# Bound-free transitions (Saha equation)

- Bound-free transitions occur between atomic state and an unbound state.
- 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, eg need λ≤ 91.2 nm to ionize hydrogen from the n=1 level.

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### The Saha equation

- Gives the distribution of atoms in different 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:

• 
$$\Delta E = \chi_I + \frac{1}{2}m_ev^2$$

• where  $\chi_I$  is the ionization potential.

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### 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:

- $-dN_0^+(\upsilon)$  is the number of ions in the ground state with the free electron having velocity between  $\upsilon$  and  $\upsilon + d\upsilon$ .
- $-N_0$  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  $g_e$ . ie  $g = g_0^+ g_e$

### Statistical weight of free electron

• 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,

$$dp_1 dp_2 dp_3 = 4\pi p^2 dp = 4\pi m_e^3 v^2 dv$$

• 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 v 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 the integral

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

was used.

### 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<sup>j</sup>*, *N*<sup>+</sup> by *N<sup>j+1</sup>*, etc.

## Ionization of hydrogen - I

• Define the degree of ionization *x* by

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

• ie 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,

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

- a quadratic equation for the degree of ionization. To apply, we need
  - $-P_{\text{gas}}$  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  $U^+ = 1$ .
- Alas, 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.

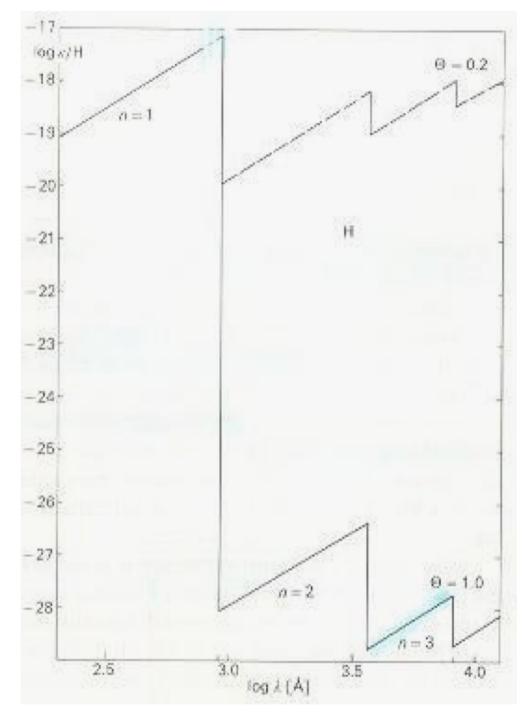
### Bound-free absorption cross-section

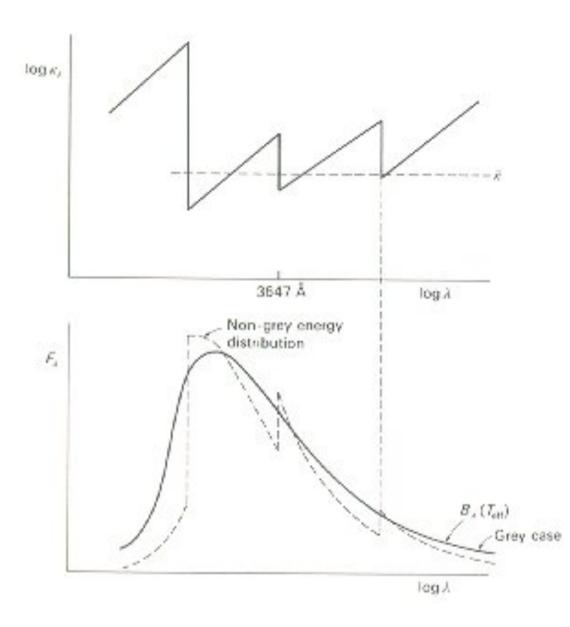
• Bound-free absorption provides an important source of continuum opacity. For a hydrogen-like atom in a level with principal quantum number n, with ionization potential  $\chi_n$ , the bound-free absorption cross-section  $\sigma_{bf}$  is given by

$$\sigma_{bf} = 0$$
 for  $\nu < \frac{\chi_n}{h}$   
 $\sigma_{bf} \propto \frac{g(\nu, n, l)}{n^5 \nu^3}$  otherwise

