LASER ACTION IN C IV PLASMAS

A) INTRODUCTION

The theoretical study of decaying plasma has been crucial in the development of short wavelength and X-Ray lasers (Matthews *et al.*, 1988). The purpose of this work is to study the adiabatic expansion of C IV plasmas and to identify the conditions under which population inversions occur. The results provide an explanation of the intensity anomalies of C IV lines in Wolf-Rayet stars and Quasars.

This paper is divided into 9 sections, B) Description of the plasma model. C) Various constraints the plasma parameters must obey. D) Important physical processes occurring in the plasma. E) Detailed description of the theoretical model used in our plasma simulation. F) How gain is computed. G) Results and astronomical evidence. H) Conclusion. Appendix A: Atomic data used in computing rate coefficients. Appendix B: Ionization equilibrium computation. Appendix C: Computer Program analysis

B) THE PLASMA MODEL

A plasma consists of one or more elements in various stages of ionization. Its main constituents are positively charged ions, free electrons, neutral atoms, and electromagnetic radiation from discrete and continuous spectra.

In this work, we consider a monatomic (element A), stationary, and spatially homogeneous plasma, free of magnetic fields. Label A refers to all ionization stages of element A: neutral (A I), singly ionized (A II), doubly ionized (A III), ... Element A is characterized by a density n_A cm^{-3} and a temperature T_A Kelvin, and the free electrons by a density n_e and a temperature T_e. Furthermore, each stage of ionization X of element A is characterized by a density $n_A^{(x)}$; then $n_A = \sum_x n_A^{(x)}$

All particles of the plasma are assumed to be at the same temperature $T = T_e = T_A$. Under the plasma conditions considered in this work, this is a reasonable approximation, especially since T_A is used only to calculate the ionization equilibrium of element A (See appendix B)

C) APPLICABILITY OF THE PLASMA MODEL

ENERGY DISTRIBUTION OF THE FREE ELECTRONS

The mass of the electron is much smaller than that of any ion. The free electrons are thus much more mobile than the ions. Their energy distribution in a plasma is described by Maxwell-Boltzmann statistics. This distribution function holds if the mean de Broglie wavelength of the plasma electrons is appreciably smaller than the mean distance between them (Vedenov, 1965). This puts an approximate upper limit on n_e of

$$n_e \ll 1.2 \times 10^{15}\, T^{3/2} \mathrm{cm}^{-3}, \tag{1}$$

In all cases studied in this work, we are well below this upper limit of validity.

An approximate lower limit of validity can be derived as follows. An electronic Maxwellian distribution will hold if a sufficient number of elastic collisions occur between the free electrons to allow enough energy exchanges between them to establish a

Maxwellian energy distribution. This will be the case if the plasma is sufficiently dense. A crude estimate of the lower limiting value of n_e for a lithium-like ion C IV is:

$$n_e > 10^{10}\text{cm}^{-3}, \tag{2}$$

Since we consider plasmas with $n_e = 10^{12}$ to 10^{15}cm^{-3}, we expect the Maxwellian distribution to be a reasonable approximation to the actual distribution function of the free electrons in the plasma. A sufficiently dense plasma also insures that the response time of the distribution to a change in the plasma parameters is sufficiently rapid that the distribution remains Maxwellian at all times.

EQUILIBRIUM POPULATION OF THE LEVELS

Plasmas in complete thermodynamic equilibrium (CTE) can only exist under very special conditions and are thus very rarely observed. However, there exists a large class of plasma in which each volume element fulfils all thermodynamic equilibrium laws derived for plasmas in CTE except for Planck's radiation law. Such plasmas are said to be in local thermodynamic equilibrium (LTE).

In these plasmas, the level population densities are determined solely by collisional processes which are assumed to occur rapidly enough such that the population densities respond instantaneously to any change in the plasma conditions. The population densities thus depend entirely on the local values of the plasma parameters. Furthermore, each physical process is accompanied by its's inverse and, by the principle of detailed balance, these pairs of processes occur at equal rates. The advantage of this model is that the atomic cross-sections of the various physical processes are not needed to calculate the population densities. These are determined solely by the laws of statistical mechanics.

NON-EQUILIBRIUM POPULATION OF THE LEVELS:

Plasmas that don't obey the LTE model are called non-LTE plasmas. The population densities of the energy levels of ions in non-LTE plasmas must be obtained from the rate coefficients of the individual collisional and radiative processes occurring within the plasma. Several models which take into account some or most of these processes have been proposed; of these, the most useful and general is the Collisional-Radiative (CR) model. This model was first proposed and applied to hydrogenic ions by Bates et al. (1962a,b). Since then, much work has been done using the CR model, especially in modelling short wavelength lasers.

D) PHYSICAL PROCESSES OCCURRING IN A PLASMA

Let e denote an electron, hν a photon, and N_i^x an X-times ionized atom (ion X) in state i, n^+ is the ion density (N^{x+1}) and n_e is the electron density. Then the physical processes occurring within the plasma and included in the CR model can be described as follows (rate coefficients are a function of T)

i) *Collisional ionization* by electron impact:

$$N_i^x + e \rightarrow N^{x+1} + e + e, \tag{3}$$

The rate coefficient of this process is denoted by $S_i(T)$. The number of such processes occurring per unit volume per unit time is given by $n_i n_e S_i(T)\text{cm}^{-3}s^{-1}$

ii) *Three-body recombination*: inverse of process (i):

$$N^{x+1} + e + e \rightarrow N_i^x + e, \tag{4}$$

The rate coefficient: $\alpha_i(T)$, and the number of processes $n_e^2 n^+ \alpha_i(T)$.

iii) *Radiative recombination*: It predominates over process (ii) in low-density plasmas.

$$N^{x+1} + e \rightarrow N_i^x + \mathrm{h}\nu, \tag{5}$$

The rate coefficient $\beta_i(T)$, and the number of processes: $n_e n^+ \beta_i(T)$.

iv) *Collisional excitation* by electron impact:

$$N_i^x + e \rightarrow N_j^x + e, \tag{6}$$

Rate coefficient $C_{ij}(T)$, number of processes: $n_i n_e C_{ij}(T)$.

v) *Radiative transition*

$$N_j^x \rightarrow N_i^x + \mathrm{h}\nu, \tag{7}$$

Einstein probability coefficient: A_{ij}; and number of processes: $n_j A_{ji}$.

These are the main physical processes which occur in a plasma under most conditions. (see appendix A for computation of rate coefficients) The plasma is also assumed to be optically thin such that all radiation emitted within the plasma escapes without being absorbed. (Thus neglecting photoexcitation and photoionization)

By including all the above collisional and radiative processes into a rate equation for each quantum level of a specific stage of ionization of our atom we obtain the following differential equation for the time development of the population density n_i of a level i.

$$\begin{aligned} \dot{n}_i \equiv \frac{dn_i}{dt} &= -n_e n_i S_i - n_e n_i \sum_{j \neq i}^{\infty} C_{ij} - n_i \sum_{j=1}^{i-1} A_{ij} \\ &+ n_e \sum_{j \neq i}^{\infty} n_j C_{ji} + \sum_{j=i+1}^{\infty} n_j A_{ji} + \{\beta_i + \alpha_i n_e\} n_e n^+ \quad , \end{aligned} \tag{8}$$

There is such an equation for each and every discrete level $i = 1, 2, 3, \cdots, \infty$. Thus, we obtain an infinite number of coupled differential equations describing the population densities of all the discrete levels.

