Determining the Absorption Coefficient

It would be Good to know how to determine the coefficients of the Equation of Transfer!

The Absorption Coefficient

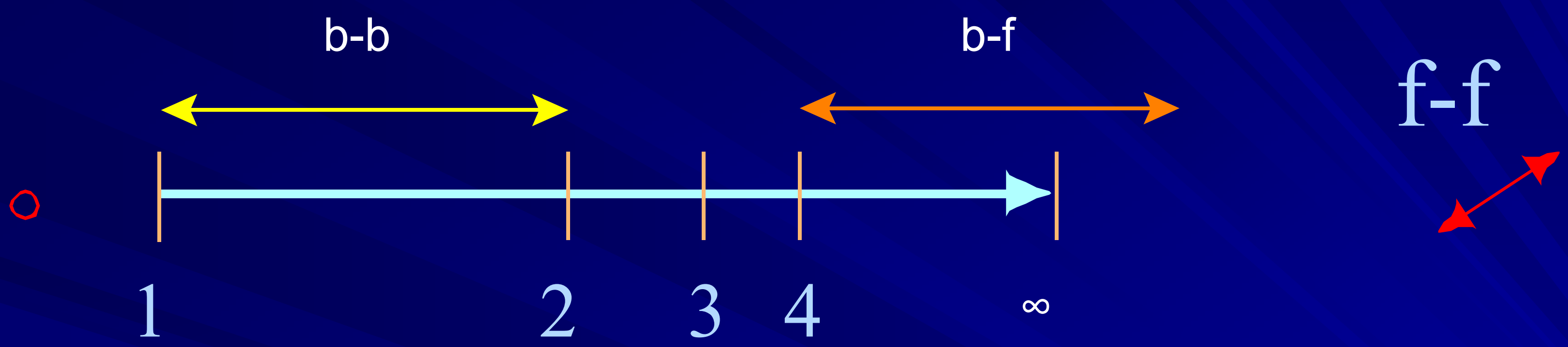
- Occupation Numbers
  - N = Total Number of an Element
  - $N_{i,I}$ = Number in the proper state (excitation and ionization)
- Thermal Properties of the Gas (State Variables: P_g, T, N_e)
- Atomic/Molecular Parameters: Excitation and Ionization Energies, Transition Probabilities, Broadening Parameters

Bohr Theory

The One Electron Case

- e = Electron Charge (ESU)
- Z = Atomic number of the nucleus
- m💧 = reduced mass of the nucleus
  - $m_{nucleus} * m_e / (m_{nucleus} + m_e) \sim m_e$
- N = principal quantum number
- r_n = effective orbital radius
- v_n = speed in orbit

Bohr Model



- Total Energy (TE) = Kinetic Energy(KE) + Potential Energy(PE)
- PE is Negative
- For a bound state TE< 0
- Therefore: |KE| < |PE|

$$E_{i,n} = \frac{1}{2} m' v_n^2 - \frac{Ze^2}{r_n}$$

n = Excitation "stage"
i = Ionization Stage:
I = neutral, II=first ionized

Continuing ...

Combine the Energy and Radial Force Equations

Energy: $$E_{i,n} = \frac{1}{2} m' v_n^2 - \frac{Ze^2}{r_n}$$

Force: $$F_n = -m' \frac{v_n^2}{r_n} = -\frac{Ze^2}{r_n^2}$$

Substituting mv^2 $$E_{i,n} = -\frac{Ze^2}{2r_n}$$

Bohr Postulates

Angular Momentum is Quantitized

$$m' v_n r_n = n\frac{h}{2\pi} = n\hbar$$

$$v_n = \frac{nh}{2\pi m' r_n}$$

Now put v into the force equation:

$$-m'\left(\frac{nh}{2\pi m'}\right)^2 r_n^{-3} = -\frac{Ze^2}{r_n^2}$$

$$\frac{n^2h^2}{4\pi^2 m' r_n} = Ze^2$$

$$r_n = \frac{n^2h^2}{4\pi^2 m' Ze^2}$$

Now put r into the energy equation:

