# The chemical equilibrium

Suppose you have the following reaction:

$$A + B \leftrightarrow C + D \tag{1}$$

We have two arrows, because the reaction can happen in two ways. However, if you wait long enough, at a certain point, the reaction rate for $A + B \to C + D$ and the reaction rate for $A + B \leftarrow C + D$ will be closer and closer together, so the number densities of $A$, $B$, $C$ and $D$ will converge to certain values. Then, we can say that they reached "equilibrium." In this article, we will find a formula that these number densities satisfy.

In the last article, we have seen that the chemical potential is conserved in the equilibrium, i.e.

$$\mu_A + \mu_B = \mu_C + \mu_D \tag{2}$$

If we now express the number density in terms of the chemical potential, temperature and other relevant quantities, our job is done. Earlier, we learned that the Bose-Einstein distribution and the Fermi-Dirac distribution can be approximated as the Maxwell-Boltzmann distribution in the limit ($e^{(\epsilon-\mu)/kT} \gg 1$). This is the case of our interest, so we have

$$N_i = \frac{1}{h^3} \int \frac{d^3p d^3q}{e^{(\epsilon-\mu_i)/kT}} \tag{3}$$

where $i$ can be $A$, $B$, $C$, $D$. Using

$$\epsilon = E_i + \frac{p^2}{2m} \tag{4}$$

where $E_i$ is whateever the energy the particle $i$ has when $p = 0$, we get

$$n_i \equiv \frac{N_i}{V} = \left(\frac{m_i kT}{2\pi\hbar^2}\right)^{3/2} e^{(-E_i+\mu_i)/kT} \tag{5}$$

(**Problem 1.** Show this!)

We also know that the reaction (1) can produce energy. Let's denote the energy change upon reaction $A + B \to C + D$ by

$$\Delta E = E_C + E_D - E_A - E_B \tag{6}$$

Then, (2) implies

$$\frac{n_C n_D}{n_A n_B} = \left(\frac{m_C m_D}{m_A m_B}\right)^{3/2} e^{-\Delta E/kT} \tag{7}$$

**Problem 2.** Repeat the above calculation for $2A + B \leftrightarrow C$

# Summary

- The number density of particles during chemical equilibrium can be derived from the Maxwell-Boltzmann distribution and the conservation of chemical potential. The final result has a factor $e^{-\Delta E/kT}$ where $\Delta E$ is the energy change during the reaction.