Atomic processes in gaseous nebulae

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Abstract. The atomic physics relevant to gaseous nebulae is critically examined using modelling software with particular emphasis on radio recombination lines (RRLs). The theoretical spectral line intensities can be deduced if we know the population structure of the bound electrons in the gas under non-thermal equilibrium conditions. The population structure of hydrogen is solved for various environments using a capture-collision-cascade (C^3) model that incorporates an ambient radiation field. Effects of an ambient radiation field on the population structure is examined and processes that are stimulated by a radiation field are included in the model. This has been done as a preliminary investigation to extend the model to a photoionization code.

1. Introduction

The understanding of the physics of ionized gasses is crucial to many subjects in astronomy. Emission spectra can be observed from numerous astronomical objects and the study of spectral lines in these spectra has yielded valuable information regarding the most elementary atomic processes occurring in the Universe and has proven to be an essential tool in astronomy.

Gaseous nebulae are often permeated by an external radiation field, generally from a nearby star or stars and the cosmic microwave background radiation (CMBR). To model the theoretical spectrum that we would expect to see from a specific nebula, it is necessary to have a detailed knowledge of the atomic processes occurring within the nebula.

A special class of spectral lines results from transitions between highly excited atomic states. These arise when an electron is captured by an ion into an energy level with a large principal quantum number n. If the downward cascading electron makes transitions between levels with small energy differences, it can produce photons that are in the radio regime. Spectral lines that result from this process that are in the radio regime are referred to as radio recombination lines (RRLs).

A model for hydrogen plasmas that is applicable to a large portion of the electromagnetic spectrum, in particular to the radio regime, has been developed. Hitherto, models for gaseous nebulae have focused on transitions at optical and infra-red wavelengths, while the importance of processes involving levels with large principal quantum numbers have not always been recognised.

The model simulates the influences of the ionizing radiation, free particle temperature and density on the excited level population structure of hydrogen. From this, the expected spectral line intensities can be calculated. The model considers an unbounded pure hydrogen plasma permeated by an external radiation field. Stimulated processes are important in the Rayleigh-Jeans limit, so it is necessary to investigate the influence of the incident radiation field on the population structure.

The model was coded in the programming language C using the MinGW compiler on a Windows XP platform. The code was written completely independently using algorithms described in literature and no existing codes were copied.

2. Atomic Level Populations

The level populations of states within an atom or ion would follow a Boltzmann distribution if the system were in thermodynamic equilibrium (TE). Menzel [1] introduced a correction factor b_n to compensate for the degree of departure from TE of the level population. In this scheme, the Saha-Boltzmann equation becomes

$$N_n = b_n N_e N_i \left(\frac{h^2}{2\pi m_e k_B T_e} \right)^{3/2} n^2 \exp\left(\frac{\chi_n}{k_B T} \right) . \tag{1}$$

The b_n factors are called departure coefficients and b_n equal to unity indicates strict TE. The level populations of a gas described by a specific electron temperature T_e and electron density N_e are solved if the departure coefficients for all levels are known.

The condition of statistical balance can be used to set up balance equations of the processes affecting the populations of each energy level of the atoms. These balance equations are coupled and need to be solved simultaneously to give the departure coefficients.

Equating all the atomic processes filling and emptying level n, gives the statistical balance equation

$$\begin{aligned} & N_e N_i \left(\alpha_n^r + \alpha_n^s + N_e C_{i,n}\right) + \sum_{m>n} N_m \left(A_{mn} + N_e C_{mn} + B_{mn} J_\nu\right) + \sum_{k<n} N_k \left(N_e C_{kn} + B_{kn} J_\nu\right) \\ = \; & N_n \left[\alpha_n^p + N_e C_{n,i} + \sum_{k<n} \left(A_{nk} + N_e C_{nk} + B_{nk} J_\nu\right) + \sum_{m>n} \left(N_e C_{nm} + B_{nm} J_\nu\right) \right] . \end{aligned} \tag{2}$$

The left-hand side contains all processes that populate level n. The terms represent radiative recombination, stimulated recombination, three-body recombination, spontaneous emission, collisional de-excitation, stimulated emission, collisional excitation and absorption, respectively.

