Excitation, ionisation and gas thermodynamical properties

We have looked at the population of the different energy and ionisation levels. let's now look at how partial ionisation can affect the gas equation of state.

The gas equation of state is

(1) $$P_g = nkT$$

$n =$ total number of free particles per unit volume

non degenerate gas

(2) $$P_g = \frac{\mathcal{R}}{\mu}\rho T$$

$\mathcal{R} =$ gas constant per mole

$\mu =$ mean molecular weight $=$ mass per mole of free particle

$\rho =$ mass density

non relativistic condition

$1 \text{ mole} = 6.22 \cdot 10^{23} \text{ atoms} = \mathcal{N}_0$

Definition of the atomic mass unit $\quad AMU = \frac{M(O^{16})}{16} = \frac{M(C^{12})}{12} \simeq \frac{M(H)}{1}$

$M(O^{16})$ = rest mass of the neutral atom O^{16}

Because μ depends on the number of free particles in a given mass of chosen matter, μ is impacted by the processes of ionisation, dissociation, nuclear reaction

$\longrightarrow$ change of equation of state

$\rightarrow$ $\boxed{\text{let's move to atomic mass unit}}$ $\leftarrow$

n, the density in number of a mixture of k constituents

n_k of the particles of type k

$$n = \sum_k n_k$$

m_k the mass of particle of type k

total density of the gas $\rho = \sum_k m_k n_k$

A_k the mass per atomic unit of the particle k

$$A_k = \frac{m_k}{H} = \frac{m_k}{m_H}$$

The general definition of μ, in AMU

$$\mu = \frac{\sum_k \frac{m_k n_k}{H}}{\sum_k n_k} = \boxed{\frac{\sum_k A_k n_k}{\sum_k n_k} = \frac{\rho}{H n}}$$

x_k = The <u>relative</u> abondance <u>in mass</u> of the particle k
= nb in grams of particle k per gram of composite matter

$$x_k = \frac{m_k n_k}{\rho} = \frac{H A_k n_k}{\rho}$$

One can write n_k in fonction of x_k $\quad n_k = \frac{\rho x_k}{H A_k}$

$$\rightarrow \quad \sum_k x_k = \frac{\sum m_k n_k}{\rho} = 1$$

Let's express μ in fonction of x_k:

$$\boxed{\mu =} \frac{\sum \cancel{A_k} \frac{\cancel{\rho} x_k}{\cancel{H A_k}}}{\sum \frac{\cancel{\rho} x_k}{\cancel{H} A_k}} = \frac{\sum_k x_k}{\sum_k \frac{x_k}{A_k}} = \boxed{\frac{1}{\sum_k \frac{x_k}{A_k}}}$$

In astrophysics, some of the particles are electrons, which were liberated through ionization of neutral particles (atoms, molecules at sufficiently low temperature.

$$n = n_e + \sum_i n_i$$

E_i the number of free particles coming from the ionization of a particle of type i

The density in number of e^-, $n_e = \sum_i E_i n_i = \sum_i E_i \frac{\rho x_i}{A_i H}$

$$\boxed{n_e = \frac{\rho}{H} \sum_i E_i \frac{x_i}{A_i}}$$

we write $n = n_e + \sum_i n_i$ in fonction of $\frac{\rho x_i}{H A_i}$

$$n = \frac{\rho}{H} \sum_i E_i \frac{x_i}{A_i} + \sum_i \frac{\rho x_i}{H A_i} = \frac{\rho}{H} \sum_i (1+E_i) \frac{x_i}{A_i}$$

$$n = \frac{\rho}{H} \sum_i \bar{n}_i x_i \quad \text{avec} \quad \boxed{\bar{n}_i = \frac{1+E_i}{A_i}}$$

$\left(\mu = \frac{\rho}{H n}\right)$ we get

$$\boxed{\mu = \frac{1}{\sum_i \bar{n}_i x_i}}$$

mean ionization (Chandrasekhar)

If a medium is fully ionized (good approximation of stellar interiors), the number of liberated particles by an atom of atomic number Z_i and atomic mass A_i is $Z_i + 1$

$$\bar{n}_i = \frac{(Z_i + 1)}{A_i}$$

Example:

