Chapter #: Modeling Atomic Populations

Models are employed to relate spectral emission measurements to the properties of the plasma being observed. This chapter will give an overview of the types of models which could be used, which leads to the motivation for the model under evaluation.

#.# Atomic Processes

An atom in one state can transition to another state by interacting with something. These interactions are divided into two broad categories: collisional, and radiative. Radiative transitions are interactions with the electromagnetic field such that a photon is produced or absorbed to account for the change in energy between the two states. Collisional transitions account for the change in energy by other particles (electrons or atoms) gaining or losing energy.

An example of a radiative process is spontaneous emission. The rate of this transition is contained in the Einstein coefficient A_{ij} between states i and j, which has units of inverse time. There cannot be a spontaneous transition upward in energy since this would require emitting a photon of negative energy. For simplicity of notation here, upward transitions have $A_{ij} = 0$, as well as $A_{ii} = 0$.

An example of a collisional process is electron-impact excitation and de-excitation. The likelihood of an electron passing near the atom inducing a transition to another level is contained in a cross section σ_{ij}, which has units of area, and depends on the relative velocity between the electron and atom. To calculate the total rate, the cross-section must be averaged over the distribution of relative velocities and multiplied by the electron density $R_{ij} = n_e \langle \sigma_{ij} \mathbf{v} \rangle$. Also for convenience here $R_{ii} = 0$.

If collisional transitions from the ground state to the ith state are now combined with spontaneous emissions, this gives a rate equation for the density of atoms in the ith state.

$\frac{\partial n_i}{\partial t} = n_1 R_{1i} - n_i \Sigma_j A_{ij}$ (#.#)

This is called coronal equilibrium. This is valid when radiative processes happen much faster than collisional ones for the level of interest, which occurs when the electron density is sufficiently low. As the electron density increases, collisional transitions between levels may not be neglected. This can be accounted for by simply including all the other levels.

$\frac{\partial n_i}{\partial t} = \Sigma_j n_j (R_{ji} + A_{ji}) - n_i \Sigma_j (R_{ij} + A_{ij})$ (#.#)

This constitutes a collisional-radiative model. Other processes can also be included, such as ionization and recombination, but they all take a similar form with separate rate coefficients.

R_i^{ion} = ionization rate from level i

$R_i^{2B-recomb}$ = 2-body recombination from ion (radiative recombination)

$R_i^{3B-recomb}$ = 3-body recombination from ion

$\frac{\partial n_i}{\partial t}$ can be split into a “gain” term that depends on all other levels plus the environment and a “loss” term which depends only on the ith level plus environment.

$\frac{\partial n_i}{\partial t} = G_i - n_i L_i$

$G_i = \Sigma_j n_j (R_{ji} + A_{ji}) + n_{ion}(R_i^{2B-recomb} + R_i^{3B-recomb})$

$L_i = \Sigma_j (R_{ij} + A_{ij}) + R_i^{ion}$

#.# Kinetic Theory

The previous discussion is fine for a system that does not depend on position, or depends on position only weakly. However, the effect of spatial variations will now be considered. The atoms being observed are typically part of a low density gas. If the atoms are ionized they will feel forces from macroscopic electric and magnetic fields as well as collision forces. For neutral atoms, only collisions affect their motion. At the most detailed level the evolution of a gas can be described by the Boltzmann equation.

$$\frac{\partial f}{\partial t} + \nabla_x \cdot (f\mathbf{v}) + \nabla_v \cdot (f\mathbf{a}) = \frac{\partial f}{\partial t}|_{collisions} \quad \textbf{(\#.\#)}$$

$$f = f(\mathbf{x}, \mathbf{v}, t),\ \mathbf{a} = \mathbf{a}(\mathbf{x}, \mathbf{v}, t)$$

This requires information of not only the density of the gas at every location in space, but also its distribution in velocities. For a neutral gas, and neglecting the force of gravity, the acceleration term will go to zero.

This says nothing of the atomic processes which are of interest. The extension is to describe each atomic level as a gas with its own evolution. Transitions between levels, as well as ionization and recombination, are included into a source term s_i. An index is also added to signify that each level has it's own evolution.

$$\frac{\partial f_i}{\partial t} + \nabla_x \cdot (f_i\mathbf{v}) + \nabla_v \cdot (f_i\mathbf{a}) = \frac{\partial f_i}{\partial t}|_c + s_i \quad \textbf{(\#.\#)}$$

$$s_i = s_i(\mathbf{x}, \mathbf{v}, t)$$

To see how s_i relates to the atomic processes already discussed, the first moment of this equation will be taken.

$$\frac{\partial n_i}{\partial t} + \nabla \cdot (n_i\mathbf{v}_i) = \int d\mathbf{v} s_i = S_i \quad \textbf{(\#.\#)}$$

S_i, the first moment of s_i, provides the link since $\frac{\partial n_i}{\partial t} = S_i$ in the absence of spatial variations. The only detail is how to go backward to s_i with rate terms R_{ij}, R_i^{ion}, etc.. . These rates are an integral over both atomic velocities and electron velocities. This gives rise to a velocity dependent electron-impact excitation rate as seen in eq. #.#.

$$R_{ij} = \int d\mathbf{v} \hat{f}_i(\mathbf{v}) \int d\mathbf{v}' |\mathbf{v}' - \mathbf{v}| f_e(\mathbf{v}') \sigma_{ij}(\mathbf{v}' - \mathbf{v}) = \int d\mathbf{v} \hat{f}_i(\mathbf{v}) r_{ij}(\mathbf{v}) \quad \textbf{(\#.\#)}$$

where $\hat{f}_i = \frac{1}{n_i} f_i$

This means that $n_i R_{ij}$ is the first moment of $f_i r_{ij}$. So, s_i can be written vary similarly to S_i by replacing all the n_i with f_i, R_{ij} with r_{ij}, etc. with the understanding that they are functions in velocity space.

$$s_i = g_i - f_i l_i$$

$$g_i = \Sigma_j f_j (r_{ji} + A_{ji}) + f_{ion}(r_i^{2B-recomb} + r_i^{3B-recomb})$$
$$l_i = \Sigma_j (r_{ij} + A_{ij}) + r_i^{ion}$$

#.# Solution for Helimak

For the purpose of the Helimak, the collision term will be neglected since the mean free path is larger than the chamber. Also, a solution of equilibrium is being sought, which reduces the equations to be solve to #.#

$$\nabla_x \cdot (f_i \mathbf{v}) = s_i \quad \text{#.#}$$

For a single direction and speed, eq. #.# can be re-arranged such that f_i can be directly integrated from the boundary (x=0) along a chosen direction as in eq. #.#.

$$f_i(x, v) = \int dx \frac{\partial f_i}{\partial x} + f_i(0, v) = \int dx \frac{1}{v} s_i + f_i(0, v) \quad \text{#.#}$$

Once $f_i(\mathbf{x}, \mathbf{v})$ is calculated, the first two moments give the total population densities and velocities.

$$n_i(\mathbf{x}) = \int d\mathbf{v} f_i(\mathbf{x}, \mathbf{v})$$

$$\mathbf{v}_i(\mathbf{x}) = \frac{1}{n_i} \int d\mathbf{v} \mathbf{v} f_i(\mathbf{x}, \mathbf{v})$$

For the Helimak, the solution should possess axial symmetry, which reduces the spatial dimension of the problem by one, and a reflection symmetry in the vertical direction. The distribution in velocity space should also have reflection symmetry in the azimuthal direction.