

1 Bose-Einstein condensation and Statistical mechanics

We start defining the partition function in the grand-canonical ensemble:

$$Z = \prod_i \sum_{n_i=0}^{\infty} e^{-\beta(\varepsilon_i - \mu)n_i} \quad (1)$$

where μ is the chemical potential and $\beta = \frac{1}{k_B T}$. Also, ε_i is the energy of the state i and n_i the number of particles in that state. The sum over n_i shows the possible combinations of number in every state i . With them, we can define the total energy and the total number of particles with $E = \sum_i \varepsilon_i n_i$ and $N = \sum_i n_i$.

Now, we can define the partition function of a particular state Z_i as

$$Z_i = \sum_{n_i=0}^{\infty} e^{-\beta(\varepsilon_i - \mu)n_i} = \sum_{n_i=0}^{\infty} (e^{-\beta(\varepsilon_i - \mu)})^{n_i} \quad (2)$$

Notice that the sum converges only if $e^{-\beta(\varepsilon_i - \mu)} < 1$. It implies that $\varepsilon_i - \mu > 0$ for any energy ε_i . Thus, the chemical potential is bounded by the energy of the states. As the ground state ε_0 is the smallest energy, the chemical potential μ should be smaller than the ground state energy. This fact is important for the physics of the system. Let us to analyse implications of this fact.

Considering this condition for the chemical potential, we use the geometric serie to get

$$Z_i = \frac{1}{1 - e^{-\beta(\varepsilon_i - \mu)}} \quad (3)$$

We can get the number of particles in the state i using that $n_i = \frac{1}{\beta} \frac{1}{Z_i} \frac{\partial Z_i}{\partial \mu}$. Hence,

$$n_i = \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1} \quad (4)$$

and the total number of particles is

$$N = \sum_{i=0}^{\infty} n_i = \sum_{i=0}^{\infty} \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1} \quad (5)$$

We will set apart the ground state $i = 0$:

$$N = \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1} + \sum_{i=1}^{\infty} \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1} \quad (6)$$

We will call $N_0 = \frac{1}{e^{\beta(\varepsilon_0 - \mu)} - 1}$. Notice that when $\mu \rightarrow \varepsilon_0$ we can expand in series and to get

$$N_0 \approx \frac{1}{\beta(\varepsilon_0 - \mu)} \quad (7)$$

We observe that when the chemical potential approaches to the ground state energy, the number of particles in this state is big.

If we go to the particles out of the ground state, since $\mu < \varepsilon_0$, we have that

$$\sum_{i=1}^{\infty} \frac{1}{e^{\beta(\varepsilon_i - \mu)} - 1} < \sum_{i=1}^{\infty} \frac{1}{e^{\beta(\varepsilon_i - \varepsilon_0)} - 1} \quad (8)$$

It means that there is a limit for the number of particles in the higher energy states.

We will compute the total number of particles. For this, we will work in a thermodynamical limit, where the number of particles and the volume are big enough. In this limit, we will approximate the sum with an integral:

$$\sum_{i=0}^{\infty} \rightarrow \int d^3l \quad (9)$$

where l is a quantum number that defines the state.

First we will analyse free bosons. For this, we will take as our volume a square box of length L . The quantum state for a free particle in this box is given by

$$\varepsilon = \frac{\hbar^2 k^2}{2m} \quad (10)$$

where the momentum component is given by $k_i = \frac{2\pi l_i}{L}$. In this case, we have that the minimum energy (ground state) corresponds to take $k = 0$. Furthermore, we can write a differential of l in terms of k as $dl_i = \frac{L dk_i}{2\pi}$. Hence, $d^3l = \frac{V}{(2\pi)^3} d^3k$ and using spherical coordinates, the sum becomes

$$\sum_{i=0}^{\infty} \rightarrow \frac{4\pi V}{(2\pi)^3} \int_0^{\infty} k^2 dk \quad (11)$$

We can write this integral in terms of the energy rather than in terms of the momentum. Thus,

$$\sum_{i=0}^{\infty} \rightarrow \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \int_0^{\infty} \sqrt{\varepsilon} d\varepsilon \quad (12)$$

