$$

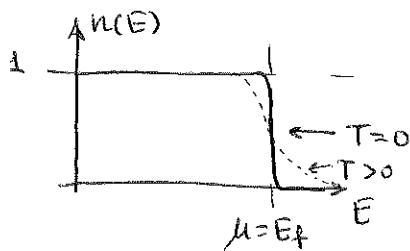
② Fermions  
Fermi-Dirac distribution

$$n(E_k) = \frac{1}{e^{(E_k - \mu)/k_B T} + 1} < 1$$

③ Bosons  
Bose-Einstein distribution

$$n(E_k) = \frac{1}{e^{(E_k - \mu)/k_B T} - 1}$$

Fermions at  $T \rightarrow 0$   $e^{\frac{E_k - \mu}{k_B T}} \rightarrow \begin{cases} 0 & \text{if } E_k - \mu \ll 0 \\ \infty & \text{if } E_k - \mu > 0 \end{cases}$



$$n(E_k) \rightarrow \begin{cases} 1 & \text{if } E_k - \mu < 0 \\ 0 & \text{if } E_k - \mu > 0 \end{cases}$$

$$n(E_k) = \frac{1}{e^{(E_k - E_F)/k_B T} + 1}$$

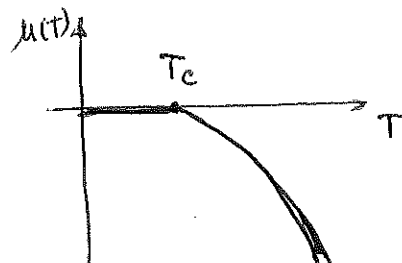
Bosons : as ~~above~~  $n(E_k) \geq 0 \Rightarrow$  for  $E_k = 0$   $e^{-\mu/k_B T} > 1$   
thus  $\mu(T) < 0$

Normally, to find  $\mu$ , we need to evaluate

$$N = \frac{V}{2\pi^2} \int_0^\infty \frac{k^2 dk}{e^{(\hbar^2 k^2/2m - \mu)/k_B T} - 1}$$

$$T_c = \frac{2\pi\hbar^2}{m k_B} \left( \frac{N}{2.61 V} \right)^{3/2}$$

For  $T < T_c$  Bose-Einstein condensate is formed



Another type of boson - photon  
massless  $E_k = \hbar ck = \hbar \omega$ ,  $\mu = 0$

Thermal radiation spectrum  $\Rightarrow$  black body spectrum

$$N_k = \frac{d_k}{e^{E_k/k_B T} - 1}, \text{ usually written for } \omega$$

$$d_k \text{ (or } d\omega) = 2 \cdot \frac{1}{8} \frac{4\pi k^2 dk}{V^3/V} = \frac{V}{\pi^2} k^2 dk = \frac{V}{\pi^2 c^3} \omega^2 d\omega$$

$$dN_\omega = \frac{V}{\pi^2 c^3} \frac{\omega^2}{e^{\hbar\omega/k_B T} - 1} d\omega$$

Typically we use energy density  $f(\omega) = \frac{\hbar\omega \cdot dN_\omega}{V \cdot d\omega}$

$$f(\omega) = \frac{\hbar\omega^3}{\pi^2 c^3 (e^{\hbar\omega/k_B T} - 1)}$$

