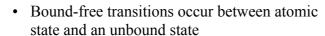
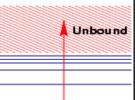
# Bound-free transitions (Saha equation)



- Free electron can have a range of kinetic energies => bound-free transitions produce continuous opacity (not just at lines)
- A minimum photon energy is needed to ionize an atom from a given level, e.g., need λ≤ 91.2 nm to ionize hydrogen from the n=1 level.



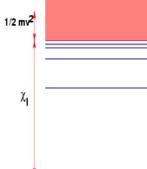


## The Saha equation

- Gives the distribution (relative number densities) of atoms in successive stages of ionization.
   Simplest case: a neutral atom and its first stage of ionization.
- Energy difference between ground state of atom, and free electron having velocity v, is:

$$\Delta E = \chi_I + \frac{1}{2} m_e v^2$$

• where  $\chi_I$  is the ionization potential.





#### Boltzmann

• The Boltzmann law suggests:

$$\frac{dN_0^+(v)}{N_0} = \frac{g}{g_0} \exp\left[-\frac{(\chi_I + 1/2m_e v^2)}{kT}\right] dv$$

where:

- $-dN_0^+(v)$  is the number of ions in the ground state with the free electron having velocity between v and v+dv
- $-N_0$  is number of atoms in ground level
- $-g_0$  is the statistical weight of the atom in the ground state
- g is the product of the statistical weight of the ion in its ground state  $g_0^+$ , and the differential statistical weight of the electron  $g_e$ . i.e.,  $g = g_0^+ g_e$

## Statistical weight of free electron

- Uncertainty principle tells us phase space is quantised into cells with volume h<sup>3</sup>
- For the electron, with two spin states,

$$g_e = \frac{2 \, dx_1 dx_2 dx_3 dp_1 dp_2 dp_3}{h^3}$$

- The volume  $dx_1 dx_2 dx_3$  contains one electron, so  $dx_1 dx_2 dx_3 = 1/N_e$ , where  $N_e$  is the electron density.
- Since the electrons have an isotropic velocity distribution,

$$dp_1dp_2dp_3=4\pi p^2dp=4\pi m_e^3v^2dv$$

· which gives,

$$\frac{dN_0^+(v)}{N_0} = \frac{g_0^+}{g_0} \frac{8\pi m_e^3}{N_e h^3} \exp\left[-\frac{(\chi_I + 1/2m_e v^2)}{kT}\right] v^2 dv$$

## Eliminating velocity

• We don't care about the electron velocity. Integrating over all possible  $\upsilon$  gives,

$$\frac{N_0^+ N_e}{N_0} = \frac{2g_0^+}{g_0} \left(\frac{2\pi m_e kT}{h^2}\right)^{3/2} e^{-\frac{\chi_I}{kT}}$$

• where we use the integral

$$\int_0^\infty e^{-x^2} x^2 dx = \frac{\sqrt{\pi}}{4} \qquad x = \sqrt{\frac{m_e}{2kT}} v$$



### Finally... the Saha equation

• For the ground state, Boltzmann's law gives,

$$\frac{N_0}{N} = \frac{g_0}{U(T)}$$
 and  $\frac{N_0^+}{N^+} = \frac{g_0^+}{U^+(T)}$ 

• Substituting these gives us Saha's equation,

$$\frac{N^{+}N_{e}}{N} = \frac{2U^{+}(T)}{U(T)} \left(\frac{2\pi m_{e}kT}{h^{2}}\right)^{3/2} e^{-\frac{\chi_{I}}{kT}}$$

- where N and N<sup>+</sup> are the number densities of neutral and once-ionized atoms, and U and U<sup>+</sup> are the corresponding partition functions.
- Saha's equation for any two neighbouring states of ionization is just the same, replace N by  $N^j$ ,  $N^+$  by  $N^{j+1}$ , etc.

## Ionization of hydrogen - I

• Define the degree of ionization x by

$$X = \frac{N^+}{N + N^+}$$

• For a neutral gas x = 0, for a fully ionized gas x = 1. Left hand side of Saha equation is then,

$$\frac{N^+ N_e}{N} = \frac{x}{1-x} N_e$$

- Next, eliminate  $N_e$  by writing it in terms of the gas pressure.
- If  $N_H = N + N^+$  is the total number of hydrogen nuclei, then can write the pressure of the electrons as:

$$P_e = N_e kT = (N_H + N_e)kT \frac{N_e}{N_H + N_e} = P_{gas} \frac{N_e}{N_H + N_e}$$

## Ionization of hydrogen - II

• Each ionized atom gives one electron, so for pure hydrogen  $N_e = N^+$  and

$$P_e = \frac{x}{1+x} P_{gas}$$

• The Saha equation can then be written,

$$\frac{x^2}{1-x^2} = \frac{1}{P_{aas}} \frac{2U^+(T)}{U(T)} \left(\frac{2\pi m_e}{h^2}\right)^{3/2} (kT)^{5/2} e^{-\frac{\chi_I}{kT}}$$

- a quadratic equation for the degree of ionization. To apply, we need
  - $-P_{\rm gas}$  and T. Ionization increases with the temperature (collisions become more violent) and decreases with increasing pressure at fixed T (more recombinations).
  - The partition functions. In practice, can take U = 2 (the ground state value) and  $U^+ = 1$ .
- Even a small abundance of other elements can provide lots of electrons if the ionization potential is low. So the pure hydrogen case is of limited applicability.

