Intensity Opacity

- In a general case level populations depend on collisions (gas temperature) and radiation.
- Change in level population can be described by arrivals – departures:

$$\frac{dn_i}{dt} = \sum_{j \neq i} n_j P_{ji} - n_i \sum_{j \neq i} P_{ij}$$

- where P_{ij} are transition rates per particle.
  n_i is the number of particles in level i per unit volume.

Transition processes

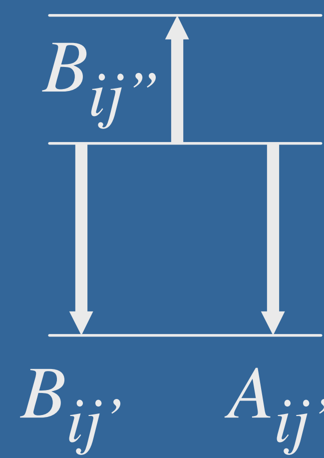
Two type of interaction make particle to "move" between energy levels: interaction with radiation and collisions with other particles. Thus we can split the expression for the rates into radiative rates and collisional rates:

$$P_{ij} = R_{ij} + C_{ij}$$

Radiative processes include absorption, emission and stimulated emission in *b-b* and *b-f*. Collisional processes include non-elastic collisions.

Transition rates (cont'd)

- Radiative rates can be expressed through Einstein probabilities:



$$R_{ij} = \begin{cases} A_{ij} + B_{ij} \cdot \bar{J}_{ij}, & i > j \\ B_{ij} \cdot \bar{J}_{ij}, & i < j \end{cases}$$

$$\bar{J}_{ij} = \frac{1}{4\pi} \oint d\Omega \int d\nu I_\nu(\mu) \varphi_{ij}(\nu - \nu_0)$$

- Computational recipes for non-elastic collisions exist but are not very reliable ☹

Statistical Equilibrium

Equation of statistical equilibrium:

$$n_i \sum_{j \neq i} \left(R_{ij} + C_{ij} \right) = \sum_{j \neq i} n_j \left(R_{ji} + C_{ji} \right)$$

or substituting the expression for the rates:

$$\sum_{j<i} \left[n_i A_{ij} - \left(n_j B_{ji} - n_i B_{ij} \right) \bar{J}_{ij} \right] -$$

$$\sum_{j>i} \left[n_j A_{ji} - \left(n_i B_{ij} - n_j B_{ji} \right) \bar{J}_{ij} \right] + \sum_{j} \left(n_i C_{ij} - n_j C_{ji} \right) = 0$$

or reformulating this as a SLE: $\mathbf{An} = 0$

Solving for Statistical Equilibrium

In most situations the level population reaches a balance very quickly, faster than most of other dynamic events in stellar atmospheres.

The equation of statistical equilibrium is:

$$\frac{dn_j}{dt} = 0 \Rightarrow \sum_{i \neq j} n_i P_{ij} = n_j \sum_{i \neq j} P_{ji}$$

$$\begin{pmatrix} -\sum_{i\neq 1} P_{1,i} & P_{1,2} & \cdots & P_{1,M} \\ P_{1,2} & -\sum_{i\neq 2} P_{2,i} & & \vdots \\ \vdots & & \ddots & P_{M-1,M} \\ P_{1,M} & \cdots & P_{M,M-1} & -\sum_{i\neq M} P_{M,i} \end{pmatrix} \cdot \begin{pmatrix} n_1 \\ n_2 \\ \vdots \\ n_{M-1} \\ n_M \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

- If all collisional and radiative rates are known from calculations or measurements and we also know the radiation field, we can solve this SLE and derive level populations.
- We have *M-1* independent equations (the sum of all equations is a trivial equality), therefore, we can only derive *the relative level populations* (e.g. fractions of the total number of atoms seating on each level):

$$n_j^* = n_j \Big/ \sum_i n_i = n_j \Big/ N_{\mathrm{species}}$$

and the additional equation will be: $\sum_{i=1}^{M} n_i^* = 1$

Molecular/Ionization equilibrium equations

- Equations connecting the density of each molecule to the densities of its constituents (chemical reaction equations)
- Equations connecting the density of each ion to the densities of the corresponding neutral and electrons
- In addition we have certain parameters specified: *abundances* (fraction of atoms of a given type among all atoms in all incarnations), *electric neutrality* and the *local physical conditions* (e.g. *pressure* and *temperature*) which give the total number of particles.

Equations: definitions

- Abundances Z_{atom} is the ratio $n_{\text{atom}} / n_{\text{total}}$
- $X_{\text{Atom}}^{\text{Species}}$ is the number of particular atoms in a particular species (e.g. $X_{\text{H}}^{\text{H}_2\text{O}} = 2, \quad X_{\text{C}}^{\text{H}_2\text{O}} = 0$)
- X^{Species} is the total number of atoms in a particular species (e.g. $X^{\text{H}_2\text{O}} = 3$)
- q^{species} charge of a given species $X^{\text{TiO+}} = +1$

Equations: simple ones

- Abundances (X is the number of atoms in a given species):

$$Z_{\text{Atom}} = \frac{\sum_{\text{species}} n_{\text{species}} \cdot X^{\text{Species}}_{\text{Atom}}}{\sum_{\text{species}} n_{\text{species}} \cdot X^{\text{Species}}}$$

- Total number of particles:

$$n_e + \sum_{\text{species}} n_{\text{species}} = n_{\text{total}} = P/kT$$

- Charge conservation (q is the electric charge):

$$\sum_{\text{species}} n_{\text{species}} \cdot q^{\text{species}} = n_e$$

Equations: Chemistry

- Chemical reaction in which species A and B form AB can be described by kinetic equation:

$$\frac{n_A n_B}{n_{AB}} = K(T) = \left(\frac{2\pi kT}{h^2}\right)^{\frac{3}{2}} \left(\frac{m_A m_B}{m_{AB}}\right)^{\frac{3}{2}} \frac{U_A U_B}{U_{AB}} e^{-\frac{D_{AB}}{kT}}$$

- Ionization can be described in exact same way:

$$\frac{n_{A^+} n_e}{n_A} = K(T) = \left(\frac{2\pi m_e kT}{h^2}\right)^{\frac{3}{2}} \frac{2U_{A^+}}{U_A} e^{-\frac{I_A}{kT}}$$

Saha equation!

Unknowns and equations

- One reaction equation for each species (except electrons).
- One equation per each atom (abundances).
  The sum of all abundances makes a trivial equality 1=1 so we are one equation short.
- The electric neutrality and the total pressure/density gives the two missing equations.
- Solution is non-trivial as we have to deal with a large system on non-linear equations.