

Mean Molecular Weight

The thermodynamic relations between P , ρ , and T , as well as the calculation of stellar opacity requires knowledge of the system's mean molecular weight (defined as the mass per unit mole of material, or, alternatively, the mean mass of a particle in Atomic Mass Units). Recall that a mole of any substance contains $N_A = 6.02252 \times 10^{23}$ atoms. Thus, the number density of ions is related to the mass density, ρ , by

$$n = \frac{\rho}{\mu m_a} = \frac{\rho N_A}{\mu} \quad (5.1.1)$$

where m_a is the mass that is equivalent to 1 A.M.U. If the mass fraction of species i is x_i , then its number density is

$$n_i = \frac{x_i \rho N_A}{A_i} \quad (5.1.2)$$

where A_i is the atomic weight of the species. The number density of all ions in a volume of gas is then

$$n_I = \sum_i n_i = \rho N_A \sum_i \frac{x_i}{A_i}$$

or

$$n_I = \frac{\rho N_A}{\mu_I} \quad \text{where} \quad \mu_I = \left(\sum_i \frac{x_i}{A_i} \right)^{-1} \quad (5.1.3)$$

To compute the contribution of (massless) electrons to the mean molecular weight, let Z_i be the atomic number of species i , and f_i be the species' ionization fraction, *i.e.*, the fraction of electrons of i that are free. The number density of electrons is therefore

$$n_e = \rho N_A \sum_i \left(\frac{x_i}{A_i} \right) f_i Z_i \quad (5.1.4)$$

or

$$n_e = \frac{\rho N_A}{\mu_e} \quad \text{where} \quad \mu_e = \left(\sum_i \frac{Z_i x_i f_i}{A_i} \right)^{-1} \quad (5.1.5)$$

Note that in the case of total ionization ($f_i = 1$), this equation simplifies greatly. Since $Z_i/A_i = 1$ for hydrogen, and $\sim 1/2$ for everything else,

$$\mu_e = \left(X + \frac{1}{2}(Y + Z) \right)^{-1} = \left(X + \frac{(1 - X)}{2} \right)^{-1} = \frac{2}{1 + X} \quad (5.1.6)$$

From the definitions above, the total number density of particles is

$$n = n_I + n_e = \frac{\rho N_A}{\mu}$$

where the mean molecular weight is defined as

$$\mu = \left[\frac{1}{\mu_I} + \frac{1}{\mu_e} \right]^{-1} \quad (5.1.7)$$

The Ionization Fraction

The calculation of mean molecular weight requires knowledge of the chemical composition of the material and the ionization fraction. To calculate ionization fraction, one needs the Saha equation.

In general, the Saha equation can be used to compute ionization fractions over most of the star. It does, however, require that the gas be in thermodynamic equilibrium. This is true throughout the star, as at high densities, collisions will control the level populations. This approximation only breaks down in the solar corona, where the densities become very low.

The Saha equation also breaks down in the centers of stars, where high densities cause the ionization energies of atoms to be reduced. (Obviously, if the mean distance between atoms is d , then there can be no bound states with radii greater than $\sim d/2$.) In the case of the hydrogen atom, the Bohr radius of level n is

$$a_n = (n + 1)^2 \frac{\hbar^2}{m_e e^2} = 5.28 \times 10^{-9} (n + 1)^2 \text{ cm}$$

Thus, if the particle density is

$$\rho \sim \frac{\mu m_a}{4/3\pi(2a_0)^3} \sim 0.3 \mu \text{ g cm}^{-3}$$

then all the hydrogen is necessarily *pressure ionized*. In practice, the Saha equation begins to break down at nuclear distances of $\sim 10 a_0$, which corresponds to $\sim 2.7 \times 10^{-3} \mu \text{ g-cm}^{-3}$. To correct for this effect, the Saha equation is normally used until it begins to show decreasing ionization fractions toward the center of the star. When this happens, complete ionization is assumed.

To derive the Saha equation, begin by considering the Boltzmann equation, which states that the number of atoms in level i relative to level j is

$$\frac{n_i}{n_j} = \frac{\omega_i}{\omega_j} e^{-\chi_{ij}/kT} \quad (5.2.1)$$

where ω_i is the statistical weight of the level i (*i.e.*, the number of separate, individual states that are degenerate in energy), and χ_{ij} is the difference in energy between the two levels. The number of atoms in level i relative to the number in *all levels* is thus

$$\begin{aligned} \frac{n_i}{n} &= \frac{\omega_i}{\omega_0 e^{+\chi_{i0}/kT} + \omega_1 e^{+\chi_{i1}/kT} + \omega_2 e^{+\chi_{i2}/kT} + \dots} \\ &= \frac{\omega_i e^{-\chi_i/kT}}{\omega_0 + \omega_1 e^{-\chi_1/kT} + \omega_2 e^{-\chi_2/kT} + \dots} \\ \frac{n_i}{n} &= \omega_i \frac{e^{-\chi_i/kT}}{u} \end{aligned} \quad (5.2.2)$$

where χ_i is the energy difference between the i^{th} level and the ground state. The variable u is the partition function for the atom (or ion). Because u is a function of temperature, it is sometimes written $u(T)$.

