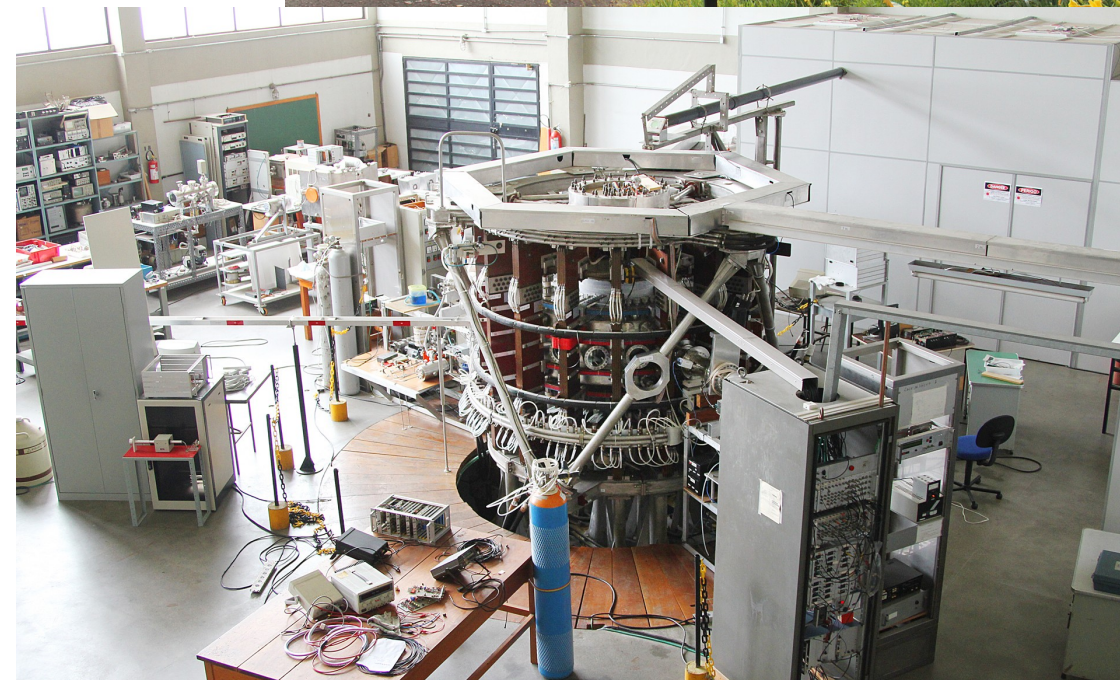


# PGF5112 - Plasma Physics I

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- **Thermodynamic equilibrium states**

- Distribution function of plasmas in thermodynamic equilibrium
- General principle of *detailed balance and binary collisions*
- *The Maxwell distribution function (particles without internal states)*
- *The Boltzmann distribution function (particles with internal states)*
- *Equilibrium in the presence of an external force*

- **Degree of ionization and the Saha equation**

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# Under equilibrium conditions, collisions between particles do not result in changes of the distribution function

- The characteristics of a plasma in thermodynamic equilibrium can be understood from the kinetic Boltzmann equation

$$\frac{\partial f_\alpha}{\partial t} + \mathbf{v} \cdot \nabla f_\alpha + \frac{q_\alpha}{m_\alpha} (\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_\alpha = \sum_{\beta} C_{\text{coll}}[f_\alpha, f_\beta]$$

– Note that, in the collision operator sum,  $\beta$  also takes the value of  $\alpha$

- In a closed system, and in the absence of external forces, the equilibrium state is spatially homogeneous. In this case, the kinetic equation reduces to simply

$$\sum_{\beta} C_{\text{coll}}[f_\alpha, f_\beta] = \sum_{\beta} \int_{\Omega} \int_{v_\beta} \left[ f_\alpha(\mathbf{v}'_\alpha) f_\beta(\mathbf{v}'_\beta) - f_\alpha(\mathbf{v}_\alpha) f_\beta(\mathbf{v}_\beta) \right] g_{\alpha\beta} \sigma_{\alpha\beta} (g_{\alpha\beta}, \Omega) d\Omega d^3v_\beta = 0$$

– Where  $g_{\alpha\beta} = |\mathbf{v}_\alpha - \mathbf{v}_\beta|$  is the relative velocity between particles

