## Plasma ionization. Saha equation.

([2], p.184-187; [11] p.382-390, 402-408)

How to make plasma? The most natural way is to heat a gas to high temperature. High-speed electrons collide with atoms and tear away electrons from atomic orbits. The degree of ionization depends on temperature. A general relation between the degree of ionization and temperature can be obtained from a statistical description of plasma in thermodynamic equilibrium.

Consider  $N_{a0}$  atoms in volime V. Then, as a result of an ionization process there are  $N_i$  ions and  $N_e = N_i$  electrons. The number of remaining neutral atoms is

$$N_a = N_{a0} - N_i$$

Consider a single nucleus. If it has a bound electron then this is an atom, otherwise it is ion. According to statistical physics the probability electron is in the energy state  $\epsilon_k$  is

$$w_k = A \exp\left(-\frac{\epsilon_k}{T}\right)$$

where A is a constant. Negative  $\epsilon_k$  correspond to bound states, and positive  $\epsilon_k$  correspond to continuum.

In hydrogen atom the energy of the bound states is given by the Bohr formula:

$$\epsilon_k = -\frac{me^4}{2\hbar^2 k^2} \quad \mathbf{SI} : \epsilon_k = -\frac{me^4}{32\pi^2 \epsilon_0^2 \hbar^2 k^2}$$

where k = 1, 2, ... For simplicity consider only the lowest level.



Figure 1: The energy energy levels of hydrogen atom The abscissa denotes the position coordinate of the electron (the distance between the proton and electron), r, in units of the Bohr radius  $a_0$ , where  $a_0 = \frac{\hbar^2}{me^2}$  **SI** : $a_0 = \frac{4\pi\epsilon_0\hbar^2}{me^2}$ .

For simplicity consider only the lowest level k = 1:

$$\epsilon = -\frac{me^4}{2\hbar^2} = -I$$

where I = Ry = 13.6 eV is the ionization potential.

Constant A can be found from the condition that the total probability is 1:

$$\sum_{k} w_k = 1$$

Thus,

$$A = \left[\sum_{k} \exp\left(-\frac{\epsilon_k}{T}\right)\right]^{-1} = \left[\exp\frac{I}{T} + \sum_{\epsilon_k > 0} \exp\left(-\frac{\epsilon_k}{T}\right)\right]^{-1}$$

The states with  $\epsilon_k > 0$  are in the continuum. Thus, the second term (partition function) can estimated as an integral in the phase space. In the quasi-classical approximation, each energy state corresponds to an elementary cell in the phase space (p, r), the volume of which  $(2\pi\hbar)^3$ :

$$\sum_{\epsilon_k > 0} \to \int \frac{d^3 p d^3 r}{(2\pi\hbar)^3}$$

where p is momentum.

Each electron occupies 1 elementary cell in the phase space (p, r) of volume  $(2\pi\hbar)^3$ . This is Pauli's exclusion principle.

In the continuum state we can neglect the energy of interaction between electron and nucleus, and assume that energy  $\epsilon_k = p^2/2m$ . Then,

$$\sum_{\epsilon_k>0} \exp\left(-\frac{\epsilon_k}{T}\right) = \int \frac{d^3 p d^3 r}{(2\pi\hbar)^3} \exp\left(-\frac{p^2}{2mT}\right) =$$
$$= \frac{V}{(2\pi\hbar)^3} \int_0^\infty 4\pi p^2 dp \exp\left(-\frac{p^2}{2mT}\right) =$$
$$= \frac{4\pi V}{(2\pi\hbar)^3} (2mT)^{3/2} \int_0^\infty dx \, x^2 \exp\left(-x^2\right) =$$
$$= \frac{V m^{3/2} T^{3/2}}{2^{3/2} \pi^{3/2} \hbar^3} = \frac{V}{V_Q}.$$

Here we assumed that the space is uniform and isotropic and used the following relations:

$$\int d^3r = V$$

is volume available for electron;

$$\int_0^\infty dx \, x^2 \exp\left(-x^2\right) = \sqrt{\pi}/4$$
$$x = p/\sqrt{2mT}$$

Also, we defined "quantum volume"  $V_Q$  as

$$V_Q = \frac{2^{3/2} \pi^{3/2} \hbar^3}{m^{3/2} T^{3/2}} = \left(\sqrt{\frac{2\pi}{mT}} \hbar\right)^3 \equiv \lambda_B^3$$

where

$$\lambda_B = \frac{\sqrt{2\pi}\hbar}{\sqrt{mT}} = \sqrt{4\pi}\frac{\hbar}{p}$$

where  $p = \sqrt{2mT}$  is momentum.

