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**XSNQ-U — A NON-LTE EMISSION AND
ABSORPTION COEFFICIENT SUBROUTINE**

MASTER

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XSNQ-U — A NON-LTE EMISSION AND ABSORPTION COEFFICIENT SUBROUTINE

Abstract

This report describes the non-LTE atomic-state computer program, XSNQ-U. The original classified report was issued in 1971 (Ref. 1). Since then, important changes and improvements have been included.

XSNQ-U provides frequency-dependent emission and absorption coefficients for a material not in LTE (local thermodynamic equilibrium). As in XSNB,² an LTE opacity subroutine, a compromise has been sought between accuracy and computer speed. The result, XSNQ-U, is intended for use as a subroutine in any transport code. This report surveys the basic non-LTE equations for the average ion model, as pioneered by Grasberger,^{3,4} and gives details for the approximations and technique used in XSNQ-U. Also included are some illustrative numerical examples.

Since the writing of the classified report, the code has been modified by W. H. Grasberger and J. E. Ramus to handle the case of multiple elements. The extension is straight forward and would only make the notation more cumbersome if the single-element notation of this report were replaced by the multiple-element notation. Also, the method of solving the rate equations by using analytical differentials as discussed in the classified report has been replaced by a more direct incremental differences scheme, which is discussed in the present version.

1. Introduction

Consider a gas of uniform density at a point in time and space. Assume that the radiative and hydrodynamic changes in the gas occur more slowly than the time to establish a Maxwellian velocity distribution in either the ions or electrons. Therefore, let the electrons and ions have Maxwellian velocity distributions with associated kinetic temperatures. Further assume kinetic equilibrium; namely, that the ion and electron kinetic temperature, θ , are the same.

The subsequent time evolution of the gas can be calculated by using the equation of transfer and the material heating equation. Included in these equations are terms describing the radiative properties of the plasma. These

absorption and emission coefficients are functions of the number of bound and free electrons per atom. The state populations are established by electron detachment and recombination processes, both radiative and collisional (non-radiative electron-ion interactions). Since the populations are partly determined by radiation, they cannot be calculated unless the radiation field is specified.

In the approximation known as local thermodynamic equilibrium (LTE), we assume that the state populations are as they would be if the gas were in thermodynamic equilibrium at the local kinetic temperature θ . This would be true if the radiation field were essentially Planckian at the local temperature or if electron-ion collision processes were dominant. This assumption permits use of the steady-state Boltzmann-Saha equations which are functions only of the elemental composition, mass density, and temperature.

Suppose, however, the radiation field is non-Planckian and the resulting radiative electron transition rates are not overwhelmed by collisional rates. State populations must then be found from equations that incorporate explicitly the coupling of the state populations to the radiation field as a function of time. These form the non-LTE rate equations.

The changing population values will change the absorption and emission of the gas. These properties in turn affect the transport of radiation and the heating of the gas. The complete set of non-LTE equations, including the transport equation, the materials heating equation and the population rate equations are therefore coupled. The goal of the model given in this report is a stable separate package in which the rate equations can be advanced in time using explicit values of θ and the radiation field. This would be done in the same inline subroutine form as XSNB. Using these explicit values for the populations to calculate emission and absorption, the energy and transport equations would then be advanced a calculational cycle.

It is worth emphasizing that non-LTE is a condition quite different from "non-equilibrium" where the kinetic temperatures of the ions and electrons are different, but the level populations are given by the Saha and Boltzmann equations. If the radiative field is strong enough, the material density is low enough, or the time of interest short, the true level populations will be unrelated to these equations and in their place we must use the non-LTE equations.

2. Radiative Emission and Absorption

The equation of transfer, in the absence of scattering, is

$$\frac{1}{\rho c} \frac{dI_\nu}{dt} = \frac{1}{\rho c} \frac{\partial I_\nu}{\partial t} + \frac{1}{\rho} \vec{\omega} \cdot \nabla I_\nu = \epsilon_\nu - \kappa_\nu I_\nu, \quad (2.1a)$$

where ϵ_ν and $\kappa_\nu I_\nu$ represent the amount of radiant energy emitted or absorbed from the beam of intensity I_ν in the interval $d\nu$ about frequency ν per unit time, per unit solid angle, per unit mass.