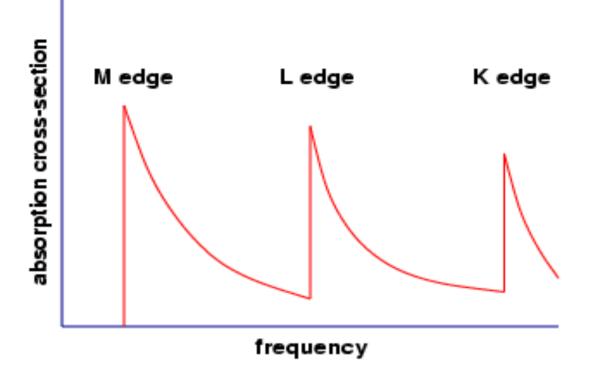
- Here g is the bound-free Gaunt factor -- a slowly varying correction factor to the simple scaling.
- Properties:
  - Absorption cross-section has sharp rises, absorption edges, at the frequency where the atom in a given level can be ionized.
  - At frequencies higher than the edge:  $\sigma_{bf} \propto v^{-1}$
  - 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.
- 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 ~ 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  $\nu^{-3}$  tail (becoming closer to  $\nu^{-3.5}$  at high  $\nu$ ). Very hard to absorb these.
- Seeing the absorption at low energies → measurement of the column density towards an X-ray source.

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

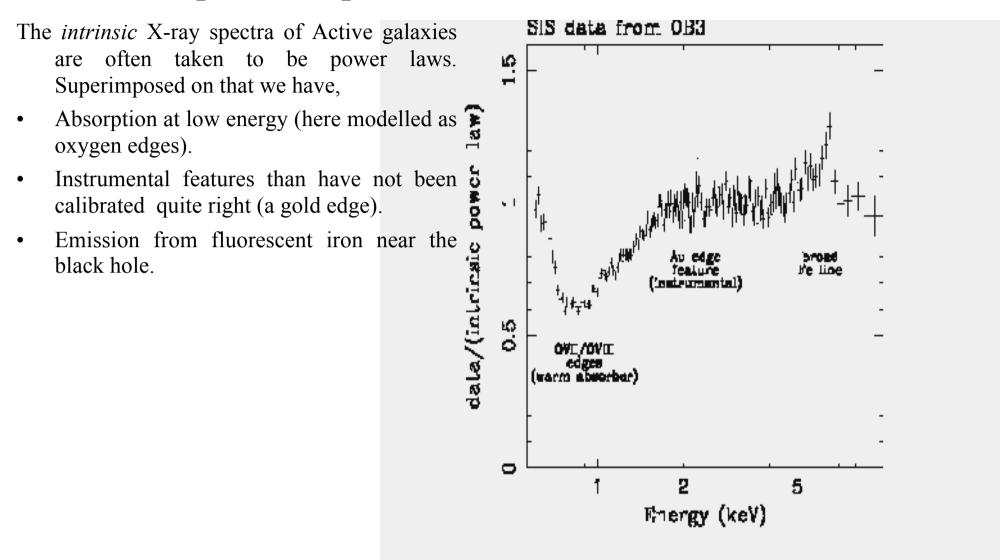


Figure 2.2: Ratio of the tull band SISC spectrum of MCG+6-30-15 obtained during OB3 to the best fitting intrinsic power-law. The intrinsic continuum is defined by fitting a power-law to the 2-4 keV range (since there is negligible X-ray reprocessing over this range). Galactic absorption is included with a column density of  $N_{\rm H} = 4.1 \times 10^{22}$  cm<sup>-2</sup>.

### 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  $log(P_{gas})$  at a fixed  $T=10^4$  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?