Thus,  $\lambda_B$  is a De Broglie wavelength of electrons for thermal motion.

The physical volume V per electron is equal to the total plasma volume divided by the number of electrons, that is:

$$V = n_e^{-1}$$

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Thus, the partition function of the free states is:

$$\sum_{\epsilon_k > 0} \exp\left(-\frac{\epsilon_k}{T}\right) = \frac{V}{V_Q} = \frac{1}{\lambda_B^3 n_e}$$

Thus, constant A:

$$A = \left(\exp\frac{I}{T} + \frac{1}{\lambda_B^3 n_e}\right)^{-1}.$$

Therefore, the probability  $w_a$  of an proton to have a bound electron is:

$$w_a = \frac{\exp\left(I/T\right)}{\exp\left(I/T\right) + 1/\lambda_B^3 n_e}$$

The corresponding probability for ions is:

$$w_i = 1 - w_a \equiv \frac{1/\lambda_B^3 n_e}{\exp\left(I/T\right) + 1/\lambda_B^3 n_e}$$

Then, the relative ion density is:

$$\frac{n_i}{n_a} = \frac{w_i}{w_a} = \frac{1}{n_e \lambda_B^3} \exp\left(-I/T\right)$$

or

$$\frac{n_i n_e}{n_a} = \frac{1}{\lambda_B^3} \exp\left(-I/T\right)$$

Note that electrons, ions and atoms have internal degrees of freedom, which affect their partition functions. For instance, electrons have two spin states, "up" and "down", thus statistical weight for electrons  $g_e = 2$ . Because of this each energy levels can be occupied by two electrons. Therefore, in the last equation we should replace  $n_e$  with  $n_e/g_e$ .

Taking into account the statistical weights for ions  $g_i$  and atoms  $g_a$  we write:

$$\frac{n_e n_i}{n_a} = \frac{g_i g_e}{g_a} \frac{\exp\left(-I/T\right)}{\lambda_B^3} \equiv K(T)$$

K(T) is the equilibrium constant.

The degree of ionization is defined as

$$\alpha = n_e/n_{a0} = n_i/n_{a0}$$

where  $n_{a0}$  is the total number of atoms and ions. Then  $n_a = (1 - \alpha)n_{a0}$  and the final equation for the ionization degree is:

$$\frac{\alpha^2}{(1-\alpha)} = \frac{g_i g_e}{g_a} \frac{\exp\left(-I/T\right)}{\lambda_B^3 n_{a0}}$$

This is Saha equation.



Figure 2: The degree of ionization,  $\alpha$ , of hydrogen plasma in thermodynamic equilibrium for different plasma densities (in cm<sup>-3</sup>). *J* is the ionization potential.

This plot shows that the characteristic temperature of ionization is much lower than the ionization potential. This is because the large factor  $1/\lambda_B^3 n_{a0}$  in the Saha equation. This ratio can be written as

$$\left(\frac{n^{-1/3}}{\lambda_B}\right)^3,$$

cubed ratio of the distance between the particles and the De Broglie wavelength. For example, for  $n_{a0} = 10^{15}$  and T = I = 13.6 eV, this factor is  $1.7 \cdot 10^8$ .

We have considered only the ground state of the atom and continuum, and neglected the higher bound state. How accurate is this approximation? Since the ionization occurs at  $T \ll I$ , and the energy difference between the ground state and the next energy level is  $\frac{3}{4}I$ , the probability of the transition to this level is  $\exp\left(-\frac{3}{4}I/T\right)$ , very small. The electron has much higher probability of transition to continuum than to the higher energy level. The reason for this is that the number of the available states in the continuum is very large, and even though the probability of transition to each of them is lower the total probability of the transition to the continuum is much higher than for the higher bound states.