The integral of Eq. (2.1a) over all directions and frequencies gives the net loss of material energy, E_m . This can be written as the material energy equation,

$$\frac{\partial E_m}{\partial t} = S - \int_0^\infty \int_{4\pi} (\epsilon_\nu - \kappa_\nu I_\nu) d(h\nu) d\Omega, \quad (2.1b)$$

where S includes any hydrodynamic work and nuclear source energy per mass per time. This change can be related through a specific heat to a change in material temperature. Temperature in turn helps determine ϵ_ν and κ_ν .

A relation between ϵ_ν and $\kappa_\nu I_\nu$ can be derived^{5,6} by using the Einstein coefficients of emission and absorption to calculate the transition probabilities.

Let E_n and E_m represent two, not necessarily discrete, energy states of an atom. Absorption by the system of a photon of energy,

$$h\nu = E_n - E_m, \quad (2.2)$$

results in a transition from lower state n to higher state m . The Einstein absorption coefficient β_{nm} is defined such that the probability of absorbing a photon from a beam of intensity I_ν per unit time, per unit solid angle, per atom is $\beta_{nm} I_\nu$. The rate at which energy is absorbed from the beam by an elemental mass unit due to transitions from state n to state m can be written as

$$\kappa_\nu(n,m) I_\nu = \frac{N_n}{\rho} \beta_{nm} I_\nu h\nu, \quad (2.3)$$

where N_n is the number density of particles in state n .

Notice that β_{nm} is constant for a specified ionic state and is independent of the radiation field. We would have to specify the state of the entire plasma to determine β_{nm} because distant, free and bound electrons screen the local charge. If we ignore the number and location of other ions and electrons, we greatly reduce the number of specific configurations for which separate β_{nm} need be calculated. However, the coefficients will then no longer be exactly independent of atomic populations.

Nevertheless, we will make the following approximations:

- For discrete states, the coefficient β_{nm} applies to all electrons making the transition from level n to level m, where the levels are of principal quantum numbers n and m.
- For levels n and m, β_{nm} is not a function of the populations of the other levels or free states.

These assumptions permit us to restrict the electron population calculations to just those of the principal quantum levels. The total free-electron population is directly given by subtracting the total level population from Z. The free-electron velocity distribution is already given through the assumption of a kinetic temperature.

To see how these assumptions can go wrong, consider the following ionic configurations for an atom of charge Z:

Electron populations	Ia	Ib	IIa	IIb
n=1 K shell	1	2	2	2
n=2 L shell	0	0	0	0
n=3 M shell	0	0	0	1

Clearly the Einstein coefficient, β_{12} , for an electron transition from the K to L shell in ion Ib is different from Ia because the nuclear charge as seen by the jumping electron will be effectively reduced because of the presence of the other bound electron. Similarly, the M shell electron in ion IIb will reduce the K shell binding energy of IIb as compared with IIa thus making the value of β_{12} for IIa different from IIb.

We can compensate for this by calculating the coefficients using screened charges. In this way, the coefficients will in fact depend on the populations. However, we will assume that the dependency is small enough to allow use of the method described below to solve for emission coefficients in terms of absorption coefficients.

A third approximation, which follows from the first two, is:

- Only the average number of electrons per atom in a level need be calculated, rather than the number of atoms having a specific configuration. (Average ion approximation.)

This assumption is crucial, for without it a time-dependent calculation of the nonequilibrium ionization of a high Z atom could require following the population of hundreds of possible electron configurations. (For a review of the ionic non-LTE problem see Tarter.⁵)

Let P_n then be the average number of electrons per atom in level n. We can now write

$$N_n \approx NP_n, \quad (2.4)$$

where N is the plasma number density.

The simplification brought by the average ion approximation adds a complication. By writing transition rates for levels instead of states, we must account for the degeneracy of the final level. Let the availability of level m be given as

$$Q_m = 1 - \frac{P_m}{g_m}, \quad (2.5)$$

where g_m is the statistical weight of level m; $2m^2$ for discrete states.