$$E_{i,n} = -\frac{Ze^2}{2r_n} = -\frac{2\pi^2 m' Z^2 e^4}{n^2h^2}$$

Hydrogen

Atomic Parameters

- $Z = 1$
- m🌢 $= 1836.1\ (1)\ /\ 1837.1 = 0.99946\ m_e = 9.1033(10^{-28})$ gm
- e = electron charge $= 4.803(10^{-10})$ esu
- $h = 6.6252(10^{-27})$ erg s
- $k = 1.380622(10^{-16})$ erg K
- $E_{i,n} = -2.178617(10^{-11})\ /\ n^2$ ergs $= -13.5985\ /\ n^2$ eV
  - $1\ \text{eV} = 1.6021(10^{-12})$ erg
- For $n = 1$: $E_{i,1} = -13.5985$ eV $= -109678\ \text{cm}^{-1}$
  - $1\ \text{eV} = 8065.465\ \text{cm}^{-1}$
  - $E_{i,n} = -109678\ /\ n^2\ \text{cm}^{-1}$

Continuing

- Note that all the energies are negative and increasing
  - n = ❄ ==> $E_{i,❄} = 0$
  - The lowest energy state has the largest negative energy
- For hydrogen-like atoms the energies can be deduced by multiplying by Z^2 and the proper m💧.
  - Li^{++} (Li III): $3^2(-13.60) = -122.4$ eV
  - hν = 122.4 eV = 122.4(1.6021(10^{-12}) ergs) = 1.96(10^{-10}) ergs
  - ν = 2.9598(10^{16}) Hz ==> λ = 101 Å
- What is the temperature?
  - hν = kT ==> T = 1.4(10^6) K

Specifying Energies

Energies are usually quoted WRT the ground state (n=1)

- Excitation Potential: $\chi_{i,n} \equiv E_{i,n} - E_{i,1}$
  - For an arbitrary n it is the absolute energy difference between the nth state and the ground state (n=1).
    - This means $\chi_{i,1} = 0$ and that $\chi_{i,❄} = -E_{i,1}$
- $\chi_{i,❄}$ $\equiv$ Ionization Energy (Potential)
  = Energy needed to lift an electron from the ground state into the continuum (minimum condition)
- $\chi_{i,❄} = E_{i,❄} - E_{i,1}$

Ionization

Energy Requirement: $E_m = \chi_{i,❄} + \varepsilon$

- ε goes into the thermal pool of the particles (absorption process)
- One can ionize from any bound state
- Energy required is: $E_{i,n} = \chi_{i,❄} - \chi_{i,n}$
- Energy of the electron will be: $h\nu - E_{i,n}$

A Free "Orbit"

- Consider the quantum number n′
- $n = \sqrt{-1}n'$ which yields a positive energy
- n′ = a positive value

$$E_{i,n'} = h\nu + E_{i,n}$$

$$\frac{2\pi^2 m' e^4 Z^2}{h^2 n'^2} = h\nu - \frac{2\pi^2 m' e^4 Z^2}{h^2 n^2}$$

The solution for the orbit yields a hyperbola

Bound Transitions

- Consider a transition between two bound states (a,b) => (n_a,n_b) [n's are the quantum numbers]

$$h\nu = E_{i,n_b} - E_{i,na}$$

$$= \frac{-2\pi^2 m' e^4 Z^2}{h^2 n_b^2} + \frac{2\pi^2 m' e^4 Z^2}{h^2 n_a^2}$$

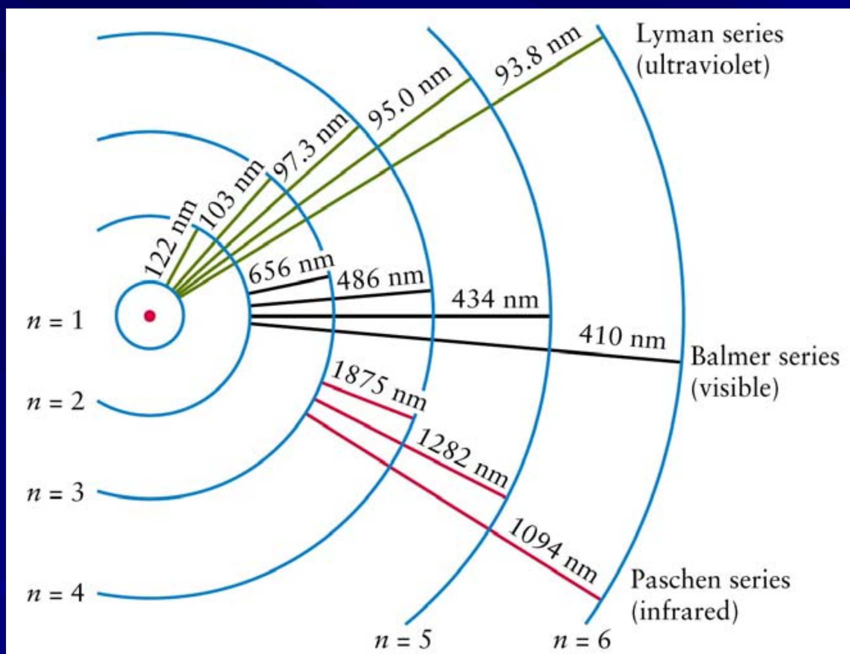
$$\nu = \frac{-2\pi^2 m' e^4 Z^2}{h^3}\left[\frac{1}{n_b^2} - \frac{1}{n_a^2}\right]$$

