

Chapter 3C

The excitation ratio N_B/N_A increases as the excitation potential get smaller. Also, as T increases, the higher energy levels become more populated. One should see that as T goes to infinity, $N_B/N_A = g_B/g_A$. Hence, line strength depends on T and the total number of atoms of a particular atomic species that are present in the gas, that is, the **abundance**. Line strength will vary from one element to another for the same temperature, because the excitation potentials are different for different atoms.

If we express the excitation potential in electron volts, equation (3-12) becomes:

$$\text{Log}(N_B/N_A) = (5040.4/T) (E_A - E_B) + \log(g_B/g_A) \quad (3-18)$$

Sometimes this expression may be a convenient form of the Boltzmann excitation equation for doing computations, at least it was in the days before hand calculators.

Do RJP-52, 53, 54, 55, 56, 57.

3-4C. Ionization

If the energy of excitation exceeds a certain critical value, the electron is detached from the atom during the collision or after absorbing a photon. This critical energy is called the ionization potential. Ionization of some or all of the atoms results in what is called an **electron gas** that moves independently of the ions. The electron gas has its own density and exerts a separate pressure aside from the pressure exerted by the ions. The notation for ionization states is as follows:

I: neutral atom, e. g., HI, Fe I

II: one electron lost, e.g., HII, Fe II

III: 2nd stage of ionization, 2 electrons lost, e. g., Fe III. There can be no HIII.

Etc.

The ionization potential, χ (script upper case Greek chi), for HI is 13.6eV, whereas it is only a few eV for most metals. Hence, metals are ionized even in cool stellar atmospheres.

Now we derive a form of the Boltzmann excitation equation in terms of the state of ionization. In so doing, we arrive at the Boltzmann partition function.

Let N_{ij} be the number of atoms per unit volume that are in the i th ionization stage and the j th excitation level.

The range for i is 1 to $Z+1$, for complete ionization. The ground state of energy is $j=1$. Let $j=1$ correspond to $E=0$ and that $E>0$ for $j>1$. Then, relative to the ground state, $j=1$, we have for the j th level and i th stage of ionization:

$$\frac{N_{ij}}{N_{i1}} = \frac{g_{ij}}{g_{i1}} e^{-E_{ij}/kT}$$

where $E_{ij} = (E_j - E_0)_i$ is the excess energy of level j over the ground state. E_{ij} is called the excitation potential of level j .

Now

$$N_i = \sum_{j=1}^{\infty} N_{ij}$$

This is the total no. of atoms per unit volume that are in the i th state of ionization. From (3-14) we

have

$$N_{ij} = \left(\frac{N_{i1} g_{ij}}{g_{i1}} \right) e^{-E_{ij}/kT}$$

Inserting (3-16) into (3-15) we obtain:

$$N_i = \sum_{j=1}^{\infty} \left(\frac{N_{i1}}{g_{i1}} \right) g_{ij} e^{-E_{ij}/kT}$$

or
$$N_i = \frac{N_{i1}}{g_{i1}} \sum_j g_{ij} e^{-E_{ij}/kT} \quad (3-18)$$

Let
$$B_i \equiv \sum_{j=1}^{\infty} g_{ij} e^{-E_{ij}/kT} \quad (3-19)$$

B_i is called the partition function

Now find the ratio of (3-16) to (3-18) :

$$\frac{N_{ij}}{N_i} = \frac{N_{i1} \left(\frac{g_{ij}}{g_{i1}} \right) e^{-E_{ij}/kT}}{\frac{N_{i1}}{g_{i1}} B_i}$$

$$= \frac{g_{ij}}{B_i} e^{-E_{ij}/kT} \quad (3-20)$$

Or
$$\log_{10} \left(\frac{N_{ij}}{N_i} \right) = \log_{10} \left(\frac{g_{ij}}{B_i} \right) - \frac{5040}{T} E_{ij} \quad (3-21)$$

where E_{ij} is in eV. The above equations are forms of the Boltzmann equation. The partition function, B_i , is the sum, over all bound energy levels of an atom, of the product of the statistical weights and the Boltzmann factor $e^{-E_{ij}/kT}$. As $n \rightarrow \infty$ B_i diverges. However j does not really exist for very high levels, because atomic perturbations smear these levels and prevent them from being populated. Hence, each term in the summation of (3-19) should be multiplied by

a probability, p_{ij} , that the level exists. In many cases, most atoms are in the ground state. As $j \rightarrow \infty$ $p_{ij} \rightarrow 0$. In fact $p_{ij} = 0$ for all levels except $j=1$. Then $p_{i1} = 1$