- Therefore, in such an equilibrium, one has  $f_\alpha(\mathbf{v}'_\alpha) f_\beta(\mathbf{v}'_\beta) = f_\alpha(\mathbf{v}_\alpha) f_\beta(\mathbf{v}_\beta)$ 
  - There are no changes in the distribution function as a result of collisions between particles



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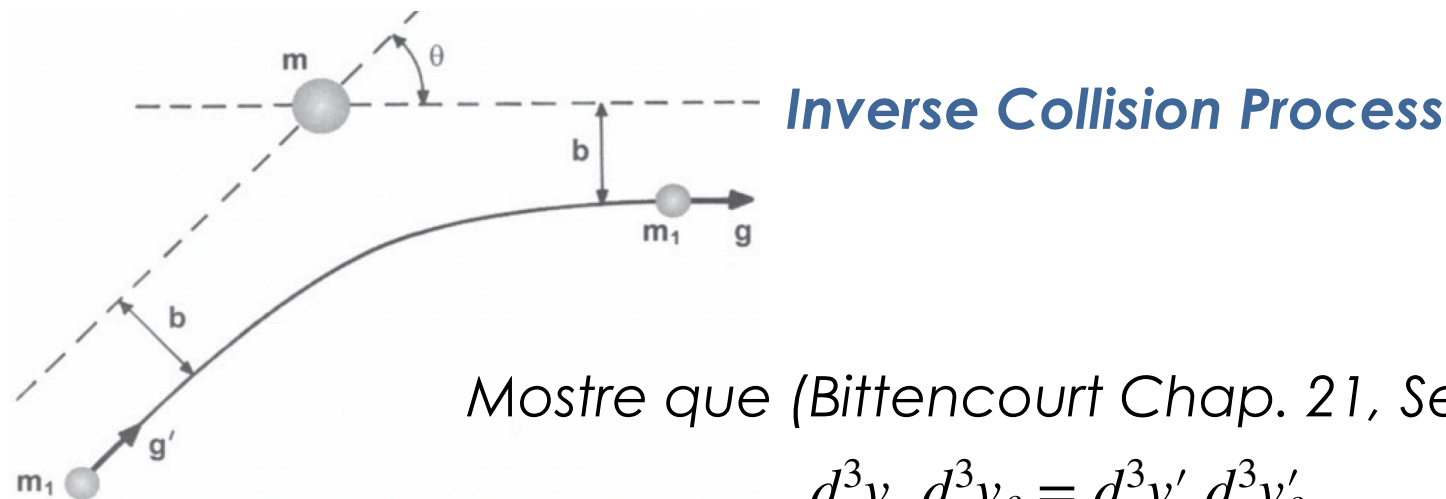
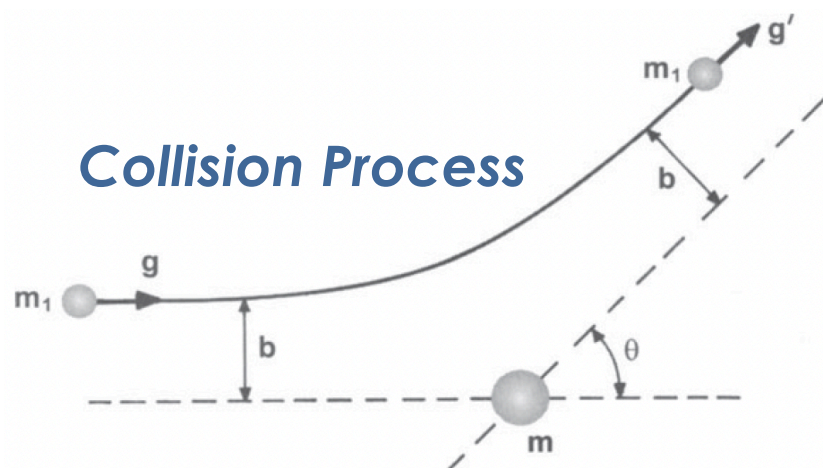
# In thermodynamic equilibrium, a given collision process is perfectly balanced by its respective inverse collision process