We can now write the average ion absorption rate as

$$\kappa_{\nu}(n,m) I_{\nu} = \frac{N}{\rho} F_n Q_m \beta_{nm} I_{\nu} h\nu. \quad (2.6)$$

For the reverse process, we note that an emission of a photon can occur either spontaneously or be induced by the presence of a radiation field. The probability that an atom in a higher state m will be stimulated by a radiation field of intensity I_{ν} to emit a photon of energy $h\nu$ per unit time, per unit solid angle is $\beta_{nm} I_{\nu}$, where β_{nm} is the Einstein coefficient for induced emission. The photon will be emitted into the direction of I_{ν} . The probability of a spontaneous emission of a photon of energy $h\nu$ occurring per unit time, per unit solid angle is simply the Einstein coefficient α_{nm} . The spontaneous emission is isotropic and independent of external radiation.

Using the notation developed above, the emission rate of a mass element due to transitions from state m to state n is

$$\epsilon_{\nu}(m,n) = \frac{N P_m Q_n}{\rho} \left(\alpha_{mn} + \beta_{mn} \right) I_{\nu} \quad h\nu. \quad (2.7)$$

The total emission and absorption of the gas at photon energy $h\nu$ are given by the sum of all energetically possible state transitions, both free and bound:

$$\epsilon_{\nu} = \sum_{m,n} \epsilon_{\nu}(m,n), \quad \kappa_{\nu} I_{\nu} = \sum_{n,m} \kappa_{\nu}(n,m) I_{\nu}. \quad (2.8)$$

Recall that in the strict definition, the Einstein coefficients are atomic quantities and do not depend on state populations or the strength of the radiation field. Therefore, we can calculate them for any condition and apply them for all conditions. In particular, we will solve for them under conditions of complete equilibrium. In what follows, we will assume that the approximate coefficients we have defined can be solved for in the same way.

For a gas in complete equilibrium, the radiation field is given by the Planck function B_{ν} , and the rate of each radiative or collisional process must be balanced in detail by the rate of its inverse. This means that for each transition, we may write

$$\epsilon_{\nu}^O(m,n) = \kappa_{\nu}^O(n,m) B_{\nu}, \quad (2.9)$$

where the superscript denotes equilibrium values. This gives

$$\frac{N}{\rho} P_m^O Q_n^O \left(\alpha_{mn} + \beta_{mn} B_{\nu} \right) h\nu = \frac{N}{\rho} P_n^O Q_m^O \beta_{nm} B_{\nu} h\nu,$$

or

$$B = \frac{\frac{\alpha_{mn}}{\beta_{mn}}}{\frac{P_n^O Q_m^O \beta_{nm}}{P_m^O Q_n^O \beta_{mn}} - 1} = \frac{\frac{2h}{c^2} \nu^3}{3^{h\nu/\theta} - 1}, \quad (2.10)$$

where the right side is the Planck function. Equating terms,

$$\frac{\alpha_{mn}}{\beta_{mn}} = \frac{2h}{c} \nu^3, \quad \frac{\beta_{nm}}{\beta_{mn}} = \frac{P_m^0 Q_n^0}{P_n^0 Q_m^0} e^u, \quad u = h\nu/\theta. \quad (2.11)$$

With two equations in three unknowns, we can replace the emission coefficients α_{mn} and β_{nm} with terms involving β_{nm} and write β_{nm} as a function of $\kappa_V^0(n,m)$. First, from the definition of β_{nm} we have,

$$\beta_{nm} = \frac{\rho \kappa_V^0(n,m)}{n P_n^0 Q_m^0 h\nu}. \quad (2.12)$$

From the above equations, we can write

$$\beta_{mn} = \frac{P_n^0 Q_m^0}{P_m^0 Q_n^0} e^{-u} \beta_{nm} = \frac{\rho \kappa_V^0(n,m)}{N P_m^0 Q_n^0 h\nu} e^{-u}, \quad (2.13)$$

and

$$\alpha_{mn} = \frac{2h}{c} \nu^3 \beta_{mn} = \frac{\rho \kappa_V^0(n,m)}{N P_m^0 Q_n^0 h\nu} B_V (1 - e^{-u}). \quad (2.14)$$