Example: solar core:  $n = 10^{26} \text{ cm}^{-3}$ ,  $T = 10^3 \text{eV} \approx 10^7 \text{K}$ . (Note:  $\hbar = 6.582 \times 10^{-16} \text{eV} \cdot \text{s}$ ,  $m = 5.69 \times 10^{-16} \text{eV} \cdot \text{s}^2 \text{cm}^{-2}$ ).

$$\lambda_B = \frac{\sqrt{2\pi}\hbar}{\sqrt{mT}} \simeq 2 \cdot 10^{-9} \text{cm}$$
$$\lambda_B^3 n \simeq 1$$
$$\frac{\alpha^2}{1-\alpha} = \exp\left(-\frac{13.6}{10^3}\right) \approx 1$$
$$\alpha \simeq 0.6$$

Ionization is not necessary complete in the solar core.

Example: solar surface: 
$$n = 10^{16} \text{ cm}^{-3}$$
,  
 $T \simeq 6000 \text{ K} \simeq 0.5 \text{ eV}$ .  
 $\lambda_B \simeq 9.6 \cdot 10^{-8} \text{ cm}$   
 $1/\lambda_B^3 n \simeq 10^5$   
 $\frac{\alpha^2}{1-\alpha} = \frac{1}{n\lambda_B^3} \exp\left(-\frac{13.6}{0.5}\right) \simeq 2 \cdot 10^{-7}$   
 $\alpha \approx 4 \cdot 10^{-4}$ 

This is weakly ionized plasma.

## Elementary processes in plasma

The Saha equation describes ionization of plasma in thermal equilibrium. When plasma is not in thermodynamic equilibrium it is important to study elementary processes of ionization and recombination, which occur because of particle collisions.

The most important processes are:

- 1. Ionization by electron impact
- 2. Photoionization
- 3. Recombination

## Ionization by electron impact

Consider ionization due electron collisions:

$$e + H \to H^+ + e + e$$

First, we find the cross-section of this process. Consider collision of two electrons. Ionization will occur when the energy transferred to the electron in the bound state exceeds the ionization potential.



Figure 3: Electron collision.

Calculate the energy of the initially stationary electron after the collision. For large collision distances  $\rho$ , the electron will move in the direction perpendicular to velocity of the fast electron.

Acceleration in the perpendicular direction is:

$$w_{\perp} = \frac{e^2}{m} \frac{\rho}{(\rho^2 + v^2 t^2)^{3/2}},$$

Then, the velocity change is:

$$v_{\perp} = \frac{e^2}{m} \int_{-\infty}^{\infty} \frac{\rho dt}{(\rho^2 + v^2 t^2)^{3/2}}$$

$$v_{\perp} = \frac{e^2}{mv\rho} \int_{-\infty}^{\infty} \frac{dx}{(1+x^2)^{3/2}} = \frac{2e^2}{mv\rho}$$

The corresponding energy change is

$$\epsilon = \frac{mv_{\perp}^2}{2} = \frac{2e^4}{mv^2\rho^2} = \frac{e^4}{W\rho^2}$$

where  $W = mv^2/2$  the initial electron energy. Thus,  $\rho^2 = \left(\frac{e^4}{W\epsilon}\right)$ .

Define the differential cross-section as:

$$d\sigma = |2\pi\rho d\rho| = \frac{\pi e^4}{W\epsilon^2} d\epsilon.$$

Ionization will occur when the energy transfer is greater than the ionization potential:  $\epsilon \geq I$ . However, the energy transfer cannot exceed the initial energy W.

Therefore, the total ionization cross-section is obtained by integrating the differential cross-section from I to W:

$$\sigma_i = \int_I^W d\sigma = \int_I^W \frac{\pi e^4}{W \epsilon^2} d\epsilon = \frac{\pi e^4 (W - I)}{W^2 I}$$

This is so-called Thompson's formula.