- The condition  $f_\alpha(\mathbf{v}'_\alpha) f_\beta(\mathbf{v}'_\beta) = f_\alpha(\mathbf{v}_\alpha) f_\beta(\mathbf{v}_\beta)$  can be understood on the basis of the general principle of detailed balance
  - Under equilibrium conditions, the effect of each type of collision is exactly compensated by the effect of the corresponding inverse collision

$$f_\alpha(\mathbf{r}, \mathbf{v}_\alpha, t) = \frac{d^6 N_\alpha}{d^3 r d^3 v_\alpha} \rightarrow d^6 N_\alpha = f_\alpha(\mathbf{r}, \mathbf{v}_\alpha, t) d^3 r d^3 v_\alpha$$

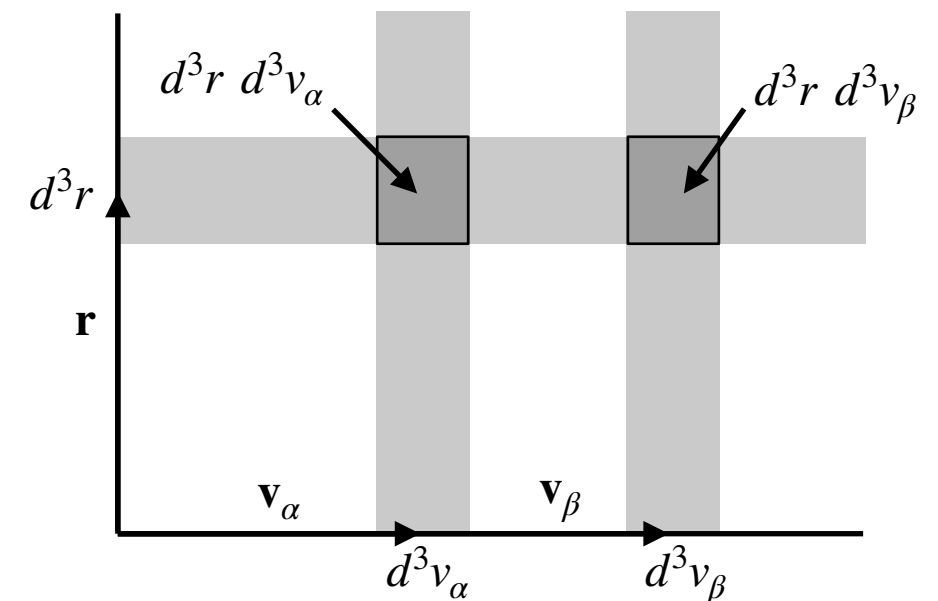
$$\left[ f_\alpha(\mathbf{r}, \mathbf{v}_\alpha) d^3 r d^3 v_\alpha \right] \left[ f_\beta(\mathbf{r}, \mathbf{v}_\beta) d^3 r d^3 v_\beta \right] = \left[ f_\alpha(\mathbf{r}, \mathbf{v}'_\alpha) d^3 r d^3 v'_\alpha \right] \left[ f_\beta(\mathbf{r}, \mathbf{v}'_\beta) d^3 r d^3 v'_\beta \right]$$

$$f_\alpha(\mathbf{v}_\alpha) f_\beta(\mathbf{v}_\beta) = f_\alpha(\mathbf{v}'_\alpha) f_\beta(\mathbf{v}'_\beta)$$



Mostre que (Bittencourt Chap. 21, Sec. 2.2):

$$d^3 v_\alpha d^3 v_\beta = d^3 v'_\alpha d^3 v'_\beta$$



# In thermodynamic equilibrium, a given collision process is perfectly balanced by its respective inverse collision process

- **The condition  $f_\alpha(\mathbf{v}'_\alpha)f_\beta(\mathbf{v}'_\beta) = f_\alpha(\mathbf{v}_\alpha)f_\beta(\mathbf{v}_\beta)$  has a profound meaning:**
  - The sum of the logarithms of the distribution function is conserved during elastic collisions

$$f_\alpha(\mathbf{v}_\alpha)f_\beta(\mathbf{v}_\beta) = f_\alpha(\mathbf{v}'_\alpha)f_\beta(\mathbf{v}'_\beta)$$

$$\ln \left[ f_\alpha(\mathbf{v}_\alpha)f_\beta(\mathbf{v}_\beta) \right] = \ln \left[ f_\alpha(\mathbf{v}'_\alpha)f_\beta(\mathbf{v}'_\beta) \right]$$

$$\ln f_\alpha(\mathbf{v}_\alpha) + \ln f_\beta(\mathbf{v}_\beta) = \ln f_\alpha(\mathbf{v}'_\alpha) + \ln f_\beta(\mathbf{v}'_\beta)$$