E) THE THEORETICAL MODEL

We consider what happens when the plasma in the outer layers of a star rapidly expands. To focus our discussion we consider Wolf-Rayet stars. The atmospheres of these stars depart seriously from LTE. We consider the state of plasma at the base of the extended atmosphere of a Wolf-Rayet star, roughly where its 'photosphere' would lie. We make the reasonable assumption that the conditions there will also correspond to non-LTE. Hence to obtain the relative concentrations of differing ionization stages of an element at a particular electron density (n_e) and electron temperature (T_e) we use the non-LTE method of House (1964) (see Appendix B). It is well known that Wolf–Rayet stars are undergoing a high–speed mass loss. We assume that this plasma expands adiabatically, for which the plasma density N and T_e are related by $T_e N^{1-\gamma}$=const. We assume $\gamma = 5/3$; for the actual plasma the value will be slightly smaller. The flow is supersonic and to a first approximation, the plasma is assumed to be 'frozen' during the rapid fall of temperature, for which a factor of 5 is assumed. (The same factor for the fall in the temperature has been used by Gudzenko *et al.*, 1966, and Varshni and Lam, 1976.)

To examine deviations from LTE it is useful to define the normalized population density of level i as

$$\rho_i = \frac{n_i}{n_i^E} \quad , \tag{9}$$

$$n_i^E \equiv Z_i n_e n^+ \quad , \tag{10}$$

$$Z_i = \{\omega_i/2\omega^+\}(h^2/2\pi m_e k T_e)^{3/2} \exp(\chi_i/kT_e) \quad , \tag{11}$$

where n_i^E is the Saha equilibrium population density of level i, ω_i is the statistical weight of level i, ω^+ is the partition function of the ion and χ_i is the ionization potential of the level i.

Dividing eq.(8) by n_i^E and using eq.(9), the set of equations (8) becomes

$$\dot{\rho}_i \equiv \frac{\dot{n}_i}{n_i^E} = -\left(n_e S_i + n_e \sum_{j\neq i}^{\infty} C_{ij} + \sum_{j=1}^{i-1} A_{ij} \right) \rho_i + n_e \sum_{j\neq i}^{\infty} C_{ij}\rho_j + \sum_{j=i+1}^{\infty} \frac{Z_j}{Z_i} A_{ji}\rho_j + \frac{1}{Z_i}\{\alpha_i n_e + \beta_i\}, \tag{12}$$

with i = 1,2,3,$\cdots,\infty$. (We used the fact that $Z_i C_{ij} = Z_j C_{ji}$ from the principle of detailed balance)

To solve this set of equations, the following assumptions are used:

(i) For all levels i located above a sufficiently high lying level, r, the population density is assumed to be given by the Saha-Boltzmann equilibrium equation instead of by Eq. (8). Thus, in this case, we have $\rho_{i>r} = 1$. The infinite set of equations (12) thus become a finite set of r coupled equations which can be solved for ρ_i, $i = 1, 2, \cdots, r$.

(ii) The infinite sums appearing in Eq. (12) can be cut off at a sufficiently high–lying level $s > r$ above which the rate coefficients involving these states contribute little.

(iii) The time derivative, Eq. (12), can be put equal to zero for all the levels $i \leq r$ except for the lowest levels without causing significant error.

TABLE 1. Population coefficients for various Collisional-Radiative models.

0	$n_i = Z_i r_i^{(0)} n^+ n_e$ $\rho_i = r_i^{(0)}$			$\dot{\rho}_i = 0$
Steady State	$r_{i>r}^{(0)} = 1$ $r_{i>s}^{(0)} = 0$	— —	— —	
1	$n_i = Z_i[r_i^{(0)} n^+ n_e + r_i^{(1)} n_1 / Z_1]$ $\rho_i = r_i^{(0)} + r_i^{(1)} \rho_1$			$\dot{\rho}_{i>1} = 0$
H I	$r_1^{(0)} = 0$ $r_{i>r}^{(0)} = 1$ $r_{i>s}^{(0)} = 0$	$r_1^{(1)} = 1$ $r_{i>r}^{(1)} = 0$ $r_{i>s}^{(1)} = 0$	— — —	$\dot{\rho}_1 \neq 0$
2	$n_i = Z_i[r_i^{(0)} n^+ n_e + r_i^{(1)} n_1 / Z_1 + r_i^{(2)} n_2 / Z_2]$ $\rho_i = r_i^{(0)} + r_i^{(1)} \rho_1 + r_i^{(2)} \rho_2$			$\dot{\rho}_{i>2} = 0$
C IV	$r_1^{(0)} = 0$ $r_2^{(0)} = 0$ $r_{i>r}^{(0)} = 1$ $r_{i>s}^{(0)} = 0$	$r_1^{(1)} = 1$ $r_2^{(1)} = 0$ $r_{i>r}^{(1)} = 0$ $r_{i>s}^{(1)} = 0$	$r_1^{(2)} = 0$ $r_2^{(2)} = 1$ $r_{i>r}^{(2)} = 0$ $r_{i>s}^{(2)} = 0$	$\dot{\rho}_1 \neq 0$ $\dot{\rho}_2 \neq 0$

$r_i^{(0)}$ is the relative contribution to level i from the ion level (n^+),
$r_i^{(1)}$ is the contribution to level i from level 1, and
$r_i^{(2)}$ is the contribution to level i from level 2.

0) In the steady state model all the time derivatives are zero and the population density n_i depends only on the ion level density n^+.

1) In the quasi-steady state model some time derivatives are non-zero. For Hydrogen-like ions, the time derivative of the lowest level is non-zero; the excited level density n_i depends on the ground level density n_1, and the ion level density n^+.

2) For Lithium-like ions, such as C IV ions, the unusually small energy gap between the first and second quantum states leads to a relatively large population in the second level. Thus the time derivative of state 1 and 2 is non-zero and all excited states depend on the first and second quantum levels as well as the ion level.

For hydrogen-like ions if we substitute from the above table back into Eq.(12) we obtain the following set of coupled linear equations for $i = 2, 3, \ldots r$,

$$
\begin{aligned}
-\left(n_e S_i + n_e \sum_{j\neq i}^{s} C_{ij} + \sum_{j=1}^{i-1} A_{ij}\right)(r_i^{(0)} + r_i^{(1)}\rho_1) \\
+ n_e C_{i1}\rho_1 + n_e \sum_{\substack{j\neq i\\ j=2}}^{r} C_{ij}(r_j^{(0)} + r_j^{(1)}\rho_1) + \sum_{j=i+1}^{r} \frac{Z_j}{Z_i} A_{ji}(r_j^{(0)} + r_j^{(1)}\rho_1) \\
+ \sum_{j>r}^{s} \{n_e C_{ij} + \frac{Z_j}{Z_i} A_{ji}\} + \frac{1}{Z_i}\{\beta_i + \alpha_i n_e\} = 0, \qquad (13)
\end{aligned}
$$

We can group the ρ_1 terms and obtain,

$$
\begin{aligned}
\Bigg[-\left(n_e S_i + n_e \sum_{j\neq i}^{s} C_{ij} + \sum_{j=1}^{i-1} A_{ij}\right) r_i^{(0)} + n_e \sum_{\substack{j\neq i\\ j=2}}^{r} C_{ij} r_j^{(0)} + \sum_{j=i+1}^{r} \frac{Z_j}{Z_i} A_{ji} r_j^{(0)} \\
+ \sum_{j>r}^{s} \{n_e C_{ij} + \frac{Z_j}{Z_i} A_{ji}\} + \frac{1}{Z_i}\{\beta_i + \alpha_i n_e\}\Bigg] + \qquad (14) \\
\Bigg[-\left(n_e S_i + n_e \sum_{j\neq i}^{s} C_{ij} + \sum_{j=1}^{i-1} A_{ij}\right) r_i^{(1)} + n_e \sum_{\substack{j\neq i\\ j=2}}^{r} C_{ij} r_j^{(1)} + \sum_{j=i+1}^{r} \frac{Z_j}{Z_i} A_{ji} r_j^{(1)} + n_e C_{i1}\Bigg]\rho_1 = 0;
\end{aligned}
$$