Ionized hydrogen $\quad Z = 1 \quad A = 1.00794$

$$\bar{n}_H = \frac{2}{1.008} = 1.984 \simeq 2$$

Ionized helium $\quad Z = 2 \quad A = 4.0026$

$$\bar{n}_{He} = \frac{3}{4.004} = 0.7492 \sim 0.75 \sim \frac{3}{4}$$

For all heavy elements - fully ionized

a good approximation is $A_i \sim 2 Z_i$

$$\bar{n}_i \simeq \frac{1}{2} \qquad (Z_i > 2)$$

let's define X, Y et Z so that

X the abundance in mass of hydrogen $= x(H)$

Y helium $= x(He)$

Z of the elements heavier than He

since $\sum_i x_i = 1$ $\qquad Z = 1 - X - Y$

$$\mu = \frac{1}{\sum_i \bar{n}_i x_i} \qquad \mu = \frac{1}{\bar{n}_H X + \bar{n}_{He} Y + \bar{n}_Z Z} \simeq \frac{1}{2X + \frac{3}{4} Y + \frac{1}{2} Z}$$

μ is not sensitive to the detail of the abundance of the heavy elements. (atomic number $Z > 2$)

- For a star only composed of hydrogen $Y = 0$ $\qquad \mu = \frac{1}{2}$
- For a star only composed of helium $\qquad X = 0 \; Y = 1$ $\qquad \mu \sim \frac{4}{3}$
- Iff no helium, no hydrogen $\quad X = Y = 0 \qquad \mu = 2$

As a consequence, for a full ionization (stellar interiors)

$$\frac{1}{2} \lesssim \mu \lesssim 2$$

- In the case of a fully neutral medium

$$\bar{n}_i = \frac{1}{A_i} \qquad \left(\bar{n}_i = \frac{1+E_i}{A_i} \right)$$

$$\mu = \frac{1}{\sum_i \frac{x_i}{A_i}} \qquad \text{equivalent to} \qquad \frac{1}{\mu} = \sum_i \frac{x_i}{A_i}$$

- In the case of a partially ionized medium (stellar envelope)

$$\frac{1}{A_i} \leq \bar{n}_i \leq \frac{(Z_i+1)}{A_i}$$

One can define the mean number of free e^- per atom/ion

$$\frac{n_e}{n} = \frac{\sum_j E_j \frac{X_j}{A_j} \frac{\rho}{H}}{\sum_j \frac{X_j}{A_j} \frac{\rho}{H}} = \boxed{E = \frac{\sum_j \frac{X_j}{A_j} E_j}{\sum_j \frac{X_j}{A_j}}}$$

If the medium is neutral $E_j = 0 \Rightarrow E = 0$

We can write $E = \frac{1/\mu_e}{1/\mu_0}$ $\qquad \mu_e = E \mu_0$

It comes

Pression of ions + neutral atoms $P_0 = n_0 kT = \frac{k \rho T}{\mu_0 m_H} = \frac{\mathcal{R}}{\mu_0} \rho T$

Electronic pressure $P_e = n_e kT = \frac{\mathcal{R}}{\mu_e} \rho T = \frac{\mathcal{R}}{\mu_0} E \rho T$

Total pressure $P_g = P_0 + P_e = \frac{\mathcal{R}}{\mu_0} (1+E) \rho T = \frac{\mathcal{R}}{\mu} \rho T$

$$\Rightarrow \quad \frac{1}{\mu} = \frac{1+E}{\mu_0} \quad \Rightarrow \quad \boxed{\mu = \frac{\mu_0}{1+E}}$$

$$\Rightarrow \quad \boxed{\frac{P_g}{P_e} = \frac{1+E}{E}}$$

Ionized H : $\frac{P_g}{P_e} \sim 2$

cool star : $\frac{P_e}{P_g} \longrightarrow 0$

Full equation of state : $P_{tot} = P_g + P_{rad}$

$$P_{tot} = \underbrace{\frac{\mathcal{R}}{\mu}}_{\text{depends on the gas composition}} \rho T + \frac{1}{3} a T^4 = \frac{\mathcal{R}}{\mu \beta} \rho T \quad \text{with} \quad \beta = \frac{P_g}{P}$$

Physical properties of the partially ionised media

We now distinguish between the ≠ ionization levels

$$\nu_j = \frac{\text{number of atoms and ions of element } j}{\text{total number of atoms and ions}}$$

$$\sum_j \nu_j = 1$$

$$X_i^s = \frac{\text{number of atom } i \text{ in ionization } s}{\text{total number of atoms and ions of element } i}$$

$$\sum_s X_i^s = 1$$

$$E = \frac{\text{number of free electrons}}{\text{total number of atoms and ions}}$$

$$E = \sum_i \nu_i \sum_{0}^{z_i} s\, X_i^s$$

We can define

$$Y_i^s = \sum_{r=s+1}^{Z_i} X_i^r$$

total number of atoms i in a ionization state $> s$ relative to the number of atoms and ions of element i