Now let's generalize this equation to electrons in the continuum. Let n_i be the number of atoms in all levels (defined as n above), and let state $i+1$ be that where an excited electron is in the continuum with momentum between p and $p + dp$. The Boltzmann equation then gives

$$\frac{dn_{i+1}}{n_i} = \frac{d\omega_{i+1}}{\omega_i} \exp\left(-\frac{\chi_i + p^2/2m_e}{kT}\right)$$

where χ_i is the energy needed to ionize the ground state of the atom, and $d\omega_{i+1}$ is the statistical weight of the ionized state.

Now consider that $d\omega_i$ has two components: one from the ion (ω_{i+1}), and other from the free electron ($d\omega_e$). The former is just the statistical weight of the ground state of the ion, while the latter can be computed using the exclusion rule. Since each quantum cell in phase space can have only two electrons in it (spin up and spin down), then the number of degenerate states in a volume h^3 is

$$d\omega_e = 2 \frac{d^3x d^3p}{h^3} = 2 \frac{dV d^3p}{h^3} = \frac{2}{h^3} dV 4\pi p^2 dp \quad (5.2.3)$$

Thus

$$\frac{dn_{i+1}}{n_i} = \frac{8\pi p^2}{h^3} \frac{\omega_{i+1}}{u_i(T)} \exp\left(-\frac{\chi_i + p^2/2m_e}{kT}\right) dV dp$$

The number of electrons in volume $\int dV = 1/n_e$, so the total number of electrons in all continuum states is therefore

$$\frac{n_{i+1}}{n_i} = \frac{\omega_{i+1}}{u_i(T)} \frac{8\pi}{n_e h^3} e^{-\chi_i/kT} \int_0^\infty p^2 \exp\left(-\frac{p^2}{2m_e kT}\right) dp$$

or, if we let $x^2 = p^2/2m_e kT$, then

$$\begin{aligned} \frac{n_{i+1}}{n_i} &= \frac{\omega_{i+1}}{u_i(T)} \frac{8\pi}{n_e h^3} e^{-\chi_i/kT} \int_0^\infty (2m_e kT) x^2 e^{-x^2} \cdot (2m_e kT)^{1/2} dx \\ &= \frac{\omega_{i+1}}{u_i(T)} \frac{8\pi}{n_e h^3} e^{-\chi_i/kT} (2m_e kT)^{3/2} \int_0^\infty x^2 e^{-x^2} dx \\ &= \frac{\omega_{i+1}}{u_i(T)} \frac{8\pi}{n_e h^3} e^{-\chi_i/kT} (2m_e kT)^{3/2} \cdot \frac{\sqrt{\pi}}{4} \end{aligned}$$

$$\frac{n_{i+1}}{n_i} = \frac{2}{n_e} \frac{\omega_{i+1}}{u_i(T)} \frac{(2\pi m_e kT)^{3/2}}{h^3} e^{-\chi_i/kT} \quad (5.2.4)$$

Finally, note that for the calculation above n_{i+1} represents those atoms of species n_i that have one electron in the continuum state, *i.e.*, ionized. It does not consider atoms of n_{i+1} that are themselves excited. (In other words, n_{i+1} in (5.2.4) only includes ionized atoms in their ground state.) To include all the excited states of n_{i+1} , we must again sum the contributions in exactly the same way as we did in (5.2.2). Thus, the statistical weight in (5.2.4) should be replaced by the partition function, and

$$\frac{n_{i+1}}{n_i} = \frac{2}{n_e} \frac{u_{i+1}(T)}{u_i(T)} \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} e^{-\chi_i/kT} \quad (5.2.5)$$

This is the Saha equation, which relates the number of atoms in ionization state $i + 1$ to the number in ionization state i . Note that if need be, we can substitute the electron pressure for the electron density using $P_e = n_e kT$, and write the Saha equation as

$$\frac{n_{i+1}}{n_i} P_e = 2 \frac{u_{i+1}(T)}{u_i(T)} \left(\frac{2\pi m_e}{h^2} \right)^{3/2} (kT)^{5/2} e^{-\chi_i/kT} \quad (5.2.6)$$

The sense of these equations is intuitive: the higher the temperature, the greater the ratio, but the higher the density (or pressure), the lower the ratio due to the greater possibility for recombinations).