This set of equations is of the form $a_i + b_i\rho_1 = 0$ for $i = 2, 3, \ldots r$. The general solution for an arbitrary value of ρ_1 is $a_i = 0$, $b_i = 0$ thus,

$$
\begin{aligned}
-\left(n_e S_i + n_e \sum_{j\neq i}^{s} C_{ij} + \sum_{j=1}^{i-1} A_{ij}\right) r_i^{(0)} + n_e \sum_{\substack{j\neq i\\ j=2}}^{r} C_{ij} r_j^{(0)} + \sum_{j=i+1}^{r} \frac{Z_j}{Z_i} A_{ji} r_j^{(0)} = \\
- \sum_{j>r}^{s} \{n_e C_{ij} + \frac{Z_j}{Z_i} A_{ji}\} - \frac{1}{Z_i}\{\beta_i + \alpha_i n_e\} \qquad (15) \\
-\left(n_e S_i + n_e \sum_{j\neq i}^{s} C_{ij} + \sum_{j=1}^{i-1} A_{ij}\right) r_i^{(1)} + n_e \sum_{\substack{j\neq i\\ j=2}}^{r} C_{ij} r_j^{(1)} + \sum_{j=i+1}^{r} \frac{Z_j}{Z_i} A_{ji} r_j^{(1)} = -n_e C_{i1} \quad (16)
\end{aligned}
$$

this is equivalent to 2 matrix equations for Hydrogen-like ions ($\rho_i = r_i^{(0)} + r_i^{(1)}\rho_1$)

$$\sum_{j=2}^{r} B_{ij} r_j^{(k)} = R_i^{(k)} \quad , \qquad i = 2, 3, \ldots, r \qquad \text{and} \qquad k = 0 \text{ or } 1 \tag{17}$$

$$R_i^{(0)} = -\sum_{j>r}^{s} \{n_e C_{ij} + \frac{Z_j}{Z_i} A_{ji}\} - \frac{1}{Z_i}\{\beta_i + \alpha_i n_e\} \quad , \tag{18}$$

$$R_i^{(1)} = -n_e C_{i1} \quad , \tag{19}$$

$$B_{ij} = \begin{cases} n_e C_{ij} + \frac{Z_j}{Z_i} A_{ji} \quad , & \text{if } i < j \qquad \text{(upper);} \\ -n_e S_i - n_e \sum\limits_{j \neq i}^{s} C_{ij} - \sum\limits_{j=1}^{i-1} A_{ij} \quad , & \text{if } i = j \qquad \text{(diagonal);} \\ n_e C_{ij} \quad , & \text{if } i > j \qquad \text{(lower);} \end{cases} \tag{20}$$

Similarly for C IV ions, ($\rho_i = r_i^{(0)} + r_i^{(1)}\rho_1 + r_i^{(2)}\rho_2$) we obtain 3 matrix equations:

$$\sum_{j=3}^{r} B_{ij} r_j^{(k)} = R_i^{(k)} \quad , \qquad i = 3, 4, \ldots, r \qquad \text{and} \qquad k = 0, 1, 2 \tag{21}$$

$$R_i^{(2)} = -n_e C_{i2} \quad , \tag{22}$$

To compute the steady state population density we must solve only one matrix equation:

$$\sum_{j=1}^{r} B_{ij} r_j^{(0)} = R_i^{(0)} \quad , \qquad i = 1, 2, 3, \ldots, r, \qquad\qquad (\rho_i = r_i^{(0)}) \tag{23}$$

The iterative method of solving linear equations, Pan and Reif (1985) is ideally suited for scanning the n_e,T_e parameter space, since we can use as initial matrix inverse the previous solution at $n_e + \delta n_e$,T_e. The rate coefficients only need be re-computed when T_e changes. Except for some sharp transitions near higher n_e, small changes in these parameters will in general produce smoothly varying solutions, thus the matrix inverse at a nearby point is a very good initial guess and the iteration converges quadratically:

We start with some matrix $\mathbf{A}_0$ that is assumed to be an *approximate* inverse of the matrix $\mathbf{B}$, so that $\mathbf{A}_0 \cdot \mathbf{B}$ is approximately the identity matrix $\mathbf{1}$. Then the recurrence,

$$\mathbf{A}_{2n+1} = 2\mathbf{A}_n - \mathbf{A}_n \cdot \mathbf{B} \cdot \mathbf{A}_n \quad , \qquad n = 0, 1, 3, 7, \ldots \tag{24}$$

will converge *quadratically* to the unknown inverse matrix $\mathbf{B}^{-1}$. This equation is known as *Hotelling's Method*. For the very first initial inverse a suitable approximation can be obtained from

$$\mathbf{A}_0 = \epsilon \mathbf{B}^{\mathrm{T}}, \tag{25}$$

ϵ is a small constant which can be set to the reciprocal of the maximum row sum times the maximum column sum of $\mathbf{B}$.

For Hydrogen-like ions, after solving the 2 matrix equations we are left with a differential equation for n_1. Since the excited state densities linearly depend on n_1, population inversion will be time dependent and a search must be made for a critical time when the laser transition has maximum gain. We can solve the differential equation for n_1 by substituting the $(r_i^{(0)}, r_i^{(1)})$ solutions of Eq.(17) back into Eq.(8) and obtain:

$$\begin{aligned}\dot{n}_1 = \quad & -n_e n_1 S_1 \quad - \quad n_e n_1 \sum_{j=2}^{s} C_{1j} \\ + \quad & \sum_{j=2}^{r} \{n_e C_{j1} + A_{j1}\} Z_j [r_j^{(0)} n^+ n_e + r_j^{(1)} n_1 / Z_1] \\ + \quad & \sum_{j>r}^{s} \{n_e C_{j1} + A_{j1}\} Z_j n^+ n_e \quad + \quad \{\beta_1 + \alpha_1 n_e\} n_e n^+ \quad ,\end{aligned} \tag{26}$$

$$\dot{n}_1 = \alpha_{\rm CR} n^+ n_e - S_{\rm CR} n_1 n_e \quad , \tag{27}$$

$$S_{\rm CR} = S_1 + \sum_{j=2}^{s} C_{1j} - \frac{1}{Z_1 n_e} \sum_{j=2}^{r} \{n_e C_{j1} + A_{j1}\} Z_j r_j^{(1)} \quad , \tag{28}$$

$$\alpha_{\rm CR} = \beta_1 + \alpha_1 n_e + \sum_{j=2}^{r} \{n_e C_{j1} + A_{j1}\} Z_j r_j^{(0)} + \sum_{j>r}^{s} \{n_e C_{j1} + A_{j1}\} Z_j \quad , \tag{29}$$

Solving the differential equation:

$$n_1(t) = \frac{\alpha_{\rm CR}}{S_{\rm CR}} n^+ + \left[n_1(t{=}0) - \frac{\alpha_{\rm CR}}{S_{\rm CR}} n^+ \right] e^{-S_{\rm CR} n_e t} \quad , \tag{30}$$

$$n_1(t \to \infty) = \frac{\alpha_{\rm CR}}{S_{\rm CR}} n^+ \quad , \tag{31}$$

Thus the final solution for H I excited state densities $(i > 1)$ is,

$$n_i = Z_i [r_i^{(0)} n^+ n_e + r_i^{(1)} n_1(t)/Z_1], \tag{32}$$

$n_1(t)$ is taken from Eq.(30), $n_1(t{=}0)$ and n^+ are obtained from the ionization equilibrium calculations of Appendix B, computed for the n_e, T_e values before the expansion. Then after the expansion we assume that these densities are 'frozen', so we divide them by the expansion factor. Eventually n_1 and n^+ relax to the cooler ionization equilibrium with an exponential time factor $S_{\rm CR} n_e$, we note that $n_1(t \to \infty)$ is merely a re-arrangement of Eq.(B-1) for the lower temperature and density.