One can write

$$E = \sum_i \sum_{s=0}^{Z_i-1} \nu_i Y_i^s$$

$$\left(E = \sum_i \sum_{s=0}^{Z_i-1} \nu_i \sum_{r=s+1}^{Z_i} X_i^r \right)$$

Example

Composit gas of hydrogen and helium both elements are ionized

$$X_i^s = \frac{\text{number of atoms } i \text{ the ionization state } s}{\text{number of atoms/ions of species } i}$$

$$H: \quad X_1^1 = \frac{H^+}{H + H^+} \quad ; \quad Y_1^0 = \frac{H^+}{H + H^+} = X_1^1$$

$$He: \quad X_2^1 = \frac{He^+}{He + He^+ + He^{++}} \qquad X_2^2 = \frac{He^{++}}{He + He^+ + He^{++}}$$

He:

$$Y_2^0 = \frac{He^+ + He^{++}}{He + He^+ + He^{++}} \qquad Y_2^1 = \frac{He^{++}}{He + He^+ + He^{++}}$$

$$Y_2^0 = X_2^1 + X_2^2 \qquad Y_2^1 = X_2^2$$

$$E = \sum_i \sum_{s=0}^{Z_i - 1} \nu_i Y_i^s = \nu_1 X_1^1 + \nu_2 \left(X_2^1 + X_2^2 \right) + \nu_2 X_2^2$$

let's simplify the naming

$$\begin{cases} X_1 = X_1^1 & X_2 = X_2^1 & X_3 = X_2^2 \\ Y_1 = Y_1^0 & Y_2 = Y_2^0 & Y_3 = Y_2^1 \end{cases}$$

we get

$$E = \nu_1 X_1 + \nu_2 \left(X_2 + X_3 \right) + \nu_2 X_3$$

$$E = \nu_1 X_1 + \nu_2 X_2 + 2 \nu_2 X_3$$

What does Saha say?

$$\frac{n_{r+1}}{n_r} P_e = 2 \frac{u_{r+1}}{u_r} \left(\frac{2\pi m_e}{h^2} \right)^{3/2} (kT)^{5/2} e^{-\frac{I_r}{kT}}$$

$$\frac{P_e}{P_g} = \frac{1+E}{E} \qquad \frac{P_g}{P_{tot}} = \frac{P_g}{P} = \beta$$

$$\frac{n_{r+1}}{n_r}\frac{P_e}{P_g} = 2\,\frac{u_{r+1}}{u_r}\left(\frac{2\pi m_e}{h^2}\right)^{3/2}(kT)^{5/2}\,\frac{1}{P_g}\,e^{-I_r/kT}$$

$$= 2\,\frac{u_{r+1}}{u_r}\left(\frac{2\pi m_e}{h^2}\right)^{3/2}(kT)^{5/2}\,\frac{1}{\beta P}\,e^{-I_r/kT}$$

let's start by the change from neutral state to 1rst ionization

$$\frac{X_1 P_e}{(1-X_1)P_g} = 2\,\frac{u_{ion}}{u_{neutral}}\left(\frac{2\pi m_e}{h^2}\right)^{3/2}(kT)^{5/2}\,\frac{1}{\beta P}\,e^{-I_1/kT}$$

$$= K_1$$

let $\omega_1 = 2\,\frac{u_{ion}}{u_{neutral}} = 2\,\frac{u_{H+}}{u_H}$

$$\frac{X_1}{(1-X_1)}\,\frac{E}{1+E} = K_1$$

We continue with .. neutral state of He : $1-X_2-X_3$

We end with a system of 4 equations with 4 unknowns.

$$
\begin{cases}
\dfrac{X_1}{1-X_1}\,\dfrac{E}{1+E} = K_1 \\[2ex]
\dfrac{X_2}{1-X_2-X_3}\,\dfrac{E}{1+E} = K_2 \\[2ex]
\dfrac{X_3}{X_2}\,\dfrac{E}{1+E} = K_3 \\[2ex]
E = \nu_1 X_1 + \nu_2 \left(X_2 + 2X_3\right)
\end{cases}
$$

$$
\left.\begin{array}{l}
\text{The partition functions are tabulated} \\
\text{The excitation pototentials as well}
\end{array}\right\} \rightarrow \underset{\text{known}}{K_1, K_2, K_3}
$$

$I_1(H) = 13.598\ eV$ $\qquad \omega_1 = 2$

$I_2(He) = 24.587\ eV$ $\qquad \omega_2 = 4$

$I_3(He) = 54.416\ eV$ $\qquad \omega_3 = 2$