- **There are four independent combinations of particle velocities whose sum remains unchanged during elastic collision**
  - Conservation of linear momentum:  $m_\alpha \mathbf{v}_\alpha + m_\beta \mathbf{v}_\beta = m_\alpha \mathbf{v}'_\alpha + m_\beta \mathbf{v}'_\beta$
  - Conservation of energy (no internal states):  $\frac{1}{2}m_\alpha v_\alpha^2 + \frac{1}{2}m_\beta v_\beta^2 = \frac{1}{2}m_\alpha v'^2_\alpha + \frac{1}{2}m_\beta v'^2_\beta$
- **Obviously,  $\ln f_\alpha(\mathbf{v}_\alpha)$  must be a linear combination:**

$$\ln f_\alpha = a_0 + a_{1x}m_\alpha v_{\alpha x} + a_{1y}m_\alpha v_{\alpha y} + a_{1z}m_\alpha v_{\alpha z} - \frac{a_2}{2}m_\alpha v_\alpha^2$$

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# Collisions always tend to evolve a distribution function to the Maxwellian equilibrium distribution function

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- Starting from  $\ln f_\alpha = a_0 + m_\alpha \mathbf{a}_1 \cdot \mathbf{v}_\alpha - \frac{a_2}{2} m_\alpha v_\alpha^2$ , one can show that

$$\ln f_\alpha = m_\alpha \left( a_0 + \frac{a_1^2}{2a_2} \right) - \frac{1}{2} m_\alpha a_2 \left| \mathbf{v}_\alpha - \frac{\mathbf{a}_1}{a_2} \right|^2$$

- Defining  $\ln C = m_\alpha \left( a_0 + \frac{a_1^2}{2a_2} \right)$  and  $\mathbf{v}_0 = \frac{\mathbf{a}_1}{a_2}$ , one obtains

$$f_\alpha = C \exp \left( -\frac{1}{2} m_\alpha a_2 |\mathbf{v}_\alpha - \mathbf{v}_0|^2 \right)$$

- This expression is known as the Maxwell-Boltzmann, or Maxwellian, equilibrium distribution function

## Exercise (Chap. 7, Sec 1.4)

- Normalize the Maxwellian distribution function using

$$n_\alpha = \int_{v_\alpha} f_\alpha d^3v_\alpha \quad (\text{Particle number density})$$

$$\mathbf{u}_\alpha = \frac{1}{n_\alpha} \int_{v_\alpha} \mathbf{v}_\alpha f_\alpha d^3v_\alpha \quad (\text{Mean fluid velocity})$$

$$\frac{3}{2} n_\alpha k_B T_\alpha = \frac{1}{2} m_\alpha n_\alpha \langle |\mathbf{v}_\alpha - \mathbf{v}_0|^2 \rangle = \frac{1}{2} m_\alpha \int_{v_\alpha} |\mathbf{v}_\alpha - \mathbf{v}_0|^2 f_\alpha d^3v_\alpha \quad (\text{Mean kinetic energy})$$

and show that

$$f_\alpha(v_\alpha) = n_\alpha \left( \frac{m_\alpha}{2\pi k_B T_\alpha} \right)^{3/2} \exp \left( -\frac{m_\alpha |\mathbf{v}_\alpha - \mathbf{u}_\alpha|^2}{2k_B T_\alpha} \right)$$

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# In thermodynamic equilibrium, inelastic collisions change the internal state of the particles

- **To account for inelastic collisions, one must take into consideration the possibility of a change in the internal state of the particles**

– The energy conservation equation must now take the total energies of the particles,  $E_{\alpha j} = \frac{1}{2}m_{\alpha}v_{\alpha}^2 + \mathcal{E}_{\alpha j}$ , with  $\mathcal{E}_{\alpha j}$  being its internal energy in state  $j$

- **This leads to**

$$\ln f_{\alpha} = a_0 + m_{\alpha} \mathbf{a}_1 \cdot \mathbf{v}_{\alpha} - a_2 \left( \frac{1}{2}m_{\alpha}v_{\alpha}^2 + \mathcal{E}_{\alpha j} \right)$$