The right-hand side includes all processes that depopulate level n. The terms represent photoionization, collisional ionization, spontaneous emission, collisional de-excitation, stimulated emission, collisional excitation and absorption, respectively.

J_ν is the mean intensity of the incident radiation field. In this work the electron number density N_e and the ion number density N_i are decoupled from the bound level populations N_n, and are taken as constant throughout the plasma. Terms involving J_ν are not included in the previous models dsescribed in Brocklehurst [2], Smits [3] or Storey & Hummer [4].

The number density N_i of atoms in level i can be substituted in the rate equation (2), using equation (1), to yield a form of the rate equation that depends on the departure coefficients. This form of the rate equation can be written in matrix form as

$$\mathbf{a} = \mathbf{b} \cdot \mathbf{X}$$

where the row vector $\mathbf{a}$ has components

$$\mathrm{a}_n = \left(\frac{2\pi m_e k_B T}{h^2} \right)^{3/2} \left(\alpha_n^r + \alpha_n^s + N_e C_{i,n}\right) \tag{3}$$

and the row vector $\mathbf{b}$ has components b_n, $n = 1, 2, 3 \ldots$.

The diagonal entries of the matrix $\mathbf{X}$ represent all the processes depopulating level n and the non-diagonal matrix elements represent all the processes populating level n. All the processes involving downward transitions into n from higher levels are above the diagonal and the processes populating n from lower levels are below the diagonal.

The departure coefficients b_n can be obtained by inverting the matrix $\mathbf{X}$ and multiplying it with vector $\mathbf{a}$ from the left. The elements of $\mathbf{a}$ and $\mathbf{X}$ depend on the electron temperature T_e, the density N_e, the external radiation field J_ν, and the rates of the individual atomic processes.

3. Atomic calculations

3.1. Bound-bound radiative processes

The Einstein A-values were computed using the expression given by Brocklehurst [5]. The explicit formula for the bound-bound matrix element of an atomic transition [6] was used.

For very high energy levels ($n > 500$), the expression in [6] is not appropriate due to the large number of terms occurring in the hypergeometric series. Instead, the approximation given by Brocklehurst [2] was used with the bound-bound Gaunt factor as given by Baker & Menzel [7].

The rate coefficients for absorption and stimulated emission were calculated using the Einstein relations.

3.2. Bound-free radiative processes

A method to compute the bound-free radial matrix elements that is based on a set of recurrence relations, satisfied by the exact matrix elements for hydrogenic atoms or ion, has been described by Burgess [8]. These simple recurrence relations allow for fast computing to very high accuracy.

The expression given in [8] for the radiative recombination coefficients α_n^r, using a Maxwellian distribution with a temperature T_e for the free electron velocities, was used. A Gaussian integration method was used to evaluate the integral in the expression for the radiative recombination. This method does the integration over an arbitrary interval, so that smaller intervals can be used for energies close to the ionization threshold when the integrand varies rapidly. A number of five-point Gaussian integrations is done starting with an interval size of $h = 10^{-4}n^{-1}$. The interval size is doubled after every five-point integration and the procedure is terminated when the sum of the integrals are accurate up to six significant digits.

The photoionization cross-section to level n for an hydrogenic atom or ion was calculated using the formula of Burgess & Seaton [9]. From this, the cross-section for stimulated emission σ_n^s was calculated using the Einstein-Milne relations.

For a plasma in an ambient radiation field with mean intensity J_ν, the rate of photoionizations is given by

$$\alpha_n^p = \int_{\chi_n/h}^{\infty} a_n^p(\nu) \frac{4\pi J_\nu}{h\nu} \, d\nu \tag{4}$$

where $a_n^p(\nu)$ is the photoionization cross-section from level n for a photon with frequency ν, and χ_n is the ionization potential of level n.