Using these results, we can write for any free- or bound-state transition, n to m and its inverse, ($n < m$),

$$\kappa_V(n,m) I_V = \kappa_V^0(n,m) \frac{P_n^0 Q_m^0}{P_n^0 Q_m^0} I_V, \quad (2.15)$$

$$\epsilon_V(m,n) = \kappa_V^0(n,m) \frac{P_m^0 Q_n^0}{P_m^0 Q_n^0} \left[B_V (1 - e^{-u}) + e^{-u} I_V \right]. \quad (2.16)$$

We here define, for later use, the monochromatic mass emission coefficient as

$$H_V(n,m) \equiv \kappa_V^O(n,m) \frac{P_m Q_n}{P_m^O Q_n^O}, \quad (2.17)$$

and Eq. (2.16) can be written as

$$\varepsilon_V(m,n) = H_V(n,m) \left[B_V(1 - e^{-u}) + e^{-u} I_V \right]. \quad (2.18)$$

If we apply the LTE approximation: namely, if we assume that the populations are always given by their equilibrium values,

$$P_n = P_n^O,$$

the radiative terms become simply

$$\kappa_V I_V = \sum_{n,m} \kappa_V(n,m) I_V = \kappa_V^O I_V, \quad (2.19)$$

$$\varepsilon_V = \sum_{m,n} \varepsilon_V(m,n) = \kappa_V^O \left[B_V(1 - e^{-u}) + e^{-u} I_V \right], \quad (2.20)$$

where κ_V^O is the total LTE mass absorption coefficient at the indicated photon energy.

Inserting these values into the equation of transfer, we have the familiar expression

$$\frac{1}{\rho c} \frac{\partial I_V}{\partial t} + \frac{1}{\rho} \vec{\omega} \cdot \nabla I_V = \kappa_V^O \left[B_V(1 - e^{-u}) + e^{-u} I_V \right] - \kappa_V^O I_V = \kappa_V^O (B_V - I_V), \quad (2.21)$$

where

$$\kappa_V' = \kappa_V^O(1 - e^{-u}). \quad (2.22)$$

The energy equation becomes

$$\frac{dE_m}{dt} = \frac{d}{dt} (c_v \theta) = \dot{S} - \int_0^\infty \left(4\pi \kappa'_v B_v - \int_{4\pi} \kappa'_v I_v d\Omega \right) d(h\nu), \quad (2.23)$$

where c_v is the specific heat.

3. Calculation of LTE Opacities

The processes contributing to κ_v^0 considered by XSNQ are the bound-bound (where significant), bound-free (where possible) and free-free.

The equilibrium occupation numbers and level energies are derived, as in XSNB,² from an iterative solution of the following equations (θ is temperature in keV):

$$p_n^0 = \frac{2n^2}{1 + \frac{317A}{\rho Z^{*0}} \theta^{3/2} e^{-E_n^0/\theta}}, \quad (3.1)$$

$$Z^{*0} = Z - \sum_{\text{all } n} p_n^0 \quad (\text{number of free electrons per atom}). \quad (3.2)$$

$$E_{n,\kappa}^0 = \bar{E}_{n,\kappa}^0 - \Delta E^0 \quad (\kappa = 1, 2, \dots, n), \quad (3.3)$$

where $\bar{E}_{n,\kappa}^0$ is the isolated ion ionization energy of sublevel κ at level n , and ΔE is the lowering of the continuum. $\bar{E}_{n,\kappa}^0$ is calculated by using either the Dirac formula for hydrogenic ions, allowing for spin and relativity, or by Pauli's approximation to this formula. These formulae are given in Appendix A, as well as a discussion of the prescription used for the lowering of the continuum. To represent the level n , we take the average of the extreme values of the sublevels, using for the effective charge of the level Z_n^{*0} :

$$E_n^0 = \frac{1}{2} (E_{n,1}^0 + E_{n,n}^0), \quad (3.4)$$

$$Z_n^* = Z - \sum_{\substack{m=1 \\ m \neq n}} P_m^0 \sigma_{n,m} + \frac{P_n^0 \sigma_{n,n}}{2n^2}, \quad (3.5)$$

where $\sigma_{n,m}$ are the Harris Mayer screening constants, listed in Appendix B. The maximum number of levels permitted by the current code is ten.