- **Following the same steps as before leads us to**

$$f_{\alpha}(v_{\alpha}, j_{\alpha}) = A \exp \left( -\frac{m_{\alpha} |\mathbf{v}_{\alpha} - \mathbf{u}_{\alpha}|^2}{2 k_B T_{\alpha}} \right) \exp \left( -\frac{\mathcal{E}_{\alpha j}}{k_B T_{\alpha}} \right)$$

– The constant  $A$  can be found from the normalization condition:  $n_{\alpha} = \int_{v_{\alpha}} f_{\alpha} d^3 v_{\alpha}$

- **Mostre que**  $A = \left( \frac{m_{\alpha}}{2 \pi k_B T_{\alpha}} \right)^{3/2} \left[ \sum_{j \text{ states}} \exp \left( -\frac{\mathcal{E}_{\alpha j}}{k_B T_{\alpha}} \right) \right]^{-1} = \left( \frac{m_{\alpha}}{2 \pi k_B T_{\alpha}} \right)^{3/2} \left[ \sum_{j \text{ energy levels}} g_j \exp \left( -\frac{\mathcal{E}_{\alpha j}}{k_B T_{\alpha}} \right) \right]^{-1}$



# In thermodynamic equilibrium, inelastic collisions change the internal state of the particles

- **Substituting the normalization constant A yields the equilibrium distribution function, which can be written as  $f_\alpha(v_\alpha, j_\alpha) = f_v(v_\alpha) f_j(j)$ , where**
  - $f_v(v_\alpha)$  is the Maxwellian distribution over the velocities of the particles and
  - $f_j(j)$  determines the distribution over the internal states of the particles, with

$$f_j(j) = \frac{\exp\left(-\frac{\mathcal{E}_{\alpha j}}{k_B T_\alpha}\right)}{\sum_{k \text{ states}} \exp\left(-\frac{\mathcal{E}_{\alpha k}}{k_B T_\alpha}\right)} = \frac{g_j \exp\left(-\frac{\mathcal{E}_{\alpha j}}{k_B T_\alpha}\right)}{\sum_{k \text{ energy levels}} g_k \exp\left(-\frac{\mathcal{E}_{\alpha k}}{k_B T_\alpha}\right)}$$

*( $g_j$  and  $g_k$  are the statistical weights determining the degeneracy of that particular energy level)*

- **Therefore, the equilibrium distribution of velocities remains Maxwellian even when inelastic collisions occur**
- **At the same time, inelastic collision lead to equilibrium distribution among the various internal states of the atoms and ions**

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# External forces can cause the equilibrium distribution function to be non-homogeneous

- Let's now calculate the equilibrium distribution while accounting for the presence of an external conservative force  $\mathbf{F}_\alpha = -\nabla U_\alpha(\mathbf{r})$

– Under this assumption, the kinetic equation becomes

$$\mathbf{v} \cdot \nabla f_\alpha + \frac{\mathbf{F}_\alpha}{m_\alpha} \cdot \nabla_{\mathbf{v}} f_\alpha = \sum_{\beta} C_{\text{coll}}[f_\alpha, f_\beta]$$

- Let's now assume that the velocity distribution is given by a Maxwellian distribution with  $\mathbf{u} = 0$  and with  $n_\alpha = n_\alpha(\mathbf{r})$  (local equilibrium):

$$f_\alpha(\mathbf{r}, v_\alpha) = n_\alpha(\mathbf{r}) \left( \frac{m_\alpha}{2\pi k_B T_\alpha} \right)^{3/2} \exp\left( -\frac{m_\alpha |\mathbf{v}_\alpha|^2}{2k_B T_\alpha} \right) = n_\alpha(\mathbf{r}) f_M(v_\alpha)$$

– Under this assumption, the collision operator vanishes and the kinetic equation becomes

$$f_M(\mathbf{v} \cdot \nabla n_\alpha) - n_\alpha \frac{\nabla U_\alpha \cdot \nabla_{\mathbf{v}} f_M}{m_\alpha} = 0$$