The stimulated emission coefficient α_n^s is found by averaging the stimulated emission cross-section $\sigma_n^s(v)$ over the velocity distribution and accounting for the stimulating radiation field. The stimulated emission coefficient is given by

$$\alpha_n^s = \int_{\chi_n/h}^{\infty} \frac{4\pi J_\nu}{h\nu} \sigma_n^s(v)\, f(v) \frac{h}{m} \, d\nu \, . \tag{5}$$

The integration involved in the calculations of the photoionization and stimulated emission coefficients were handled using a Gaussian quadrature scheme as described above for radiative recombination.

3.3. Collisional processes

The semi-empirical formulae of Vriens & Smeets [10] were used to calculate the collisional rate coefficients for collisional bound-bound and bound-free transitions. Because the values are valid over a wider range of temperature, these were used in favour of the more commonly used formulae of Gee et al. [11]. Vriens & Smeets [10] claim that their values agree within 5 to 20 % with those of Gee et al. [11].

4. Numerical methods

4.1. Transition rates close to the ionization limit

In principle, an atom has an infinite number of energy levels and thus the solution of the population structure of hydrogen requires the solution of an infinite number of coupled equations represented by equation (2). Since the atoms discussed here are not in isolation, there are physical considerations, like the density, that limit the actual number of states in which an electron can be found. Therefore, an upper cut-off n_* was introduced for the highest n level for which the rate equation will be solved explicitly. The details of how n_* was determined can be found in [12].

4.2. Matrix condensation

Burgess & Summers [13] introduced a matrix condensation technique based on Lagrange interpolation which has been used by a number of authors. The technique condenses the sizable matrix $\mathbf{X}$ to a much smaller matrix, which can be readily inverted. Because the departure coefficients vary smoothly and slowly with n, the condensation technique can be applied. The method is presented in detail in [12].

5. Hydrogen Population Structure

The departure coefficients were calculated using codes developed based on the theory and techniques discussed in the preceding sections. Results were in good agreement with other capture-collision-cascade (C^3) models The results of this work for an n-method C^3 model agree on average within 0.5 % with the results of Brocklehurst [2] and 0.3 % with that of Smits [3].

The problem of whether or not to include Lyman transitions in the calculations when determining departure coefficients was investigated. The mean free path of Lyman photons from the different energy levels was investigated under various environmental conditions by calculating the extinction coefficient of the photons explicitly. It was concluded that the escape probability of Lyman photons are negligibly small for conditions found in astronomical plasmas that produce a recombination spectrum. Therefore, it is always appropriate to assume Case B of Baker & Menzel [7] when determining departure coefficients.

Departure coefficients for C^3 models permeated by a radiation field were also calculated. In general it is important to take the ionizing radiation into account, but this cannot be described by recombination theory alone and it is necessary to do radiative transfer calculations. The radiation changes as it propagates through the gas and the gas itself will absorb photons at specific frequencies as well as emit a diffuse radiation field. The b_n problem will then depend on many more parameters than for a C^3 model, in particular it will be geometry-dependent. In this work, the effects of a radiation field on the departure coefficients was investigated, but the amplification of lines by stimulated processes was not considered.

The mean intensity of the external radiation field is represented by a blackbody spectrum with temperature T_r, multiplied by a dilution factor W that depends on geometrical considerations of the system. For a single ionizing star with a radius of R, the dilution factor at a distance d (with $d \gg R$) from the star will be given by $W \approx 0.25\,(R/d)^2$. For an O star with $R = 18R_\odot$, the dilution factor will be $W \sim 10^{-16}$ at a distance of 10 pc and $W \sim 10^{-14}$ at 1 pc.

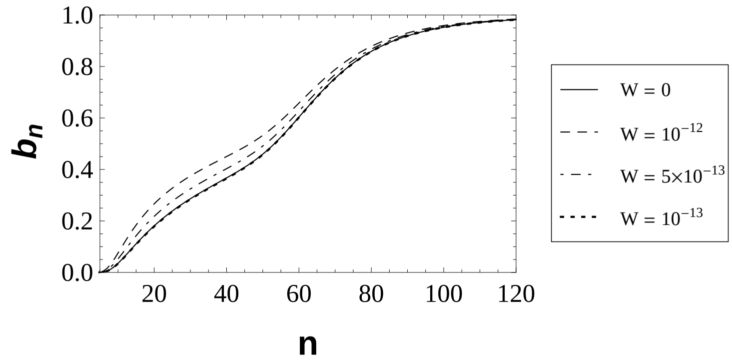

Figure 1. Effect on the population structure of hydrogen of a diluted blackbody radiation field with temperature $T_r = 40\,000\,\mathrm{K}$ with various dilution factors. Parameters for the nebula was taken as $T_e = 10^3\,\mathrm{K}$ with $N_e = 10^3\,\mathrm{cm}^{-3}$, assuming Case B. The solid line shows the population structure if no radiation field is present.