Formulae for the free-free, bound-free and bound-bound, absorption coefficients are listed below.

Free-Free:

$$\kappa_{\nu}^0(f,f) = \frac{D^0(f,f) g_{ff}}{(h\nu)^3} \text{ cm}^2/\text{gm}, \quad (3.6)$$

where g_{ff} is the free-free Gaunt factor and

$$D^0(f,f) = 2.78 \frac{(Z_n^*)^3}{A^2} \rho \theta^{-1/2} \quad (3.7)$$

Bound-Free:

$$\kappa_{\nu}^0(n,c) = F^0(n,c) \frac{P_n^0}{(h\nu)^3} g_{n,\nu}^{bf}, \quad (3.8)$$

where

$$F^0(n,c) = 12.0 \frac{(Z_n^*)^4}{A} \frac{1}{n^5}, \quad (3.9)$$

if $h\nu$ is in keV.

The total bound-free opacity is given by

$$\kappa_{\nu}^0(b,f) = \sum_{i=n}^{n \text{ max}} \kappa_{\nu}^0(i,c), \quad (3.10)$$

where n is the lowest level such that $h\nu \geq E_n$.

Bound-Bound:

Line broadening in general consists of Doppler, natural, and pressure broadening. At low densities and moderately high ion temperatures and not too high Z , Doppler broadening will dominate. Only Doppler broadening is considered in this report. For all lines we have

$$\kappa_V^O(n, m) = F^O(n, m) P_n^O Q_m^O \psi_V^O(n, m), \quad (3.11)$$

where, for large n we can approximate the hydrogenic f -value by

$$F^O(n, m) = \frac{5.17 \times 10^4}{A W_{nm}^O} \frac{nm^3}{(m^2 - n^2)^3}, \quad (3.12)$$

$$\psi_V^O(n, m) = \exp \left[-\frac{1}{2} \frac{(E_{nm}^O - h\nu)^2}{(W_{nm}^O)^2} \right], \quad (3.13)$$

and $(E_{nm}^O, h\nu, W_{nm}^O)$ are in keV

$$W_{nm}^O = 0.001036 E_{nm}^O \sqrt{\theta/A}, \quad (3.14)$$

where θ is the ion temperature in keV, assumed to be equal to the electron temperature. The quantity $F^O(n, m)$, given by Eq. (3.12), is based upon an approximation to the hydrogenic oscillator strength, valid for large values of n, m . For $n < 5$ or $m \leq 5$, this formula is replaced by its exact values as discussed in Appendix B.

4. Population Rate Equations

We return now to the non-LTE problem; namely, the situation when

$$P_n \neq P_n^O.$$

The change in P_n per unit time can be given as the difference between the number of electrons entering and leaving level n in that time. Let T stand for the electron transition-rate per atom between two levels (e.g., T_{nm}) or a level and the continuum (e.g., T_{nc}). For upward transitions (to lower energies), use the superscript U; for downward transitions, use superscript D. We can write, for level n ,

$$\frac{dP_n}{dt} = \sum_{m=1}^{n-1} (T_{mn}^U - T_{nm}^D) + \sum_{m=n+1}^{\infty} (T_{nm}^D - T_{nn}^U) + T_{cn}^D - T_{nc}^U \quad (4.1)$$

Thus, if n max levels are being followed, a coupled set of n max equations, one of this form for each level, must be integrated in time.