# External forces can cause the equilibrium distribution function to be non-homogeneous

- Using the fact that  $\nabla_{\mathbf{v}} f_M = -\frac{m_{\alpha} \mathbf{v}_{\alpha}}{k_B T_{\alpha}} f_M$ , the equation can be written as

$$f_M \mathbf{v} \cdot \left( \nabla n_{\alpha} + \frac{n_{\alpha}}{k_B T_{\alpha}} \nabla U_{\alpha} \right) = 0 \quad \rightarrow \quad \frac{\nabla n_{\alpha}}{n_{\alpha}} = -\frac{\nabla U_{\alpha}}{k_B T_{\alpha}}$$

- Since  $dU = \nabla U \cdot d\mathbf{r}$ , one has that

$$\frac{dn_{\alpha}}{n_{\alpha}} = -\frac{dU_{\alpha}}{k_B T_{\alpha}} \quad \rightarrow \quad n_{\alpha}(\mathbf{r}) = n_{\alpha 0} \exp \left[ -\frac{U_{\alpha}(\mathbf{r})}{k_B T_{\alpha}} \right]$$

- This exponential factor, responsible for the inhomogeneity, is the so-called Boltzmann factor

- An important example is for  $U_{\alpha}(\mathbf{r}) = q_{\alpha} \Phi(\mathbf{r})$  being the electrostatic energy

- In this case, the plasma density varies as

$$n_{\alpha}(\mathbf{r}) = n_{\alpha 0} \exp \left[ -\frac{q_{\alpha} \Phi(\mathbf{r})}{k_B T_{\alpha}} \right]$$



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# Degree of ionization of a gas or a plasma

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- From statistical mechanics, one can determine the degree of ionization of a gas (or plasma) in thermal equilibrium at some temperature  $T$
- A considerable degree of ionization can be achieved even when the average thermal energy of the particles is far below the ionization potential
- From statistical mechanics, one has that

$$\frac{n_a}{n_b} = \frac{g_a}{g_b} \exp \left[ -\frac{(U_a - U_b)}{k_B T} \right]$$

- Here,  $g_a$  and  $g_b$  are the statistical weights (degeneracy factor) associated to the energies  $U_a$  and  $U_b$

# Degree of ionization of a gas or a plasma

- For the particular case of a system having only 2 energy levels, the fraction of particles that are in the higher energy state ( $U_a$ ) is

$$\alpha = \frac{n_a}{n_a + n_b} = \frac{n_a}{n_b} \left( \frac{n_a}{n_b} + 1 \right)^{-1}$$

- Which can be written as

$$\alpha = \frac{(g_a/g_b) \exp(-U/k_B T)}{(g_a/g_b) \exp(-U/k_B T) + 1}$$

Element	U(eV)
Helium (He)	24.59
Argon (A)	15.76
Nitrogen (N)	14.53
Oxygen (O)	13.62
Hydrogen (H)	13.60
Mercury (Hg)	10.44
Iron (Fe)	7.87
Sodium (Na)	5.14
Potassium (K)	4.34
Cesium (Cs)	3.89

- For the ionization problem, state  $a$  is taken as that of the electron-ion pair, state  $b$  is taken as that of the neutral atom, and  $U = U_a - U_b$  is the ionization energy
  - The temperature for which  $\alpha = 0.5$  is equal to

$$(g_a/g_b) \exp(-U/k_B T_{1/2}) = 1 \quad \rightarrow \quad T_{1/2} = \frac{U}{k_B \ln(g_a/g_b)}$$