Notice that for $k = 0$ or $\varepsilon = 0$ the integral vanishes. However, from (??) we know that the ground state could get a considerable number of particles, so, we have to add by hand N_0 in the computation when we use the integral. Thus, the approximated number of particles are:

$$N \approx N_0 + \frac{V}{4\pi^2} \left(\frac{2m}{\hbar^2} \right)^{\frac{3}{2}} \int_0^{\infty} d\varepsilon \frac{\sqrt{\varepsilon}}{e^{\beta(\varepsilon - \mu)} - 1} \quad (13)$$

We will examine the limit $\mu \rightarrow \varepsilon_0$. For this case, we have set $\varepsilon_0 = 0$. Therefore, doing the integration in this limit we get

$$\frac{N_0}{N} \simeq 1 - \left(\frac{T}{T_c} \right)^{\frac{3}{2}} \quad (14)$$

where we have defined

$$T_c = \left(\frac{N}{\zeta\left(\frac{3}{2}\right)V} \right)^{\frac{2}{3}} \left(\frac{2\pi\hbar^2}{mk_B} \right) \quad (15)$$

Let us to consider the particle in presence of harmonic potential. In this case, the energy is known:

$$\varepsilon = \left(l_x + l_y + l_z + \frac{3}{2} \right) \hbar\omega \quad (16)$$

We can write $l = l_x + l_y + l_z$ and in spherical coordinates $d^3l = l^2 dl d\Omega = \frac{(\varepsilon - \varepsilon_0)^2}{(\hbar\omega)^3} d\varepsilon d\Omega$, where we have written $\varepsilon_0 = (3/2)\hbar\omega$ and $d\Omega$ is the angular part. Therefore, passing from sum to integral

$$\sum_{i=0}^{\infty} \rightarrow \frac{4\pi}{(\hbar\omega)^3} \int_{\varepsilon_0}^{\infty} (\varepsilon - \varepsilon_0)^2 d\varepsilon \quad (17)$$

As before, when the energy is in the ground state the integral vanishes, so we have to introduce the term N_0 in the number of particles. Hence,

$$N \approx N_0 + \frac{4\pi}{(\hbar\omega)^3} \int_{\varepsilon_0}^{\infty} d\varepsilon \frac{(\varepsilon - \varepsilon_0)^2}{e^{\beta(\varepsilon - \mu)} - 1} \quad (18)$$

We do a change of variables $\bar{\varepsilon} = \varepsilon - \mu$ to have

$$N \approx N_0 + \frac{4\pi}{(\hbar\omega)^3} \int_{\varepsilon_0 - \mu}^{\infty} d\bar{\varepsilon} \frac{(\bar{\varepsilon} + \mu - \varepsilon_0)^2}{e^{\beta\bar{\varepsilon}} - 1} \quad (19)$$

As in the free case, we are interested in the limit when $\mu \rightarrow \varepsilon_0$. Therefore, we can approximate the integral to

$$N \approx N_0 + \frac{4\pi}{(\hbar\omega)^3} \int_0^{\infty} d\bar{\varepsilon} \frac{\bar{\varepsilon}^2}{e^{\beta\bar{\varepsilon}} - 1} \quad (20)$$

Integrating we get

$$\frac{N_0}{N} \simeq 1 - \left(\frac{T}{T_c} \right)^3 \quad (21)$$

where in this case the critical temperature is defined as

$$T_c = \left(\frac{N}{8\pi\zeta(3)} \right)^{\frac{1}{3}} \frac{\hbar\omega}{k_B} \quad (22)$$

Notice that as in the free case as in the harmonical potential we had something like

$$N = N_0 + \alpha \int_0^{\infty} d\varepsilon \frac{\varepsilon^\tau}{e^{\beta\varepsilon} - 1} \quad (23)$$

where τ is an index depending on the case, here we had $\tau = \frac{1}{2}$ in the free case and $\tau = 2$ for the harmonical potential. We called α the constants that appeared in the construction of the density of states, which also depends on the case. It is important that $\tau > 0$ to have a convergent integral. Making a direct integration and arranging we have that

$$\frac{N_0}{N} = 1 - \left(\frac{T}{T_c} \right)^{1+\tau} \quad (24)$$

where the critical temperature in this case is given by

$$T_c = \left(\frac{N}{\alpha \Gamma(1+\tau) \zeta(1+\tau)} \right)^{\frac{1}{1+\tau}} \quad (25)$$