Maximum of this function is at W = 2I:

$$\sigma_{\rm max} = \frac{\pi e^4}{4I^2} = \pi a_B^2 = 10^{-16} \rm cm^2$$

where  $a_B$  is Bohr's radius of electron.



Figure 4: Cross-section ionization of hydrogen atom by electron impact. The solid is the experimental cross-section. the dashed line shows Thompson's formula. The ionization rate by electrons in a unit volume is:

 $n_a \langle \sigma_i v_e \rangle$ 

where the brackets denote averaging over a velocity distribution of electrons.

Then the number of electrons growths as a result of ionization as

$$\frac{dn_e}{dt} = n_e n_a \langle \sigma_i v_e \rangle$$

When the number of electrons is large then the reverse process of collisional (or triple) recombination takes place when two electrons collide with an ion and one of the becomes bound and another one carries away the released energy.

$$H^+ + e + e \to H + e$$

Let  $\sigma_*$  be the cross-section of this process. Then its rate is:

$$n_i n_e^2 \langle \sigma_* v_e \rangle = n_i n_e^2 \beta$$

where  $\beta = \langle \sigma_* v_e \rangle$  is recombination constant.

$$\frac{dn_e}{dt} = n_e n_i \langle \sigma_i v_e \rangle - \beta n_e^2 n_i$$

The recombination constant  $\beta$  can be calculated from the dynamics of collisions or more easily from the Saha equation.

Indeed, in the thermodynamic equilibrium  $dn_e/dt = 0$ :

$$n_e n_a \langle \sigma_i v_e \rangle - \beta n_e^2 n_i = 0$$
$$\beta = \frac{n_e n_a}{n_e^2 n_i} \langle \sigma_i v_e \rangle = \frac{n_a}{n_e n_i} \langle \sigma_i v_e \rangle$$

From Saha equation we know that

$$\frac{n_i n_e}{n_a} = K(T)$$

Therefore,

$$\beta = \frac{\langle \sigma_i v_e \rangle}{K(T)}$$

## Photoionization and recombination

Photorecombination:  $H^+ + e \rightarrow H + \hbar \omega$ Photoionization:  $H + \hbar \omega \rightarrow H^+ e$ 

The rate of photoionization is proportional to

density of both atoms and photons:

$$\left(\frac{dn_e}{dt}\right)_{\text{photoion}} = \mu n_a$$

where the number of photons is included in the coefficient,  $\mu$ . In the thermodynamic equilibrium the number of photons radiated in plasma is a function of temperature.

Similarly, the rate of photorecombination is:

$$\left(\frac{dn_e}{dt}\right)_{\text{photorec}} = -\gamma n_i n_e$$

A complete equation for electron density including the collision terms can written as:

$$\left(\frac{dn_e}{dt}\right) = n_e n_a \langle \sigma_i v_e \rangle - \beta n_e^2 n_i + \mu n_a - \gamma n_e n_i$$

In the local thermodynamic equilibrium (LTE) the collisional and radiative processes are balanced separately:

$$n_e n_a \langle \sigma_i v_e \rangle = \beta n_e n_i$$

$$\mu n_a = \gamma n_e n_i$$

However, in laboratory plasma, photoionization is not significant because photons escape, and if the plasma density is not very high then photorecombination is more significant then the collisional triple recombination. Then, we have a balance between the electron-impact ionization and photoionization:

$$n_e n_a \langle \sigma_i v_e \rangle = \gamma n_e n_i$$

In this case, the ionization degree depends only on plasma temperature:

$$\alpha = \frac{n_i}{n_a} = \frac{\langle \sigma_i v_e \rangle}{\gamma}$$

This is a replacement for Saha equation in low-density plasmas. This is called **coronal equilibrium** because this is valid for the solar corona.

Numerical formula for the photorecombination coefficient:

$$\gamma = \frac{4 \cdot 10^{-13}}{\sqrt{T_{\rm eV}}} \ {\rm cm}^3/{\rm s}$$