# Degree of ionization of a gas or a plasma

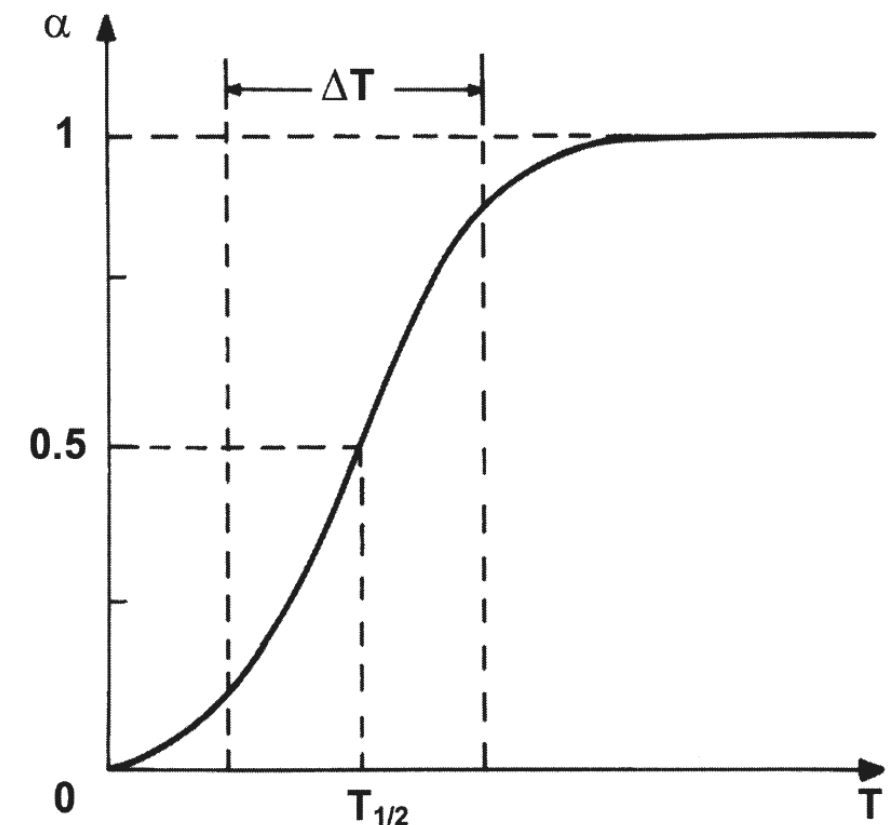
- The range in which  $\alpha$  changes from nearly zero to nearly one is defined as

$$\left. \frac{d\alpha}{dT} \right|_{T_{1/2}} = \frac{1}{\Delta T}$$

- Therefore,

$$\Delta T = \frac{4T_{1/2}}{k_B \ln(g_a/g_b)} = \frac{4U}{[k_B \ln(g_a/g_b)]^2}$$

- Since  $g_a \gg g_b$ , the curve usually looks like a step function near  $T_{1/2}$



- From quantum mechanics, one can estimate ( $h$  is the Planck's constant)

$$\frac{g_a}{g_b} = \frac{1}{\lambda_{th,e}^3 n_e} = \left( \frac{2\pi m_e k_B T}{h^2} \right)^{3/2} \frac{1}{n_e} = 2.405 \times 10^{21} \frac{T^{3/2}}{n_e}$$

( $\lambda_{th,e}$  is the electron thermal de Broglie wavelength)



# The Saha equation

- From quantum mechanics, one can estimate (T in Kelvin and  $n_i$  in  $m^{-3}$ )

$$\frac{g_a}{g_b} = \left( \frac{2\pi m_e k_B T}{h^2} \right)^{3/2} \frac{1}{n_e} = 2.405 \times 10^{21} \frac{T^{3/2}}{n_e}$$