For Lithium-like ions, after solving the 3 matrix equations we are left with a differential equations for n_1 and for n_2. These must be solved since as mentioned before, gain is time dependent. We can solve for n_1 and n_2 by substituting the solutions of Eq.(21) $(r_i^{(0)}, r_i^{(1)}, r_i^{(2)})$ back into Eq.(8) and using the constraints of table (1) we find:

$$\begin{aligned}\dot{n}_1 = \quad & -n_e n_1 S_1 \quad - \quad n_e n_1 \sum_{j=2}^{s} C_{1j} \quad + \quad n_e n_2 C_{21} \quad + \quad n_2 A_{21} \\ & + \quad \sum_{j=3}^{r} \{n_e C_{j1} + A_{j1}\} Z_j [r_j^{(0)} n^+ n_e + r_j^{(1)} n_1/Z_1 + r_j^{(2)} n_2/Z_2] \\ & + \quad \sum_{j>r}^{s} \{n_e C_{j1} + A_{j1}\} Z_j n^+ n_e \quad + \quad \{\beta_1 + \alpha_1 n_e\} n_e n^+ \quad ,\end{aligned} \tag{33}$$

$$\begin{aligned}\dot{n}_2 = \quad & -n_e n_2 S_2 \quad - \quad n_e n_2 \sum_{j\neq 2}^{s} C_{2j} \quad - \quad n_2 A_{21} \quad + \quad n_e n_1 C_{12} \\ & + \quad \sum_{j=3}^{r} \{n_e C_{j2} + A_{j2}\} Z_j [r_j^{(0)} n^+ n_e + r_j^{(1)} n_1/Z_1 + r_j^{(2)} n_2/Z_2] \\ & + \quad \sum_{j>r}^{s} \{n_e C_{j2} + A_{j2}\} Z_j n^+ n_e \quad + \quad \{\beta_2 + \alpha_2 n_e\} n_e n^+ \quad ,\end{aligned} \tag{34}$$

$$\dot{n}_1 = \alpha_1^{\mathrm{CR}} n^+ n_e + M_{21}^{\mathrm{CR}} n_2 n_e - S_1^{\mathrm{CR}} n_1 n_e \quad , \tag{35}$$

$$\dot{n}_2 = \alpha_2^{\mathrm{CR}} n^+ n_e + M_{12}^{\mathrm{CR}} n_1 n_e - S_2^{\mathrm{CR}} n_2 n_e \quad , \tag{36}$$

$$S_1^{\mathrm{CR}} = S_1 + \sum_{j=2}^{s} C_{1j} - \frac{1}{Z_1 n_e} \sum_{j=3}^{r} \{n_e C_{j1} + A_{j1}\} Z_j r_j^{(1)} \quad , \tag{37}$$

$$S_2^{\mathrm{CR}} = S_2 + \sum_{j\neq 2}^{s} C_{2j} + \frac{1}{n_e} A_{21} - \frac{1}{Z_2 n_e} \sum_{j=3}^{r} \{n_e C_{j2} + A_{j2}\} Z_j r_j^{(2)} \quad , \tag{38}$$

$$M_{21}^{\mathrm{CR}} = C_{21} + \frac{1}{n_e} A_{21} + \frac{1}{Z_2 n_e} \sum_{j=3}^{r} \{n_e C_{j1} + A_{j1}\} Z_j r_j^{(2)} \quad , \tag{39}$$

$$M_{12}^{\mathrm{CR}} = C_{12} + \frac{1}{Z_1 n_e} \sum_{j=3}^{r} \{n_e C_{j2} + A_{j2}\} Z_j r_j^{(1)} \quad , \tag{40}$$

$$\alpha_1^{\mathrm{CR}} = \beta_1 + \alpha_1 n_e + \sum_{j=3}^{r} \{n_e C_{j1} + A_{j1}\} Z_j r_j^{(0)} + \sum_{j>r}^{s} \{n_e C_{j1} + A_{j1}\} Z_j \quad , \tag{41}$$

$$\alpha_2^{\mathrm{CR}} = \beta_2 + \alpha_2 n_e + \sum_{j=3}^{r} \{n_e C_{j2} + A_{j2}\} Z_j r_j^{(0)} + \sum_{j>r}^{s} \{n_e C_{j2} + A_{j2}\} Z_j \tag{42}$$

The general solution of the coupled system of equations (35),(36) can be written as

$$n_j(t) = n_j^{\rm SS} + n_j^{(+)} e^{-\lambda^{(+)} t} - n_j^{(-)} e^{-\lambda^{(-)} t}, \qquad j = 1,2 \tag{43}$$

$$\lambda^{(\pm)} = \frac{n_e}{2}\left[S_1^{\rm CR} + S_2^{\rm CR} \pm \sqrt{(S_1^{\rm CR} - S_2^{\rm CR})^2 + 4M_{12}^{\rm CR} M_{21}^{\rm CR}}\right] \quad , \tag{44}$$

$$n_j^{\rm SS} = \frac{K_j^{\rm SS}}{\lambda^{(+)}\lambda^{(-)}} \quad , \tag{45}$$

$$n_j^{(\pm)} = \frac{n_j(t{=}0)\lambda^{(\pm)2} - K_j \lambda^{(\pm)} + K_j^{\rm SS}}{\lambda^{(\pm)}(\lambda^{(+)} - \lambda^{(-)})} \quad , \tag{46}$$

$$K_1^{\rm SS} = n_e^2 n^+ [\alpha_1^{\rm CR} S_2^{\rm CR} + \alpha_2^{\rm CR} M_{21}^{\rm CR}] \quad , \tag{47}$$

$$K_2^{\rm SS} = n_e^2 n^+ [\alpha_2^{\rm CR} S_1^{\rm CR} + \alpha_1^{\rm CR} M_{12}^{\rm CR}] \quad , \tag{48}$$

$$K_1 = n_e[\alpha_1^{\rm CR} n^+ + S_2^{\rm CR} n_1(t{=}0) + M_{21}^{\rm CR} n_2(t{=}0)] \quad , \tag{49}$$

$$K_2 = n_e[\alpha_2^{\rm CR} n^+ + S_1^{\rm CR} n_2(t{=}0) + M_{12}^{\rm CR} n_1(t{=}0)] \quad , \tag{50}$$

The steady state population densities as $t \to \infty$

$$n_1(t \to \infty) \equiv n_1^{\rm SS} = \frac{\alpha_1^{\rm CR} S_2^{\rm CR} + \alpha_2^{\rm CR} M_{21}^{\rm CR}}{S_1^{\rm CR} S_2^{\rm CR} - M_{12}^{\rm CR} M_{21}^{\rm CR}} n^+ \quad , \tag{51}$$

$$n_2(t \to \infty) \equiv n_2^{\rm SS} = \frac{\alpha_2^{\rm CR} S_1^{\rm CR} + \alpha_1^{\rm CR} M_{12}^{\rm CR}}{S_1^{\rm CR} S_2^{\rm CR} - M_{12}^{\rm CR} M_{21}^{\rm CR}} n^+ \quad , \tag{52}$$

The final solution for excited states ($i > 2$) of C IV :

$$n_i = Z_i[r_i^{(0)} n^+ n_e + r_i^{(1)} n_1(t)/Z_1 + r_i^{(2)} n_2(t)/Z_2], \tag{53}$$

Where $n_1(t)$ and $n_2(t)$ are taken from Eq.(43), to find $n_1(t{=}0)$ and $n_2(t{=}0)$ we first need to find the n^+ density by using the ionization equilibrium calculations of Appendix B on the plasma before it expands. Then by solving the steady state model Eq.(23) we can compute n_1 and n_2 for this initial state, then after the expansion we assume that these densities are 'frozen', so we divide them by the expansion factor.