## Bound-free absorption cross-section

Bound-free absorption provides an important source of continuum opacity. For a hydrogen-like atom in a level with principal quantum number n, with ionization potential  $\chi_n$ , the bound-free absorption cross-section  $\sigma_{\rm bf}$  is given by

$$\sigma_{bf} = 0 \text{ for } \nu < \frac{\chi_n}{h}$$

$$\sigma_{bf} \propto \frac{g(\nu, n, l)}{n^5 \nu^3}$$
 otherwise

- Here g is the bound-free Gaunt factor (not degeneracy), a quantum mechanical correction factor to the simple scaling
- Properties:
  - Absorption cross-section has sharp rises, absorption edges, at the frequency where the atom in a given level can be ionized

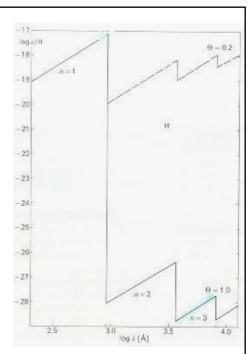
    At frequencies higher than the edge:  $\sigma_{bf} \propto v^{-3}$ The Gaunt factor is close to unity near the edge



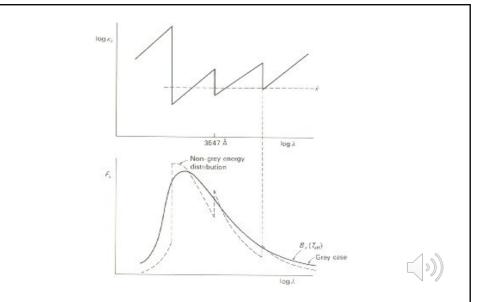
The hydrogen absorption coefficient  $\kappa$ per hydrogen atom is shown as a function of wavelength for two temperatures 5040 and 25200 K, where  $\theta = 5040/T$ 

Higher temperatures lead to higher values of  $\kappa$  in the visual spectral region (Paschen continuum, absorption from the level n = 3).

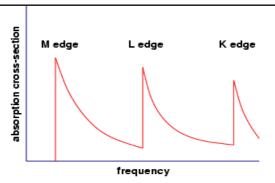
The value of  $\kappa$  at the Lyman limit is  $\sim$ the cross section of the lowest orbital  $(0.5 \times 10^{-8} \text{ cm})$  in the hydrogen atom.







Effect of wavelength-dependence of hydrogen absorption coefficient on the observed energy distribution of the star



An atom with many electrons will be characterized by a series of ionization edges as it loses electrons from successive shells.

- Heavy elements, either in the gas phase or in grains, have many inner-shell electrons. They provide large opacity to soft X-rays (below 1 keV).
- Hard X-rays (10 keV or more) see only the  $v^{-3}$  tail (becoming closer to  $v^{-3.5}$  at high v). Very hard to absorb these.
- Seeing the absorption at low energies  $\rightarrow$  measurement of the column density towards an X-ray source.



#### **Example: absorption towards an Active Galactic nucleus**

The *intrinsic* X-ray spectra of Active galaxies are often taken to be power laws. Superimposed on that we have,

- Absorption at low energy (here modelled as oxygen edges).
- Instrumental features than have not been calibrated quite right (a gold edge).
- Emission from fluorescent iron near the black hole.

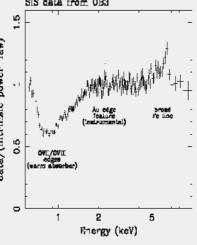




Figure 2.2: Ratio of the full band SISC spectrum of MCG=6-30-15 obtained during OB3 to the best fitting intrinsic power-law. The intrinsic continuum is defined by fitting a power-law to the 2-4 keV range (since there is negligible X-ray reprocessing over this range). Galactic absorption is included with a column density of  $N_{\rm H}=4\times10^{22}\,{\rm cm}^{-2}$ 

## Lecture 9 revision quiz

• Sanity-check integral with respect to v:

$$\frac{dN_0^+(v)}{N_0} = \frac{g_0^+}{g_0} \frac{8\pi m_e^3}{N_e h^3} \exp\left[-\frac{(\chi_I + 1/2m_e v^2)}{kT}\right] v^2 dv$$

- Plot the degree of ionization of hydrogen as a function of log(P<sub>gas</sub>) at a fixed T=10<sup>4</sup> K.
- In the spectrum of an early-type star, why is there an abrupt change in flux with wavelength across hydrogen ionization boundaries?
- Do you expect the emergent intensity to be greater at higher or lower frequencies than the ionization threshold frequency? Why?

## Lecture 9 revision quiz

- Starting from the Boltzmann excitation equation, fill in the steps to derive the Saha equation.
- Starting from the definition of the ionization fraction *x*, derive the equations for electron pressure and the quadratic form of the Saha equation.