Lecture 6:

Microphysics and NLTE

Equation of state (EOS)

- When solving a set of HD equation we will get some thermodynamic quantities of gas: e.g. pressure and internal energy (temperature). How does one get from here to the absorption/emission?
- The total absorption in a unit volume is given by:

$$\alpha_\nu = \sum_{\text{species}} \alpha_\nu^{\text{sp}} \cdot n_{\text{sp}}$$

where n_{sp} is the number density of a species.

- The source function is evaluated in a similar way:

$$S_\nu = J_\nu \cdot \sum_{\text{species}} (1 - \epsilon_\nu^{\text{sp}}) \cdot n_{\text{sp}} + B_\nu(T) \cdot \sum_{\text{species}} \epsilon_\nu^{\text{sp}} \cdot n_{\text{sp}}$$

Molecular-ionization equilibrium

- What do we know? P, T, abundances

- What else can assume in equilibrium? For chemical reactions the reactants and the product are in balance controlled by the temperature. The same is true for ionization.

- We can also assume change neutrality

Expressing what we know as equations

- Abundances (if $Z_A = n_A / n_{tot}$)

$$\sum_{sp} P_{sp} \left(n_A^{sp} - Z_A n_{tot}^{sp} \right) = 0$$

- Particle conservation (q^{sp} is charge)

$$\sum_{sp} P_{sp} \left(1 + q^{sp} \right) = P_{gas}$$

- Charge neutrality

$$\sum_{sp} P_{sp} q^{sp} = P_{elec}$$

For low temperatures ($P_{elec} << P_{gas}$)

- Abundances

$$\sum_{sp} e^{R_{sp}} \left(n_A^{sp} - Z_A n_{tot}^{sp} \right) = 0$$

- Particle conservation

$$\ln\left[\sum_{sp} e^{R_{sp}} \left(1 + q^{sp} \right) \right] = \ln P_{gas}$$

- Charge neutrality

$$\ln\left(\sum_{sp} e^{R_{sp}} q^{sp} \right) = \ln P_{elec}$$

where $R_{sp} = \ln P_{sp}$

The expression for partial pressures

- Equilibrium for two atoms and more

$$\frac{P_A \cdot P_B}{P_{AB}} = Kp^{sp}(T); \quad \frac{P_{sp+} \cdot P_{e-}}{P_{sp}} = Ip^{sp}(T)$$

$$\frac{\prod\limits_A P_A^{n_A^{sp}}}{P_{sp}} = Kp^{sp}(T); \quad \frac{P_{sp+\cdots} \cdot P_{e-}^{q_{sp}}}{P_{sp}} = Ip^{sp}(T)$$

- For "high" temperatures (>2000 K)

$$P_{sp} = \frac{Ip(T)}{Kp(T)} P_{e-}^{-q_{sp}} \prod_A P_A^{n_A^{sp}}$$

- For "low" temperatures (<2000 K)

$$R_{sp} = \log Ip(T) - \log Kp(T) - q_{sp} \log P_{e-} + \sum_A n_A^{sp} \log P_A$$

… and what are these *Kp*’s and *Ip*’s?

- Chemical equilibrium constant:

$$Kp(T) = kT\left(\frac{2\pi T}{h^2}\right)^{3/2}\left(\frac{m_A \cdot m_B \cdot \ldots}{m_{sp}}\right)^{3/2}\frac{U_A \cdot U_B \cdot \ldots}{U_{sp}}e^{-\frac{D_{sp}}{kT}}$$

- Ionization equilibrium constant:

$$Ip(T) = kT\left(\frac{2\pi T}{h^2}\right)^{3/2} m_{e^-}^{3/2} \cdot \frac{2 \cdot U_{sp^+}}{U_{sp}}e^{-\frac{I_{sp}}{kT}}$$

Let’s count equations and unknowns

- First, what are the unknowns?
  P_A and P_{e-}
- How many unknowns?
  N_A+1
- How many equations?
  N_A for abundances + total pressure + charge conservations = N_A+2!
- Help!

Solving the EOS

- Equations are non-linear so we need to use Newton-Raphson.
- Remember that N-R requires the initial guess on the same “slope” where the solution is.
- Here is an elegant way of getting one:
  1. Construct P_A’s using simply abundances
  2. Compute total pressure
  3. If it’s too small – scale up all P_A’s; too large – scale them down and repeat 2.
  4. Stop, when approximately matching

Statistical equilibrium equation

- Now that we know partial pressures for all absorbers all we need to compute opacities is level populations.
- Normally we assume equilibrium populations given by the Boltzmann distribution.
- This may not be a good guess in several situations or/and for specific transitions
- In the following we will relax this assumption and compute consistent level populations

Transition processes

Two types of interaction make a 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:

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

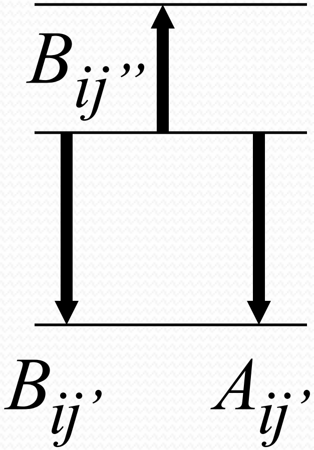
Radiative processes include absorption, emission and stimulated emission in *b-b* and *b-f* transitions. Collisional processes include non-elastic collisions.