Once we have obtained this solution for C IV we may want to compare it to the solution we would have obtained if we had used the Hydrogen-like model instead. Rather than solving two more matrix equations we can use a shortcut by setting Eq.(36) to zero ($\dot{n}_2 = 0$) we find,

$$n_2 = \frac{\alpha_2^{\mathrm{CR}}}{S_2^{\mathrm{CR}}} n^+ + \frac{M_{12}^{\mathrm{CR}}}{S_2^{\mathrm{CR}}} n_1 \quad , \tag{54}$$

$$\rho_2 = r_2^{*(0)} + r_2^{*(1)} \rho_1 \quad , \tag{55}$$

$$r_2^{*(0)} = \frac{\alpha_2^{\mathrm{CR}}}{S_2^{\mathrm{CR}}} \frac{1}{n_e Z_2}, \qquad r_2^{*(1)} = \frac{M_{12}^{\mathrm{CR}}}{S_2^{\mathrm{CR}}} \frac{Z_1}{Z_2} \quad , \tag{56}$$

$$\rho_i = r_i^{(0)} + r_i^{(1)} \rho_1 + r_i^{(2)} [r_2^{*(0)} + r_2^{*(1)} \rho_1] \quad , \tag{57}$$

$$\rho_i = r_i^{*(0)} + r_i^{*(1)} \rho_1 \quad , \tag{58}$$

$$r_i^{*(0)} = r_i^{(0)} + r_i^{(2)} r_2^{*(0)} \quad , \tag{59}$$

$$r_i^{*(1)} = r_i^{(1)} + r_i^{(2)} r_2^{*(1)} \quad , \tag{60}$$

inserting Eq.(54) into Eq.(35) we find we can express $\dot{n}_1$ as a function of α^{CR} and S^{CR}:

$$\dot{n}_1 = \alpha_1^{\mathrm{CR}} n^+ n_e + \frac{M_{21}^{\mathrm{CR}} \alpha_2^{\mathrm{CR}}}{S_2^{\mathrm{CR}}} n^+ n_e + \frac{M_{21}^{\mathrm{CR}} M_{12}^{\mathrm{CR}}}{S_2^{\mathrm{CR}}} n_1 n_e - S_1^{\mathrm{CR}} n_1 n_e \quad , \tag{61}$$

$$\dot{n}_1 = \alpha^{\mathrm{CR}} n^+ n_e - S^{\mathrm{CR}} n_1 n_e \quad , \tag{62}$$

$$\alpha^{\mathrm{CR}} = \alpha_1^{\mathrm{CR}} + \frac{M_{21}^{\mathrm{CR}} \alpha_2^{\mathrm{CR}}}{S_2^{\mathrm{CR}}} \quad , \tag{63}$$

$$S^{\mathrm{CR}} = S_1^{\mathrm{CR}} - \frac{M_{21}^{\mathrm{CR}} M_{12}^{\mathrm{CR}}}{S_2^{\mathrm{CR}}} \quad , \tag{64}$$

More simply put, the C IV model in which the excited states depended on n_1 and n_2 reduces to a Hydrogen-like model in which excited states now only depend on n_1. This can be expressed as: (for $i > 1$)

$$n_i = Z_i \left(\left[r_i^{(0)} + \frac{r_i^{(2)} \alpha_2^{\mathrm{CR}}}{S_2^{\mathrm{CR}} n_e Z_2} \right] n^+ n_e + \left[r_i^{(1)} + r_i^{(2)} \frac{M_{12}^{\mathrm{CR}} Z_1}{S_2^{\mathrm{CR}} Z_2} \right] n_1(t)/Z_1 \right), \tag{65}$$

we can substitute Eq.(63) and (64) into Eq.(30) to find $n_1(t)$, and to find $n_1(t{=}0)$ and n^+ we use the same method used for the Hydrogen-like model.

F) PLASMA LASER GAIN

The initial density of carbon atoms before expansion is taken to be 1×10^{14} cm^{-3} . Calculations will be carried out for the population densities of 32 levels of C IV for a grid of n_e and T_e values. The population inversion is often measured in terms of P, where P is given by

$$P = n_k/\omega_k - n_i/\omega_i, \tag{66}$$

where n_i and n_k are the atomic populations of the lower and upper levels, and ω_i and ω_k are the respective statistical weights. P is sometime called the 'overpopulation density' (Oda and Furukane, 1983). P is related to the fractional gain per unit distance, α , at the centre of a Doppler-broadened line by the following expression (cf. Willett, 1974)

$$\alpha = \left(\frac{\ln 2}{\pi}\right)^{1/2} \left[\frac{\omega_k A_{ki}}{4\pi}\right] \frac{P\lambda_o^2}{\Delta\nu}, \tag{67}$$

where λ_o is the centre wavelength of the transition, and $\Delta\nu$ is the linewidth. α describes the intensity of a plane wave at λ_o according to $I = I_o e^{\alpha\ell}$ where ℓ is the length over which gain occurs. In astrophysical sources, ℓ is very large, thus even a very small positive α can lead to an intense line. Unlike laboratory lasers which contain mirrors, gain is achieved only by amplified spontaneous emission (ASE) i.e. single pass lasers.

Recombination dominates in this decaying plasma, rapid cooling is necessary to favour the over-population of upper levels compared to lower levels. The upper levels are dominated by electron collisions, however below a certain level radiative decay begins to take over. Hence a population inversion can build-up between an upper level above this threshold and a lower level below this threshold.

Upper level recombination occurs mainly via three-body collisions, since radiative recombination occurs preferentially into the lower-lying quantum states. In the rate equation, the three-body recombination term depends quadratically on n_e while the radiative recombination term depends only linearly on n_e, this extra sensitivity to n_e by the three-body term requires higher electron densities to establish an over-population of the upper levels. Yet if the electron density is too high, the collisional de-excitation of the laser transition dominates.

The T_e^{-2} dependence of the three-body recombination rate along with the contradictory requirements of high temperature to initially strip the atom of the required number of electrons leads to the conclusion that significant gain occurs in a limited region of plasma parameter space.

G) RESULTS AND COMPARISON WITH ASTRONOMICAL SPECTRA

Population inversions in C IV were found to occur mostly in $n = 6 \rightarrow 5$ transitions: $6s \rightarrow 5p, 6p \rightarrow 5d, 6d \rightarrow 5p, 6f \rightarrow 5d, 6g \rightarrow 5f$ and $6h \rightarrow 5g$, figure 1 shows the $6g \rightarrow 5f$ (4658Å) gain contour plot ($\alpha\Delta\nu$), the gain decreases very rapidly at high values of n_e, decreases less rapidly at high values of T_e, and decreases slowly at high values of T_e and low values of n_e.

Wolf-Rayet stars are known to have an expanding envelope of hot ionized gases. When the speed of expansion is low, the expansion will be closer to being isothermal than adiabatic. However as the speed of expansion increases, the expansion will become more and more adiabatic, and certain spectral lines can be expected to display laser action. WC8 stars have relatively sharp lines; since the widths of the lines in an expanding shell arise from the Doppler effect, the speed of expansion of the plasma must be low and the degree of laser action is also expected to be low. The lines become wider in WC7 stars, indicating that the speed of ejection is greater than in WC8 stars; correspondingly, the degree of laser action is also expected to be greater. The lines become still wider in WC6 stars; we thus expect the degree of laser action to further increase. The three Wolf-Rayet spectra in Figure 2 demonstrate the correlation between expansion velocity and laser gain in the $6g \rightarrow 5f$ (4658Å) transition.

Laser action has also been shown to occur in He I (Nasser,1987) and many other ions, which leads us to wonder if the so-called red-shifted lines in quasars are due to laser action instead ?

The low spectral resolution survey by Craig *et al.* (1989) shows that many quasars seem to have one or two dominant lines, at various locations in the spectrum. Many of these lines are broad possibly indicating the blending of adjacent lines or high velocities. Some of the lines have P-Cygni profiles typical of high velocity outflows. All of the spectra have absorption lines not belonging to cold interstellar gases which indicates that the objects are surrounded by a thick envelope of colder gases. These last two observations indicate that laser action could be responsible for the unusual line intensities, which requires rapid cooling by adiabatic expansion and/or gas contact. However, quasar surveys suffer from the selection effect: Spectra which show similar spectral emission features as quasars but come from identifiable galactic objects are ignored or not published, such as Wolf-Rayets and central star of planetary nebula.

High spatial resolution 6cm radio surveys by the VLA (A&A) indicate that many quasars occur between pairs of highly collimated jets. Morphologically the jets look similar to the bipolar high-velocity-molecular-gas (HVMG) outflows observed by Lada *et al.* (1990) in proto-stars veiled by molecular dark clouds. Radio VLBI studies of quasar jets indicate possible super-luminal velocities in portions of the jet, however if we drop the assumption that these objects are at cosmological distances, the expansion velocity becomes reasonable for example if they were objects within our galaxy.