So:
$$B_i = p_{i1} g_{i1} e^{-E_{i1}/kT} + p_{i2} g_{i2} e^{-E_{i2}/kT} + \dots \quad (3-22)$$

or
$$B_i = p_{i1} g_{i1} e^{-0} = g_{i1}, \quad (3-23)$$

since $E_{i1} = 0$ for $j=1$ and $p_{i1} = 1$ (3-24)

For H, $j=n$ and $g_{in} = 2n^2$ ($4n^2$ if we include nuclear spin, but this doesn't affect the ratio of the g values). The excitation energy comes from

$$E_n = -13.6 \frac{Z^2}{n^2} \text{ eV} \quad (3-25)$$

To make $E_i = 0$, we add 13.6 eV to the above equation. Then we get ($Z=1$)

$$E_i - E_n = E_n = 13.6 \left(\frac{n^2 - 1}{n^2} \right) = E_{ij} \quad (3-26)$$

THE SAHA IONIZATION EQUATION (See Motz, Chap. 4.2 for a derivation.)

Valid for T.D.E. only:

$$\frac{N_{i+1}}{N_i} = A \frac{(kT)^{3/2}}{N_{e^-}} \left(\frac{2 B_{i+1}}{B_i} \right) e^{-\chi_i/kT} \quad (3-27)$$

$$A = \left(\frac{2\pi m_{e^-}}{h^2} \right)^{3/2} = 1.5 \times 10^{39} \text{ gm}^{3/2} / \text{erg}^3 / \text{sec}^2$$

Here N_{e^-} = no. density of free electrons

N_i = number density of ions in i th state of ionization,

N_{i+1} = number density of ions in the $i+1$ state of ionization,

χ_i = the ionization potential for the i th state of ionization in ergs,

and the Bs are the corresponding partition functions for the two different states of ionization.

For TDE, the no. of atoms in any state of ionization remains constant. Then:

Rate at which atoms in i th stage \rightarrow $i+1$ stage must equal the rate at which atoms in the $i+1$ stage \rightarrow i th stage.

This depends on N_{e^-} and T for given values of B_i & χ_i .

The logarithmic form of Saha's equation is often convenient to use for numerical calculations

$$\log\left(\frac{N_{i+1} N_{e^-}}{N_i}\right) = 15.38 + \log\left(\frac{2 B_{i+1}}{B_i}\right) + 1.5 \log T - \frac{5040}{T} \chi_i \quad (3-28)$$

Here χ_i is in electron volts, where $1 \text{ eV} = 1.602 \times 10^{-12}$ ergs.

For an electron gas, the ideal gas law gives

$$P_{e^-} = N_{e^-} k_B T$$

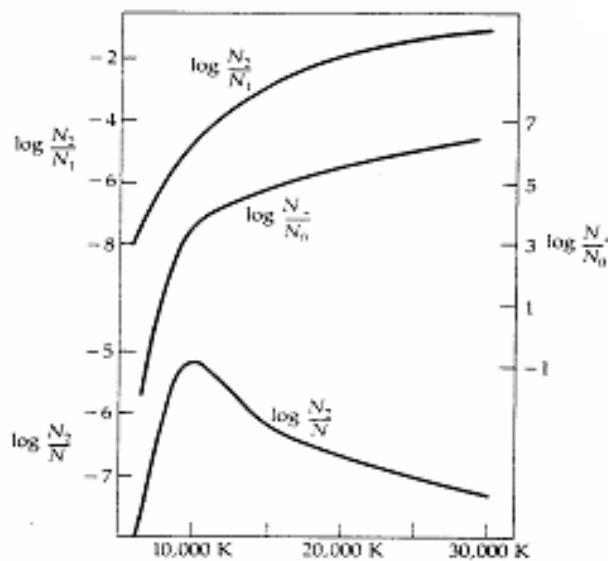
Hence,

$$\log\left(\frac{N_{i+1} P_{e^-}}{N_i}\right) = -0.48 + \log\left(\frac{2 B_{i+1}}{B_i}\right) + 2.5 \log T - \frac{5040}{T} \chi_i \quad (3-29)$$

For H: $B_1 = 2$ & $B_2 = 1$. For P_{e^-} in the range of 1 to 10 dyne/cm², H changes from almost completely neutral at 5040 K to almost completely ionized at 10,080 K. The above pressure range is found in stellar atmospheres.

Sometimes a correction factor is added to the 2 above equations that may be calculated from the known energy levels of the atoms. The value of the constant varies from atom to atom, changes slowly with temperature and has been tabulated by various workers. See for example Aller, *Atmospheres of the Sun and Stars*.