Transition rates (cont’d)

- Radiative rates can be expressed through Einstein probabilities:

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

$$\overline{J}_{ij} = \frac{1}{4\pi} \oint d\Omega \int I_\nu(\phi, \theta) \varphi_{ij}(\nu - \nu_0) d\nu$$



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

Statistical Equilibrium

Equation of statistical equilibrium $\frac{dn_i}{dt} = 0$:

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

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:

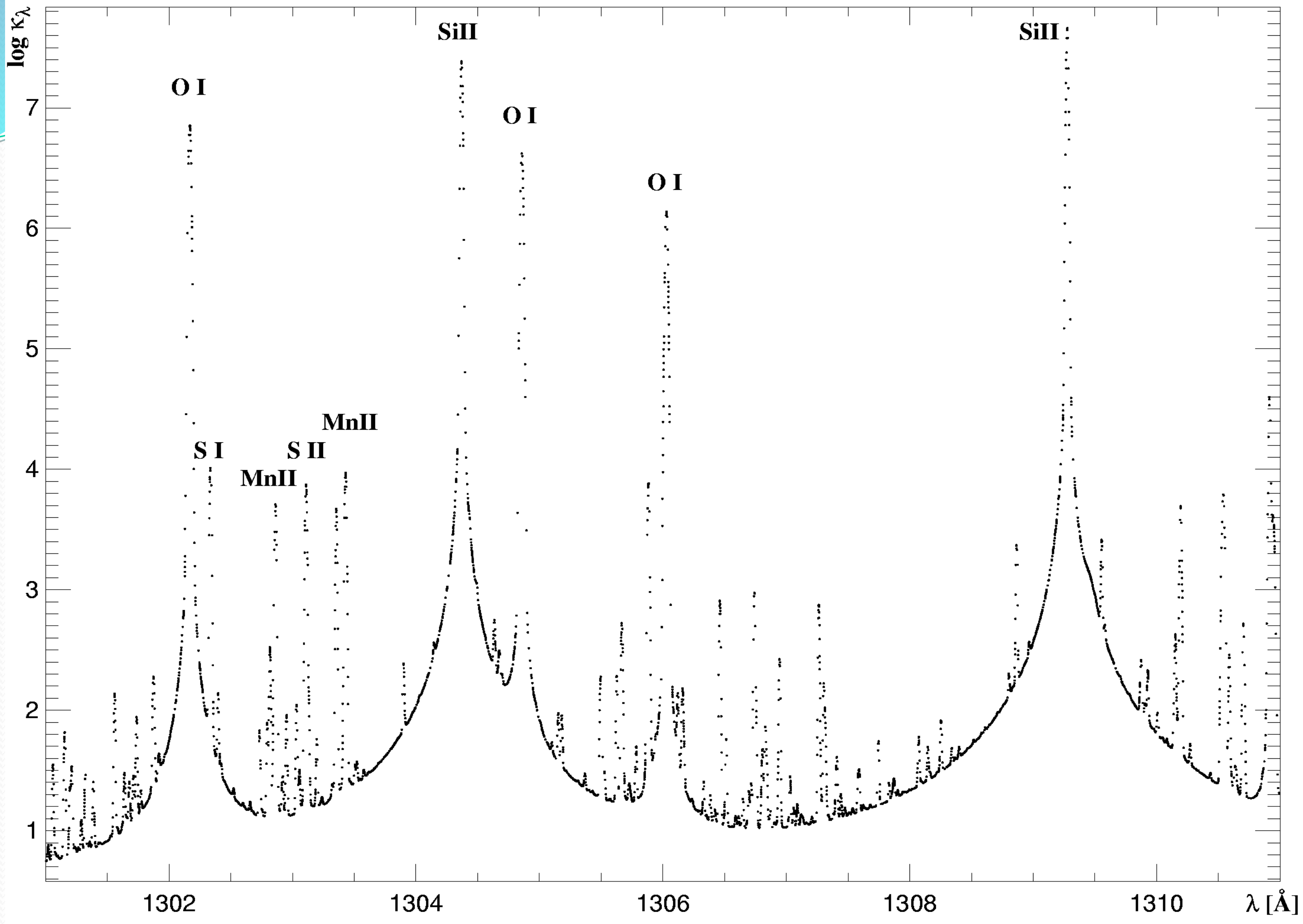
$$\mathbf{An} = 0$$

- 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):

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

and the additional equation will be:

$$\sum_{i=1}^{M} n_i^* = 1$$



Strong UV absorption by the NLTE lines of Si II in an A0 star

Ca I 6439Å