H) CONCLUSION

In this thesis we have explained the difference between LTE and non-LTE plasmas and why we must use the rate coefficients for basic physical plasma processes, instead of the simpler statistical model. We used these rates in a collisional radiative model of a recombining C IV plasma expanding adiabatically. From the solution of the level population we show how gain per unit length is computed, and why large gains occur only in limited regions of parameter space (n_e, T_e). We then compared our results to stellar spectra of Wolf-Rayet stars, and Quasars. Closer to earth, many experimental research labs have succeeded in producing laser action in decaying plasmas, and the future looks 'bright' for high power short wavelength UV or X-Ray lasers. (Matthews *et al.*, 1988)

Figure.1 : $6g \rightarrow 5f$ (4658Å) gain contour plot of C IV.

Figure.2 : Laser action in Wolf-Rayet stars at 4658Å

APPENDIX A : ATOMIC DATA

We describe in more detail how we obtain the rate coefficients. Using cross sections derived from quantum mechanical models we integrate these transition rates over the appropriate electron distribution obtained from statistical mechanics.

(a) Energy levels.

All of the levels having a principal quantum number $n \leq 6$ are treated as individual levels. Levels 7,8 and 9 remain discrete only if $\ell = 0$, otherwise they are grouped together to form a single level. For the levels with $n \geq 10$, all of the S,P,D,$\cdots$ levels are grouped together in one level. The upper limit of the levels, r and s in CR model calculation are taken as n_r =Variable and $n_s = 32$, respectively. Therefore we have 32 distinct levels in the main system, and the total number of levels whose population densities is calculated is 30.

(b) Radiative Transitions. The rates of spontaneous radiative transitions are determined by Einstein coefficients $A_{n\ell,n'\ell'}$. Einstein coefficients were calculated using the formula (Menzel and Pekeris, 1935)

$$A_{n\ell,n'\ell'} = \frac{8\pi^2 e^2 \omega_{n'\ell'}}{mc^3 \omega_{n\ell}} \nu^2_{n\ell,n'\ell'} f_{n'\ell',n\ell}, \tag{A-1}$$

where $\omega_{n'\ell'}$ and $\omega_{n\ell}$ are the statistical weights of the level $n'\ell'$ and $n\ell$, respectively, $\nu_{n\ell,n'\ell'}$ the frequency of the photon emitted as result of the transition and $f_{n'\ell',n\ell}$ is the absorption oscillator strength for the transition. When the angular momentum states ℓ or ℓ' are grouped together then,

$$A_{n\ell_i \ldots \ell_k, n'\ell_i' \ldots \ell_k'} = \frac{8\pi^2 e^2 \nu^2 \sum_{\ell_i}^{\ell_k} \sum_{\ell_i'}^{\ell_k'} \omega_{n'\ell'} f_{n'\ell',n\ell}}{mc^3 \sum_{\ell_i}^{\ell_k} \omega_{n\ell}}, \tag{A-2}$$

For transitions between unresolved levels and between resolved and unresolved levels,hydrogenic formula was used to calculate the oscillator strength (Kramers, 1923).

$$f_{n',n} = \frac{2^2}{3\sqrt{3}\pi\omega_n'} \left(\frac{1}{n'^2} - \frac{1}{n^2}\right)^{-3} \left(\frac{1}{n^3 n'^3}\right) g_I(n',n) \tag{A-3}$$

where ω_n' is the statistical weight of the level n', and $g_I(n',n)$ is the bound–bound Kramers–Gaunt factor. Analytic form for $g_I(n',n)$ has been given by Menzel and Pekeris (1935),

$$g_I(n,n) = \frac{\pi\sqrt{3}[(n-n')/(n+n')]^{2n+2n'} nn'}{(n-n')} |\Delta(n,n')| \tag{A-4}$$

where

$$\Delta(n,n') = \left[{}_2F_1\left(-n+1,-n;1;\frac{-4nn'}{(n-n')^2}\right)\right]^2 - \left[{}_2F_1\left(-n'+1,-n;1;\frac{-4nn'}{(n-n')^2}\right)\right]^2 \tag{A-5}$$

and the ${}_2F_1$ are hypergeometric functions.

(c) Collisional excitation and de–excitation rate coefficients.

The rate coefficient for collisional excitation of the $n'\ell' \rightarrow n\ell$ transition by electron impact is given by

$$C_{n'\ell',n\ell} = \int_v \sigma_{n'\ell',n\ell}(v)\, v\, f(v)\, dv \tag{A-6}$$

where v is the velocity and $f(v)$ the velocity distribution of the incident electrons. Using the Maxwellian velocity distribution

$$\frac{dn_e}{n_e} = f(v)\, dv = \frac{4v^2}{\sqrt{\pi}(2kT/m)^{3/2}} e^{-\frac{mv^2}{2kT}}\, dv \tag{A-7}$$

and expressing Equations (2-14) and (2-15) in terms of the kinetic energy E of the incident electron, we obtain

$$C_{n'\ell',n\ell} = \frac{1}{\sqrt{\pi m}} \left(\frac{2}{kT}\right)^{3/2} \int_E \sigma_{n'\ell',n\ell}(E)\, E\, e^{-\frac{E}{kT}}\, dE \tag{A-8}$$

with threshold energy units $U = E/E_{n'\ell',n\ell}$, Equation (98) becomes

$$C_{n'\ell',n\ell} = \sqrt{\frac{8}{\pi m k^3}} \frac{E^2_{n'\ell',n\ell}}{T^{3/2}} \int_1^\infty \sigma_{n'\ell',n\ell}(U)\, e^{-\frac{E_{n'\ell',n\ell}}{kT}U}\, U\, dU \tag{A-9}$$

where $E_{n'\ell',n\ell}$ is the threshold energy for the excitation of the $n'\ell' \rightarrow n\ell$ transition in Rydberg.

A very large number of excitation cross sections is required in this work. Unfortunately, the available data are but a very small fraction of the required cross sections. Most of the available data from theoretical calculations and work experimental are on the excitation from the ground state and low lying excited states. For all of the cross sections for which data exist the best experimental and theoretical data were fitted to semi–empirical formulas.

For allowed transitions between low-lying levels, the modified form of the Drawin cross section formula (1963, 1964, 1967) proposed by Millette and Varshni (1980) was used:

$$\sigma_{n'\ell',n\ell}(U) = 4\pi a_o^2 \alpha \frac{f_{n'\ell',n\ell}}{E^2_{n'\ell',n\ell}} \frac{U-\phi}{U^2} \ln(1.25\beta U), \tag{A-10}$$

$f_{n'\ell',n\ell}$ is the absorption oscillator strength, α, β and ϕ are the fitting parameters which depend on the transition. E is the kinetic energy of the incident electron, $U = E/E_{n'\ell',n\ell}$ is energy in threshold units, $E_{n'\ell',n\ell}$ is the threshold energy for the excitation of the $n'\ell' \rightarrow n\ell$ transition in Rydberg.

For transitions with $\Delta n > 3$, we used the effective Gaunt factor or $\bar{g}$ approximation developed by Van Regemorter (1962). For optically forbidden transitions without change in spin, we used the modified form of Drawin, proposed by Millette and Varshni (1980):

$$\sigma_{n'\ell',n\ell}(U) = 4\pi a_o^2 (n'/n)^3 \frac{\alpha}{E^2_{n'\ell',n\ell}} \frac{U-\phi}{U^2}, \tag{A-11}$$

where the symbols have their usual meaning.

For other optically forbidden transitions without change in spin between levels with $n \leq 6$ cross sections were calculated using the symmetrized binary encounter theory (Burgess, 1964a,b). The basic idea of the binary–encounter collision theory is that excitation of atoms by electrons is described approximately as a collision between two free electrons. In the derivation of cross section formulas it is further assumed that the atomic electrons initially have an isotropic velocity direction distribution with one constant magnitude of the velocity. This theory has been developed by Thomson (1912) and Gryzinski (1959). Mathematical corrections and discussions of the theory are given by Stabler (1964) and Vriens (1964a,b).