3-4D. Combined Boltzmann and Saha Equations



Excitation and ionization curves for hydrogen Balmer lines. The relative populations of the energy levels (N_2/N_1) from the Boltzmann equation and the ionization stages (N_+/N_0) from the Saha equation are calculated for equilibrium at the indicated temperatures. The lower curve shows the combination of the upper two with $N = N_0 + N_+$.

For any atom, assume only 3 different ionization stages are significant for a given T .

$$\frac{N_{ij}}{N} \cong \frac{N_{ij}}{N_{i-1} + N_i + N_{i+1}} = \frac{(N_{ij}/N_i)}{\frac{N_{i-1}}{N_i} + 1 + \frac{N_{i+1}}{N_i}} \quad (3-30)$$

The value of the numerator comes from the Boltzmann equation and the terms in the denominator are found from the Saha equation.

That is

$$\frac{N_{ij}}{N_i} \propto e^{-E_{ij}/kT}$$

and

$$\frac{N_{i+1}}{N_i} \propto e^{-\chi_i/kT}$$

Consider the combined results for Hydrogen. In this case, we have only 2 possibilities:

$$N = N_0 + N_+$$

For the Balmer absorption lines, their strength depends on

$$N_2/N = N_2/(N_0 + N_+) = (N_2/N_0)/[1 + (N_+/N_0)] \quad (3-31)$$

It is reasonable to assume that $N_0 \cong N_1$ for the temperature range where H is not completely ionized. Then we have

$$N_2/N \cong (N_2/N_1)/[1 + (N_+/N_0)] \quad (3-32)$$

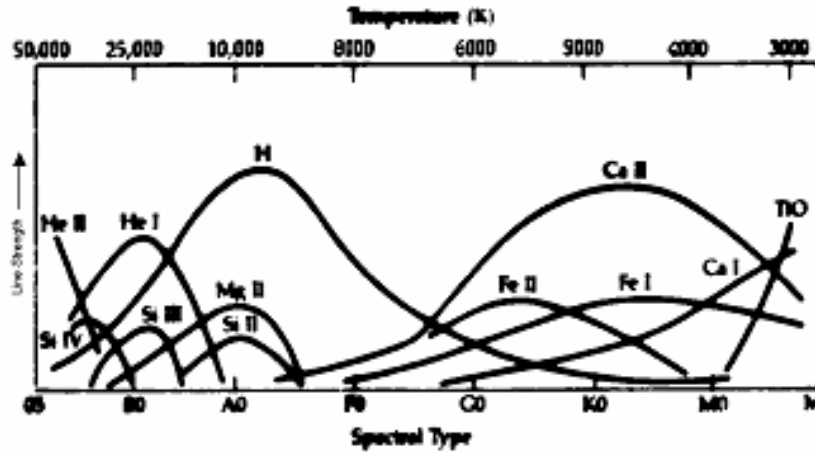
The numerator may be found from the Boltzmann equation and the denominator is found from the Saha equation. For greater precision, one uses for N_2/N_0 in (3-31), the following:

$$N_2/N_0 = N_2/(N_1 + N_2 + N_3 + \dots) = (N_2/N_1)/[1 + N_2/N_1 + N_3/N_1 + \dots], \quad (3-33)$$

where each of the ratios is found from the Boltzmann equation. The separate results for the Boltzmann and Saha equations as well as the combined results for hydrogen are shown in the diagram on the previous page. Note that the peak of the curve for the combined results is at about 10,000K, which is in agreement with the fact that the Balmer lines have their peak strength in spectral class A2. Though the ratio for N_2/N is about 6.0×10^{-6} , it is the abundance of hydrogen that produces a noticeable line in the spectrum. **Do RJP-61**

A similar calculation for other abundant elements in stellar atmospheres produces the results shown in the following figure.

Absorption lines and temperature. The strengths (equivalent widths) of the absorption lines for various ionic species are shown as a function of stellar temperature. These changes result in ionization-excitation equilibria as described by the Boltzmann-Saha equation.



One can see from this diagram, that only 2 states of ionization are usually found for a given spectral type. Therefore, one needs only 2 terms in the denominator of equation (3-30). Furthermore, note that the metals such as Ca and Fe, in addition to others not shown, are ionized even in the cooler stars. The molecule TiO is one of the most refractory of all molecules, since it exists in stellar atmospheres up to 3500K. Traces of other molecules such as water and CN are also found in the relatively cool atmospheres of giant stars.

Do RJP-58, 65, 67 & 68.