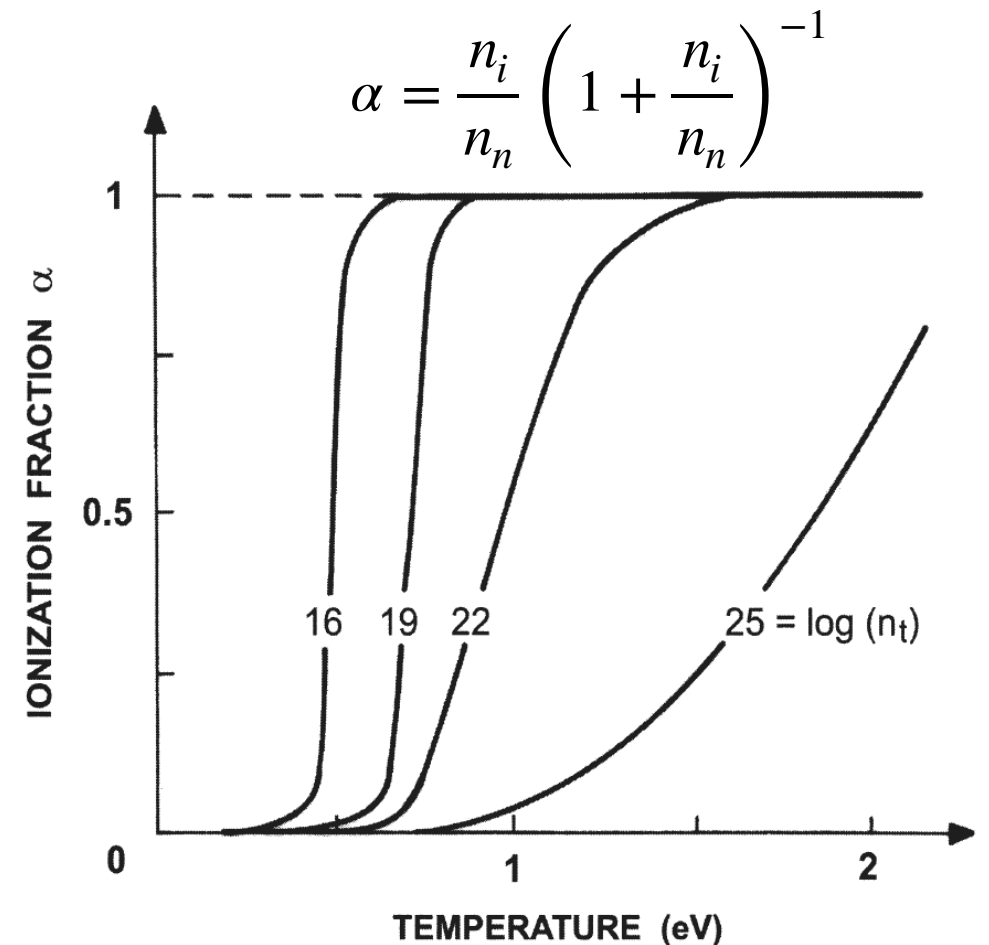
- Using this results, one can write

- This equation is known as the Saha equation

$$\frac{n_i}{n_n} = \left( \frac{2\pi m_e k_B}{h^2} \right)^{3/2} \frac{T^{3/2}}{n_e} \exp\left(-\frac{U}{k_B T}\right)$$

- Since 1 eV = 11,600 K, the Saha equation can also be written as (T in eV and  $n_e$  in  $m^{-3}$ )

$$\frac{n_i}{n_n} = 3.00 \times 10^7 \frac{T^{3/2}}{n_e} \exp\left(-\frac{U}{T}\right)$$



# Degree of ionization for some particular cases

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- **Air at room temperature**

$$n_n = 3 \times 10^{25} \text{ m}^{-3} \quad T = 300 \text{ K} \quad U = 14.5 \text{ eV (Nitrogen)}$$

$$\frac{n_i}{n_n} = 2 \times 10^{-122} \ll 1$$

- **Tokamak**

$$n_e = n_i = 1 \times 10^{20} \text{ m}^{-3} \quad T = 1 \times 10^8 \text{ K} \quad U = 13.6 \text{ eV (Hydrogen)}$$

$$\frac{n_i}{n_n} = 2.4 \times 10^{13} \gg 1$$

- **Plasma torch**

$$n_n = 3 \times 10^{25} \text{ m}^{-3} \text{ (1 Atm)} \quad T = 1 \times 10^4 \text{ K} \quad U = 13.6 \text{ eV (Hydrogen)}$$

$$\frac{n_i}{n_n} = 3 \times 10^{-4} \ll 1$$

# Degree of ionization for some particular cases

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- **Solar corona**

$$n_e = n_i = 1 \times 10^{12} \text{ m}^{-3} \quad T = 1 \times 10^6 \text{ K} \quad U = 13.6 \text{ eV (Hydrogen)}$$

$$\frac{n_i}{n_n} = 2.4 \times 10^{18} \gg 1 \quad \text{(Fully ionized plasma!!!!)}$$

- **Sun's core**

$$n_e = n_i = 1 \times 10^{32} \text{ m}^{-3} \quad T = 1 \times 10^7 \text{ K} \quad U = 13.6 \text{ eV (Hydrogen)}$$

$$\frac{n_i}{n_n} = 1.5 \quad \text{(Surprisingly, the sun's core is not fully ionized, } \alpha = 0.6, \text{ but anyway nuclear fusion reactions can occur)}$$

**Note that, from our previous definitions, the gas does not need to be fully ionized to be considered a plasma, as far as collective effects are present**

# References

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- **Thermodynamic equilibrium states**
  - *Bittencourt: Ch. 7, section 1 and 5*
  
- **Degree of ionization and the Saha equation**
  - *Bittencourt: Ch. 7, section 6*