Burgess (1964a,b) introduced a new model with a symmetrical treatment of the two interacting electrons; the binary encounter may be treated as a quantum mechanical collision between identical particles with proper symmetrization and treatment of interference between direct and exchange scattering. The initial and final atomic states are treated classically in terms of an orbiting electron with definite initial and final kinetic energy, the change in kinetic energy being related to the angle of scattering. Burgess also allowed for the acceleration of the incident electron in the same way as Thomas (1927), the kinetic energy of the incident electron before the binary encounter being set equal to E_1+E_2+U, where E_1 is the initial kinetic energy of the incident electron, E_2 is the initial kinetic energy of the atomic electron, and U is the ionization energy. In this way, Burgess showed that cross sections for direct and exchange excitation could be calculated, together with the effect of interference between direct and exchange scattering. Vriens (1966) obtained simpler formulas for the cross section than those Burgess has given, using the same transformations in Burgess's collision model,

$$\sigma(\varepsilon_1,\varepsilon_2) = (\sigma_d + \sigma_{ex} + \sigma_{int})\,F \tag{A-12}$$

where σ_d is the cross section for direct excitation,

$$\sigma_d = \frac{\pi e^4}{E_1+E_2+U}\left[\frac{1}{\varepsilon_1} - \frac{1}{\varepsilon_2} + \frac{2E_2}{3}\left(\frac{1}{\varepsilon_1^2} - \frac{1}{\varepsilon_2^2}\right)\right] \tag{A-13}$$

σ_{ex} is the cross section for exchange excitation,

$$\begin{aligned}\sigma_{ex} = {} & \frac{\pi e^4}{E_1+E_2+U}\left[\frac{1}{E_1+U-\varepsilon_2} - \frac{1}{E_1+U-\varepsilon_1}\right. \\ & \left. + \frac{2E_2}{3}\left(\frac{1}{(E_1+U-\varepsilon_2)^2} - \frac{1}{(E_1+U-\varepsilon_1)^2}\right)\right]\end{aligned} \tag{A-14}$$

σ_{int} gives the influence of interference between direct and exchange scattering:

$$\sigma_{int} = -\frac{\pi e^4}{E_1+E_2-U}\,\frac{1}{E_1+U}\,\ln\left[\frac{(E_1+U-\varepsilon_1)\varepsilon_2}{\varepsilon_1(E_1+U-\varepsilon_2)}\right] \tag{A-15}$$

F is the focussing factor, which was introduced by Burgess (1964a,b) to account for electron–positive ion collision, and is given by

$$F = 1 + (ze^4/E_1\bar{r}) \tag{A-16}$$

where $\bar{r}$ is the mean radius and z is the charge number of the ion.

Equations (A-13)-(A-15) are valid for $E_1 \geq \varepsilon_2$, while ε_2 should be replaced by E_1 for $\varepsilon_1 \leq E_1 \leq \varepsilon_2$. The appropriate classical energy band specified by ε_1 and ε_2 is not well defined; in this calculations ε_1 has been taken as the excitation energy of the transition $n'\ell' \rightarrow n\ell$ and ε_2 as the excitation energy to the next higher level with the same L or S (Cacciatore and Capitelli, 1976).

The rate coefficients for de–excitation of a bound electron from state $n\ell$ to $n'\ell'$ by electron impact are calculated from the principle of detailed balance (Drawin, 1963)

$$Z_{n\ell} C_{n\ell,n'\ell'} = Z_{n'\ell'} C_{n'\ell',n\ell} \tag{A-17}$$

where $Z_{n'\ell'}$ and $Z_{n\ell}$ are the partition functions of the states $n'\ell'$ and $n\ell$, respectively. (Eq.11)

(d) Ionization and three-body recombination rate coefficients.

The rate coefficient of the ionization by electron impact is obtained by integrating the cross section over the free electron velocity distribution, $f(v)$:

$$S_{n\ell} = \int_v \sigma_{n\ell}(v)\, v\, f(v)\, dv. \tag{A-18}$$

Using Equation (97), we obtain

$$S_{n\ell} = 2\sqrt{\frac{2}{\pi m}}\, \frac{I_{n\ell}^2}{(kT_e)^{3/2}} \int_1^\infty \sigma_{n\ell}(U) U e^{-\frac{I_{n\ell}}{kT_e} U}\, dU, \tag{A-19}$$

where $I_{n\ell}$ is the ionization potential.
Experimental cross section data was fitted to the semi-empirical formula (Drawin, 1967):

$$\sigma_{n\ell}(U) = 2.66 \pi a_o^2 \alpha \frac{\xi}{E_{n\ell}^2} \frac{U-1}{U^2} \ln(1.25 \beta U), \tag{A-20}$$

The numerical value of ξ for ionization from the ground state is given by Drawin (1967), for $n > 1$, $\xi = 1$, α and β are fitting parameters, and the other symbols have their usual meaning. The cross sections for other levels were calculated using this formula with $\alpha = 1$, and β determined from the following expression (Drawin, 1967)

$$\beta = 1 + \frac{z_{eff} - 1}{z_{eff} + 2} \tag{A-21}$$

z_{eff} denotes the effective charge number of the nucleus acting on the electron.

The rate for three–body recombination of a free electron into state $n\ell$ of an atom or ion is obtained from the principle of detailed balance.

$$\alpha_{n\ell} = Z_{n\ell} S_{n\ell} \tag{A-22}$$

where $Z_{n\ell}$ is the partition function of the state $n\ell$. (Eq.11)

(e) Radiative recombination.

The radiative recombination rate coefficient is obtained from the photoionization cross section by applying the principle of detailed balancing. The rate coefficient is then given by

$$\beta_{n\ell} = \frac{1}{c^2}\sqrt{\frac{2}{\pi}}(mkT_e)^{-3/2}\frac{\omega_{n\ell}}{\omega_i}\, e^{I_{n\ell}/kT_e} \int_{I_{n\ell}}^{\infty} (h\nu)^2\, \sigma_{n\ell}(\nu)\, e^{-\frac{h\nu}{kT_e}}\, d(h\nu) \tag{A-23}$$

where ω_i is the statistical weight of the parent ion, and the other symbols have their usual meaning. Using threshold energy units, Equation (125) becomes

$$\beta_{n\ell} = \frac{1}{c^2}\sqrt{\frac{2}{\pi}}(mkT_e)^{-3/2}\frac{\omega_{n\ell}}{\omega_i}\, e^{I_{n\ell}/kT_e} I_{n\ell}^3 \int_{1}^{\infty} U^2\, \sigma_{n\ell}(U)\, e^{-\frac{I_{n\ell}}{kT_e}U}\, d(U) \tag{A-24}$$

Cross sections were fitted to a semi-empirical formula suggested by Millette and Varshni (1980),

$$\sigma_{n\ell}(U) = \frac{C}{U^p}\left[1 + \frac{a_1}{U} + \frac{a_2}{U^2} + \ldots + \frac{a_m}{U^m}\right], \tag{A-25}$$

where C, p and $a_k,\ k = 1, \ldots, m$ are fitting parameters, and U is the energy of the incident photon in threshold units. The hydrogenic approximation was adopted to calculate the photoionization cross sections for other levels; the cross section being given by

$$\sigma_{n\ell}(\nu) = 2.815 \times 10^{29}\, \frac{g_{II}(n,\nu)}{n^5\nu^3} \tag{A-26}$$

where $g_{II}(n,\nu)$ is the Gaunt-factor, it can be approximated by the expression (Seaton, 1959)

$$g_{II}(n,\nu) = 1 + \frac{0.1728(U_n - 1)}{n^{2/3}(U_n+1)^{2/3}} - \frac{0.0496(U_n^2 + \frac{4}{3}U_n + 1)}{(U_n+1)^{4/3}} + \ldots \tag{A-27}$$

where U_n is the threshold energy of the state $n\ell$.