Figure 1 shows the effect that a diluted blackbody field has on the population structure of hydrogen for a plasma with $T_e = 10^3\,\mathrm{K}$ and $N_e = 10^3\,\mathrm{cm}^{-3}$. The radiation temperature was taken as $T_r = 40\,000\,\mathrm{K}$ to represent an O star. For a relatively dense radiation field ($W = 10^{-12}$, 5×10^{-13}), the departure coefficients are larger than they are if no radiation field were present. For less dense fields, the departure coefficients are lowered by the radiation field, as can be seen for the case $W = 10^{-13}$ in figure 1. As the density of the field decreases, the b_n values approach the $W = 0$ case asymptotically from below.

It was found that the effect that a diluted blackbody field has on the population structure of hydrogen for a plasma can be pronounced. For the example described in igure 1, the relative change on the b_n values can be as much as 45% for a relatively dense radiation field ($W = 10^{-12}$).

Even though the CMBR has a blackbody spectrum of only 3 K, it is very dense and hence affects the population structure of hydrogen atoms. The result of a 3 K blackbody radiation field on the population structure of hydrogen was examined for 16 environments with parameters $10\,\mathrm{cm}^{-3} < N_e < 10^4\,\mathrm{cm}^{-3}$ and $300\,\mathrm{K} < T_e < 20\,000\,\mathrm{K}$. The effects are most noticeable in cool clouds with low electron densities. The 3 K blackbody radiation field affects the population structures most typically for $50 < n < 150$, increasing the value of the departure coefficients slightly for these levels. In general the b_n values were altered on average by 0.2 % and at most by an average of 0.6 %.

The influence of free-free continuum on the departure coefficients was also investigated and was found to be minimal. This is consistent with the work of [14], who found that the effects of free-free radiation on the b_n values are negligible.

6. Conclusion

A comprehensive model for calculating the n-method populations of a pure hydrogen plasma has been presented. It has been assumed that the nebula is homogeneous, unbounded and permeated by a constant radiation field. Departure coefficients for bound energy levels were computed by accounting for all radiative and collisional processes, bound-bound and bound-free, via all possible transition routes. The model is comparable with the most definitive models available at present [15].

The solution for the departure coefficients presented here considers only distinct energy levels of the atoms, known as an n-model. A more complete description resolves the momentum states and a departure coefficient calculated for every angular momentum state, called an nl-model. In this model it has been assumed that the angular momentum states are populated according to their statistical weights. This n-model will serve as the basis for future studies using nl-models.

The code is valid for a larger range of temperatures than any of the current models. Because the parameters for astronomical plasmas vary greatly, this broadens the code's potential for modelling a variety of astronomical environments. Nova shells with electron temperatures $T_e < 1\,000\,\mathrm{K}$ have been detected [16], while supernova remnants have temperatures of about $10^6\,\mathrm{K}$.

The results from the model developed in this work were compared to previous calculations and found to be in good agreement. Discrepancies are small and can be explained by the different methods used to calculate atomic transition probabilities and to handle numerical and computational challenges. One of the objectives of this project was to check for systematic errors in previous calculation by independently developing code. No such errors were found.

A preliminary investigation of the effects of an external radiation field on the departure coefficients was done. In principle the external radiation field should be included in the calculations of b_n values, but the incorporation of a radiation field into such a model is not trivial and it necessitates that the geometry of the system be taken into account. It was found that the ionizing radiation from a nearby star can have a significant effect on the departure coefficients of high n levels, as can the CMBR. The influence of free-free emission on the b_n values was found to be insignificant.

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