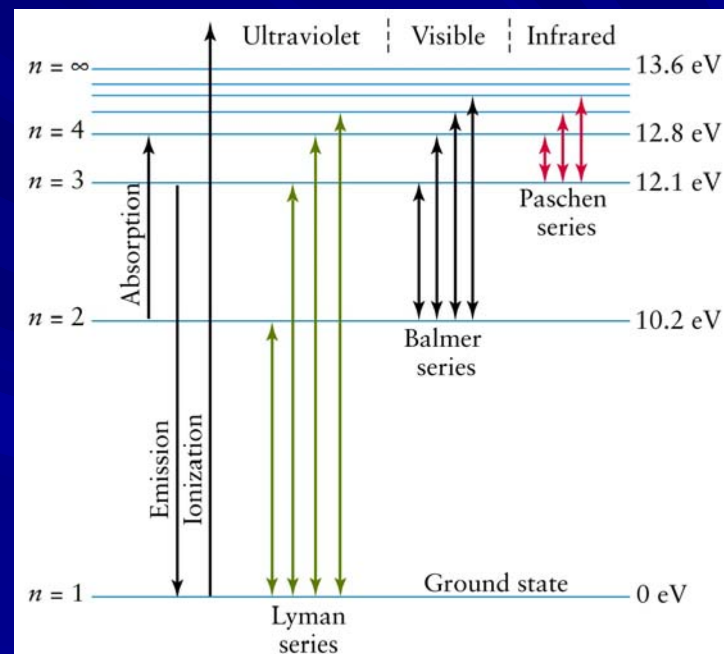
$$= -3.2883797(10^{15})\left[\frac{1}{n_b^2} - \frac{1}{n_a^2}\right]$$

m and Z for H

$$\lambda = \frac{c}{\nu} = -911.672\left[\frac{1}{n_b^2} - \frac{1}{n_a^2}\right]^{-1}$$

Hydrogen Lines





Balmer Series of H

The lower level is n = 2 ∴ $n_a = 2$

- First line (Hα) is the transition (absorption): 2 → 3.
  - For absorption: lower → upper $n_a \rightarrow n_b$
  - For emission: upper → lower $n_b \rightarrow n_a$

$$\lambda = \frac{c}{\nu} = -911.672\left[\frac{1}{3^2} - \frac{1}{2^2}\right]^{-1} = 6564.038\mathbf{A}$$

- The "observed" wavelength is 6562.3
  - The Rydberg formula gives vacuum wavelengths
- We need to account for the index of refraction of air: Edlen's Formula

Edlen's Formula

Computes the Index of Refraction of Air

- $\nu\lambda_{air} = c/n$ or $\lambda_{Vacuum} = n\lambda_{Air}$

$$(n-1)10^8 = 6432.8 + \frac{2949810}{146-\sigma^2} + \frac{25540}{41-\sigma^2}$$

- Where σ = vacuum wavenumber in inverse microns.
- For Hα: $\lambda_{Vac} = 0.6564038$ microns
- $\sigma = 1.52345$
- $n = 1.000276237$
- $\lambda_{Air} = 6562.225$ (calculated)

Series Limits

$\lambda = -911.672\ (1/❄^2 - 1/n_a^2)^{-1}$

- For $n_a = 2$ one gets λ = 3646.668 Å
  - Any photon which has λ < 3646.668 Å can move an electron from n = 2 to the continuum
- Series Limits are defined as n = ❄ to n_{Lower}

n	Limit	Name
1	912	Lyman
2	3646	Balmer
3	8204	Paschen
4	14590	Brackett
5	22790	Pfund