APPENDIX B : IONIZATION EQUILIBRIUM

The relative concentrations of various stages of ionization of an element in a monatomic non-LTE plasma under statistical equilibrium are calculated with the model of House (1964). Since the plasma is not in LTE, the individual physical processes contributing to the ionization equilibrium must be considered. House (1964) calculated the ionization equilibrium of elements between hydrogen and iron, over a wide range of temperatures, including the processes of collisional ionization, radiative and collisional recombination. The model is based on the following assumptions: (1) Each stage of ionization of element X consists only of a ground state and a continuum. (2) The monatomic plasma is optically thin. Furthermore, collisional excitation followed by auto-ionization and di-electronic recombination processes are neglected, which under certain conditions, can restrict the applicability of the model.

Let S^{+m} represent the total rate coefficient for ionization from m-times ionized atom of element X to $m+1$, β^{+m} and α^{+m} the radiative and three body recombination rate coefficients from ion $m+1$ to m. Then under statistical equilibrium, we have

$$-n_e N^{+m} S^{+m} + \{\beta^{+m} + \alpha^{+m} n_e\} n_e N^{+(m+1)} = 0 \quad , \tag{B-1}$$

N^{+m} and $N^{+(m+1)}$ are the density of ions m and $m+1$, respectively.Eq.(B-1) is a simplified version of Eq.(8) without the terms C_{ij} and A_{ij}, only the S_1, β_1 and α_1 terms remain. Equilibrium is equivalent to the steady state solution $dn_1/dt = 0$, $N^{+m} \equiv n_1$ and $N^{+(m+1)} \equiv n^+$.

The collisional ionization rate coefficient is calculated with the following simple approximate formula (Allen, 1961):

$$S^{+m} = 1.15 \times 10^{-8} f_m \frac{\zeta_m}{I_m^2} \sqrt{T_e} e^{-I_m/kT_e} \quad , \tag{B-2}$$

ζ_m is the number of electrons in the outer shell of ion m, I_m is the ionization potential of ion m in eV,

$$f_m = 3.1 - \frac{1.2}{z_m} - \frac{0.9}{z_m^2} \quad , \tag{B-3}$$

z_m is the core charge of ion m, and all other symbols have their usual meaning. The three-body recombination rate coefficient is obtained from the condition of detailed balancing

$$\alpha^{+m} = \frac{h^3}{(2\pi m_e k T_e)^{3/2}} \frac{U_m}{2U_{m+1}} e^{I_m/kT_e} S^{+m} \quad , \tag{B-4}$$

U_m is the partition function of ion m, given approximately as

$$U_m = \sum_{i=1}^{\infty} \omega_i^{+m} e^{-E_{1i}^{+m}/kT_e} \approx \omega_1^{+m} \quad , \tag{B-5}$$

The radiative recombination rate coefficient has been calculated using the well known formula of Elwert (1952) given by

$$\beta^{+m} = 5.16 \times 10^{-14} f_1 \left(\frac{I_H}{kT_e}\right)^{1/2} \frac{I_m}{I_H} n G_1(I_m/kT_e) g \quad , \tag{B-6}$$

where

$$G_1(x) = x e^x E_1(x) \quad , \tag{B-7}$$

n is the principle quantum number of the ground state of the lower stage of ionization, I_m is the ionization potential of ion of charge $+m$ in eV, I_H is the ionization potential of hydrogen, $E_1(x)$ is the first exponential integral, $f_1 = 0.8, g = 3$. The value of f_1 and g come from Allen (1961). The fraction of atoms of element X that have been ionized m times is given by

$$N^{+m} \Big/ \sum_j N^{+j}, \tag{B-8}$$

TABLE 2. Parameters used to calculate the ionization equilibrium

	Ionization stages of carbon						
	C I	C II	C III	C IV	C V	C VI	C VII
I_m(eV)	11.260	24.383	47.887	64.492	392.077	489.981	—
z_m	1	2	3	4	5	6	—
ζ_m	4	3	2	1	2	1	—
n	2	2	2	2	1	1	—
U_m	9	6	1	2	1	2	1

APPENDIX C : COLLISIONAL-RADIATIVE PROGRAM

We modified the FORTRAN4 program originally written by Nasser (1987) so that it takes advantage of the cleaner syntax of FORTRAN77 by using indentation and replacing confusing `GOTO`s with `IF..THEN..ELSE` statements. The program was adapted to Carbon (C IV or C^{+3}) by replacing the Helium oscillator strengths by carbon data from Millette (1980) as well as semi-empirical fit coefficients for collisional excitation and photo- recombination. This Ion-specific data was moved to a separate text file to reduce clutter in the main program and make it more general, so it can read other ions such as N V, O VI and He I.

The subprograms were re-written to take most of their parameters via the parameter list rather than the more anonymous `COMMON BLOCK`s, this resulted in more self-contained subroutines reducing the possibility of error from uninitialized or re-used variables.

We replaced many functions in the program by their equivalent subroutines found in Press *et al.* (1992), which are widely used and well verified numerical recipes in FORTRAN:

- `DE1X(X)`, was replaced by `EXPINT(1,X)`.
- `DGAMMA(X)` was replaced by `DEXP(GAMMLN(X))`
- `DHANKL()` and `BKL()` were both replaced by `BESSIK()` which uses `BESCHB` and `CHEBEV`.
- `LEQT2F`(...) was replaced by the iterative matrix inversion scheme eq. (2.5.11) in Press *et al.* (1992).

The matrix inversion subroutine now uses a high speed iterative scheme whose performance improves for each subsequent electron density scan. Separate testing of the inversion subroutine on a matrix filled with random numbers generated by `RAN2` of Press *et al.*(1992) confirms that it always converges, even for the most ill-conditioned matrix. General improvements to optimize the speed of the program were performed such as computation of oscillator strengths and Einstein radiative rate coefficient are now only performed once at the beginning of the program. The benefit of the increased speed was an 10-fold increase in sampling resolution of temperature and density scans of the parameter space (now computed on a regularly spaced logarithmic grid). The density sweep has been moved into the `ROCOF()` subprogram.

The `ROCOF()` subprogram which initializes the matrices and computes the population coefficients was verified by performing from basic principles the complete derivation of the quasi-steady state collisional-radiative model for one, two and three independent ground levels. `ROCOF()` can now switch between collisional-radiative models based on 1,2 or 3 independent lower levels by setting `NG` to 1,2 or 3 Number of Ground levels.

The House (1964) ionization equilibrium was improved by including all ionization stages with a relative contribution of greater than 10^{-40}. To prevent overflow and increase floating point precision, higher ionization stages are included as a function of increased temperature. The improved subroutine was tested separately and a trial plot for Carbon as a function of T_e was found to be stable for all T_e and the shape of the plots were found to be very close to Figure 1.5 in Millette (1980). The computation of various rate coefficients specific to the House (1964) ionization equilibrium subroutine were made electron density independent. They are now only computed once at the beginning of the temperature sweep. The `RATIO` subroutine was also optimized for execution speed.

Many of the subroutines were shortened by removing intermediate variables, and `RETURN` statements were all but eliminated so that conditional clauses would dominate for a clearer self-evident case-by-case analysis. Program execution control now returns to the main program only at the end of every subroutine. The layout of the program itself was shuffled in order to group the subroutines nearer to their execution points and subprograms required by other subprograms are declared first to simplify preliminary read-through of the source code by others.

Program diagnostic controls were added to the ion data file, each printout option can be easily be changed with a text-editor without the need to re-compile the main program, allowing a variable level of numerical detail at run-time.

The main fortran77 program was compiled by `f2c` a fortran-to-C converter in the public domain which is easily obtainable for most other platforms. Then we used SAS C V6.5, an optimizing C compiler for amiga computers. On an A4000 Amiga with a 68040 CPU at 25MHz, the inversion of a 32 X 32 matrix takes less than one second. Some of the plots were produced by `GnuPlot` a multi-platform public domain plotting program, with terminal type set to LaTEX in order to include equations in the plot borders.

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