Each total transition rate T is the sum of two parts — a radiative and collisional term which are given below:

	<u>Total rates</u>		<u>Radiative</u>		<u>Collisional</u>
	Downward	Emission:	bound-bound		Superelastic
$n > m$	T_{nm}^D	=	T_{nm}^{RD}	+	T_{nm}^{CD}
or $n < m$	T_{mn}^D	or	T_{mn}^{RD}	or	T_{mn}^{CD}
	Downward	Emission:	free-bound		Three body recombination
	T_{cn}^D	=	T_{cn}^{RD}	+	T_{cn}^{CD}
	Upward	Absorption:	bound-bound		Elastic
$n < m$	T_{nm}^U	=	T_{nm}^{RU}	+	T_{nm}^{CU}
or $n > m$	T_{mn}^U	or	T_{mn}^{RU}	or	T_{mn}^{CU}
	Upward	Absorption:	bound-free		Inverse of three body recombination
	T_{nc}^U	=	T_{nc}^{RU}	+	T_{nc}^{CU}

5. Calculation of Radiative Rates

Each electron jump caused by radiative absorption or emission is associated with one photon of energy $h\nu$. The number of electron transitions between two states per unit time involving radiation is, therefore, the same as the number of photons absorbed or emitted by the process. This is equal to the total radiant energy emitted in, or absorbed from, all directions per unit time per atom, divided by the energy $h\nu$ of the photon. Since a particular transition may absorb or emit photons having a range of energies, the total radiative rate is found by integrating over all energetically possible values of $h\nu$.

Consider first the case of bound-bound emission. The total number of photons emitted per atom per unit time because of spontaneous and stimulated downward electron transitions is, for $n < m$,

$$T_{mn}^{RD} = \frac{\rho}{N} \int_0^\infty \int_{4\pi} \epsilon_{\nu}(m,n) d\Omega \frac{d(h\nu)}{h\nu}. \quad (5.1)$$

Using the result of Eq. (2.16), this can be written as

$$T_{mn}^{RD} = \frac{\rho}{N} \int_0^\infty \kappa_{\nu}^O(n,m) \frac{P_m^O Q_n^O}{P_m^O Q_n^O} \left[B_{\nu}(1 - e^{-u}) \int_{4\pi} d\Omega + e^{-u} \int_{4\pi} I_{\nu} d\Omega \right] \frac{d(h\nu)}{h\nu}. \quad (5.2)$$

Before inserting the complete equilibrium form of $\kappa_{\nu}^O(n,m)$ directly in the above, recall the form of the Einstein coefficient for absorption:

$$\beta_{nm} = \frac{\rho}{N} \frac{\kappa_{\nu}^O(n,m)}{P_n^O Q_m^O h\nu} = \frac{\rho}{N} \frac{F^O(n,m)}{h\nu} \psi_{\nu}^O(n,m). \quad (5.3)$$

As mentioned earlier, if we calculate $F(n,m)$ and $\psi_{\nu}(n,m)$ by using the current non-LTE values for energy levels and effective charge, we can overcome some of the inaccuracy introduced by assuming that β_{nm} for levels n and m is independent of the populations of the other levels. These functions are calculated in the same way as given in Section 4 for the equilibrium case except

the P_n , not P_n^0 , are to be used as level populations. The absence of the superscript will indicate that a function is to be calculated with the non-LTE occupation numbers.

If we define the mean specific intensity,

$$I_\nu = \frac{1}{4\pi} \int_{4\pi} I_\nu d\Omega, \quad (5.4)$$

and substitute the modified form of $\kappa_\nu^0(n,m)$, we have

$$T_{mn}^{RD} = 4\pi \frac{c}{h} F(n,m) \frac{P_n^0 Q_m^0}{P_m^0 Q_n^0} P_m Q_n \int_0^\infty \psi_\nu(n,m) \left[B_o(h\nu)^3 + J_\nu \right] e^{-u} \frac{d(h\nu)}{h\nu}, \quad (5.5a)$$

where we have used the identity, $B_o(h\nu)^3 e^{-u} = B_\nu(1 - e^{-u})$ with

$$B_o = \frac{2}{h^2 c^2} = 5.044 \times 10^{22} \quad (5.5b)$$

for B_ν in ergs per keV per second per cm^2 per steradian. For these units, the $h\nu$ divisor at the right end of Eq. (5.5a) must be in units of ergs rather than keV.