Excitation

Move an Electron Between Bound States

- $N_{i,x}$ = Number of ions (atoms) that have been ionized to state i and excited to level x
  - $N_{i,x}$ depends upon the number of ways an electron can enter level x
    - Most levels have sublevels ΔE from the "main" energy level
    - If there are g_x of these levels then there are g_x ways of entering the level
    - g_x is called the statistical weight of the level (state)
    - Each of the sublevels has a complete set of quantum numbers
      - (n,l,m_l,m_s) or (n,l,j,m_j)

Quantum Numbers

- n: Principal Quantum Number
- ❹: orbital angular momentum quantum number
  - L = ❹(h/2π)   0 ⌨ ❹ ⌨ (n – 1)
- m❹ : - ❹ ⌨ m < + ❹
- m_s: ±½
- **j: j = l + s**   => j = l ± s   s = ½
- m_j: -j ⌨ m_j ⌨ +j

Hydrogen Quantum Numbers

- n=1: $(n = 1, l = 0, m_l = 0, m_s = \pm ½)$
- n=2: $(n = 2, l = 0, m_l = 0, m_s = \pm ½)$
- $(n = 2, l = 1, m_l = -1, m_s = \pm ½)$
- $(n = 2, l = 1, m_l = 0, m_s = \pm ½)$
- $(n = 2, l = 1, m_l = 1, m_s = \pm ½)$
- Therefore for n=1 g=2 and for n=2 g = 8
- For any H-like ion: $g_n = 2n^2$
- For any atom having level J (alternate set quantum number) with sublevels -J,...0,...+J the statistical weight is $g_J = 2J + 1$
  - J is not necessarily an integer

Notation

$$^{2S+1}L_J$$

- 2S+1: Multiplicity (Spin) $S = \sum s_i$
- L: Azimuthal Quantum Number $L = \sum$❹$_i$
- J: L+S = total angular momentum vector

Boltzmann Equation

We shall start with the state-ratio form of the equation

$$\frac{N_{i,x}}{N_{i,x'}} = \frac{g_{i,x} e^{\frac{-E_{i,x}}{kT}}}{g_{i,x'} e^{\frac{-E_{i,x'}}{kT}}}$$

The E's are with respect to the continuum.

$$= \frac{g_{i,x}}{g_{i,x'}} e^{\frac{-(E_{i,x}-E_{i,x'})}{kT}}$$

$$\frac{N_{i,x}}{N_{i,0}} = \frac{g_{i,x}}{g_{i,0}} e^{\frac{-\chi_{i,x}}{kT}}$$

χ is the excitation potential of the state

$$N_i = \sum_x N_{i,x} = \frac{N_{i,0}}{g_{i,0}} \sum p_i g_{i,x} e^{\frac{-\chi_{i,x}}{kT}}$$

p_i is the probability that the state exists

The Partition Function

- Note that p_i depends on electron pressure and essentially quantifies perturbations of the electronic states. We define the partition function U as

$$U(T) = \sum_x p_i g_{i,x} e^{\frac{-\chi_{i,x}}{kT}}$$

- These numbers are tabulated for each element as a function of ionization stage, temperature, and "pressure." The latter is expressed as a lowering of the ionization potential.

Rewrite the Boltzman Equation

$$\frac{N_{i,x}}{N_{i,0}} = \frac{g_{i,x}}{g_{i,0}} e^{\frac{-\chi_{i,x}}{kT}}$$

Number in state X WRT ground state

$$N_i = \frac{N_{i,0}}{g_{i,0}} U(T)$$

Sum $N_{i,x}$

$$\frac{N_{i,x}}{N_i} = \frac{g_{i,x}}{g_{i,0}} e^{\frac{-\chi_{i,x}}{kT}} \frac{g_{i,0}}{U(T)}$$

Substitute

$$= \frac{g_{i,x}}{U(T)} e^{\frac{-\chi_{i,x}}{kT}}$$

Example

What is the fraction of H that can undergo a Balmer transition at 5700K?

$$\frac{N_{I,2}}{N_I} = \frac{g_{I,2}}{U(T)} e^{\frac{-\chi_{I,2}}{kT}}$$

- We need g_2, $U_I(5700)$, and χ_2
  - $g_2 = 8$ (n=2)
  - $U_I(T) = 2$
  - $\chi_2 = 82259.0\ \text{cm}^{-1} = 10.20\ \text{eV} = 1.634(10^{-11})$ ergs
  - $N_2/N_I = 8/2\ e^{-(\chi/kT)} = 4\ e^{-20.76} = 3.842(10^{-9})$