Using the equation for P_n^0 , which we can write here as

$$P_n^0 = \frac{2n^2}{1 + G^0 e^{-E_n^0/\theta}}; \quad G^0 = \frac{317 A \theta^{3/2}}{\rho Z^{*0}}, \quad (5.6)$$

and recalling the definition of Q_n^0 , we can write

$$\frac{P_n^0 Q_m^0}{P_m^0 Q_n^0} = \frac{\frac{2n^2}{1 + G^0 e^{-E_n^0/\theta}} \cdot \frac{G^0 e^{-E_m^0/\theta}}{1 + G^0 e^{-E_m^0/\theta}}}{\frac{2m^2}{1 + G^0 e^{-E_m^0/\theta}} \cdot \frac{G^0 e^{-E_n^0/\theta}}{1 + G^0 e^{-E_n^0/\theta}}} = \frac{n^2}{m^2} e^{(E_n^0 - E_m^0)/\theta} = \frac{n^2}{m^2} e^{u_{nm}^0}. \quad (5.7)$$

This now gives

$$T_{mn}^{RD} = 4\pi \frac{\rho}{N} F(n,m) \frac{n^2}{2} e^{u_{nm}^0} P_m Q_n \int_0^\infty \psi_V(n,m) \left[B_0 (h\nu)^3 + J_V \right] e^{-u} \frac{d(h\nu)}{h\nu} . \quad (5.8)$$

Introduce two new assumptions:

- Assume the line width is small compared to its energy. The value of $h\nu$ in the integral can then be replaced by the line energy, E_{nm} . Also, we can place the term e^{-u} outside the integral and evaluate it at the line center, $e^{-u_{nm}^0}$.
- Further, assume the line center is close in value to u_{nm}^0 ; that is, the term $\exp [u_{nm}^0 - u_{nm}]$ can be replaced by one.

It will be convenient to factor the occupation numbers from the balance of the transition rates. Applying the above approximation, we have,

$$T_{mn}^{RD} = P_m Q_n R_{mn}^{RD} , \quad (5.9a)$$

$$R_{mn}^{RD} = 4\pi \frac{\rho}{N} \frac{n^2}{2} \frac{F(n,m)}{E_{nm}} \int_0^\infty \psi_V(n,m) \left[B_0 E_{nm}^3 + J_V \right] d(h\nu) . \quad (5.9b)$$

In general, we will refer to R as the reduced transition rate.

Note that the rate is nonlinear in occupation numbers because of the $P_m Q_n$ factors, which give a term,

$$\frac{P_m P_n}{2n^2}$$

and the term R_{nm}^{RD} , which, to account for electron screening, becomes a function of the occupation numbers of all levels.

For line absorption, we can write for the total number of photons absorbed per atom per unit time due to radiative upward electron transitions, for $n < m$,

$$T_{nm}^{RU} = \frac{\rho}{n} \int_0^\infty \int_{4\pi} \kappa_V^0(n,m) \frac{P_n Q_m}{P_n^0 Q_m^0} I_V d\Omega \frac{d(h\nu)}{h\nu} = P_n Q_m R_{nm}^{RU} , \quad (5.10a)$$

where, using the assumption that the line width is narrow compared to the resonant energy, we have

$$R_{nm}^{RU} = 4\pi \frac{\rho}{N} \frac{F(n,m)}{E_{nm}} \int_0^\infty \psi_{\nu}(n,m) J_{\nu} d(h\nu). \quad (5.10b)$$

Note we have used the above expression for κ_{ν}° that accounts for screening in the average ion.

We can develop expressions for the other radiative process considered, bound-free emission and absorption, by writing the bound-free absorption coefficient for a particular level n as

$$\kappa_{\nu}^o(n,c) = \frac{F(n,c)}{(h\nu)^3} p_n^o g_{n\nu}^{bf} \quad (5.11)$$

where g_n^{bf} is the bound-free Gaunt factor for this level and, as was done for bound-bound, $F(n,c)$ is calculated by using the non-LTE occupation values to calculate the screened effective charge $\tilde{Z}_n^*$,

$$F(n,c) = 12.0 \frac{(\tilde{Z}_n^*)^4}{A} \frac{1}{n^5}. \quad (5.12)$$

Using $\tilde{Z}^*$ as the non-LTE population of free electrons per atom, we can write the total number of photons emitted per atom per unit time caused by spontaneous and stimulated electron transitions from the continuum to level n as