Ionization

The Saha Equation

$$\frac{N_{i+1,0}}{N_{i,0}} N_e = \frac{2(2\pi mkT)^{3/2}}{h^3} \frac{g_{i+1,0}}{g_{i,0}} e^{\frac{-\chi_{i,\infty}}{kT}}$$

- This is the Saha equation. It gives the ratio of ground state populations for adjoining ionization stages. What one really wants is the number in the entire stage rather than just the ground state. Remember that $\chi_{i,0} = 0$.

$$N_{i,0} = N_i \frac{g_{i,0}}{U(T)} e^{\frac{-\chi_{i,0}}{kT}} = N_i \frac{g_{i,0}}{U(T)}$$

$$N_{i+1,0} = N_{i+1} \frac{g_{i+1,0}}{U(T)} e^{\frac{-\chi_{i+1,0}}{kT}} = N_{i+1} \frac{g_{i+1,0}}{U(T)}$$

Rewrite The Saha Equation

$$\frac{N_{i+1,0}}{N_{i,0}} N_e = \frac{2(2\pi mkT)^{3/2}}{h^3} \frac{g_{i+1,0}}{g_{i,0}} e^{\frac{-\chi_{i,\infty}}{kT}}$$

Note that m = m_e

$$\frac{N_{i+1}}{N_i} N_e = \frac{2(2\pi mkT)^{3/2}}{h^3} \frac{U_{i+1}}{U_i} \frac{g_{i+1,0}}{g_{i,0}} \frac{g_{i,0}}{g_{i+1,0}} e^{\frac{-\chi_{i,\infty}}{kT}}$$

$$\frac{N_{i+1}}{N_i} N_e = \frac{(2\pi mk)^{3/2}}{h^3} \frac{2U_{i+1}}{U_i} T^{3/2} e^{\frac{-\chi_{i,\infty}}{kT}}$$

$$P_e = N_e kT$$

$$\frac{N_{i+1}}{N_i} P_e = 0.3334 T^{5/2} \frac{2U_{i+1}}{U_i} e^{\frac{-\chi_{i,\infty}}{kT}}$$

Computing Stage Populations

- Note that the Saha Equation does not tell you the populations but:
  - $N_T = N_I + N_{II} + N_{III} + N_{IV} + \ldots$
  - Divide by N_I
  - $N_T/N_I = 1 + N_{II}/N_I + (N_{III}/N_{II})(N_{II}/N_I) + (N_{IV}/N_{III})(N_{III}/N_{II})(N_{II}/N_I) + \ldots$
  - Each of the ratios is computable and N_T is known.

Example

What is the degree of ionization of H at τ = 2/3 in the Sun?

- $T = 6035K$ and $P_e = 26.5$ dynes/cm^2
- $P_e N_{II}/N_I = 0.3334\ T^{5/2}\ (2U_{II}/U_I)\ e^{-13.598*CF/kT}$
- $U_{II} = 1$: Partition function for a bare nucleus = 1
- $U_I = 2$
- $P_e N_{II}/N_I = 9.4332(10^8)\ e^{-26.15} = 4.162(10^{-3})$

- $N_{II}/N_I = 1.57(10^{-4})$

Another Example

The Same for Neutral and First Ionized Fe.

- $T = 6035K$ and $P_e = 26.5$ dynes/cm2
- $P_e N_{II}/N_I = 0.3334\ T^{5/2}\ (2U_{II}/U_I)\ e^{-7.87*CF/kT}$
- $U_{II} = 47.4$
- $U_I = 31.7$
- $P_e N_{II}/N_I = 2.82(10^9)\ 2.68(10^{-7})$

- $N_{II}/N_I = 28.5$

Data Sources

- Atomic Energy Levels: NBS Monograph 35 and subsequent updates (NIST)
- Line Lists
  - Compute from AEL
  - MIT Wavelength Tables
  - RMT - Charlotte Moore
  - Kurucz Line Lists
  - Literature for Specific Elements
- Partition Functions
  - Drawin and Felenbok
  - Bolton in ApJ
  - Kurucz ATLAS Code
  - Literature (Physica Scripta)