$$\begin{aligned} T_{cn}^{RD} &= \frac{\rho}{N} \int_{E_n}^{\infty} \int_{4\pi} \epsilon_{\nu}(c,n) d\Omega \frac{d(h\nu)}{h\nu} \\ &= 4\pi \frac{\rho}{N} \int_{E_n}^{\infty} \kappa_{\nu}^o(n,c) \frac{\tilde{Z}^* Q_n}{\tilde{Z}^o Q_n^o} \left[B_{\nu}(1 - e^{-u}) + e^{-u} J_{\nu} \right] \frac{d(h\nu)}{h\nu}. \quad (5.13) \end{aligned}$$

Making the indicated substitutions and defining terms similarly to those for the bound-bound

$$T_{cn}^{RD} = \sum_n Q_n R_{cn}^{RD}, \quad (5.14a)$$

$$R_{cn}^{RD} = 4\pi \frac{\rho}{N} \frac{P_n^O}{\sum_n Q_n^O} F(n, c) \int_{E_n}^{\infty} e^{-u} \left[B_o (h\nu)^3 + J_v \right] g_{nv}^{bf} \frac{d(h\nu)}{(h\nu)^4}. \quad (5.14b)$$

Note that P_n^O/Q_n^O must be computed by using the non-LTE energy level E_n .

Similarly, assuming the free electrons are not degenerate, the rate for the reverse transitions, photoelectric absorption, is

$$T_{nc}^{RU} = \frac{\rho}{N} \int_{E_n}^{\infty} \int_{4\pi} \kappa_v^O(n, m) \frac{P_n}{P_n^O} I_v d\Omega \frac{d(h\nu)}{h\nu} = P_n R_{nc}^{RU}, \quad (5.15a)$$

$$R_{nc}^{RU} = 4\pi \frac{\rho}{N} F(n, c) \int_{E_n}^{\infty} J_v g_{nv}^{bf} \frac{d(h\nu)}{(h\nu)^4}. \quad (5.15b)$$

6. Calculation of Collisional Rates

Bound-Bound and bound-free electron transitions (and their inverses) can be caused by interaction with a moving free electron. No photons are created or destroyed in a collisional process. These processes are considered because of their contribution to the change in level population — which in turn will change the radiative properties of the gas — and because of their effect on the heating (or cooling) of the free electrons.

The number of collisional ionizations from the n^{th} level per atom per unit time can be written as

$$T_{nc}^{CU} = NP_n \sum_n K(n, c), \quad (6.1)$$

where $K(n, c)$ is the population-independent collisional-rate coefficient analogous to the Einstein coefficients for radiative processes.

The inverse of this process, three body recombination, is

$$T_{cn}^{CD} = N^2 \left(\sum_n \right)^2 Q_n K(c, n). \quad (6.2)$$

In equilibrium, detailed balance holds and we have

$$T_{cn}^{CU} = T_{cn}^{CD} \quad (\text{equilibrium}).$$

Thus,

$$K(c,n) = \frac{P_n^O}{N \sum_o Q_n^O} K(r,c). \quad (6.3)$$

Again we must compute P_n^O/Q_n^O by using the non-LTE energy level E_n . Factoring terms in a manner identical to that done for the radiative rates, we have

$$T_{nc}^{CU} = P_n R_{nc}^{CU}, \quad R_{nc}^{CU} = N \sum K(n,c); \quad (6.4a,b)$$

$$T_{cn}^{CD} = \sum Q_n R_{cn}^{CD}, \quad R_{cn}^{CD} = \frac{N \sum P_n^O}{\sum_o Q_n^O} K(n,c). \quad (6.5a,b)$$

Similarly, if $K(n,m)$ is the rate coefficient for collisional excitation and $m > n$, we have

$$T_{nm}^{CU} = N \sum P_n Q_m K(n,m). \quad (6.6)$$

For collisional de-excitation, we have

$$T_{mn}^{CD} = N \sum P_m Q_n K(m,n). \quad (6.7)$$

Again, applying detailed balance, $T_{nm}^{CU} = T_{mn}^{CD}$, for the equilibrium condition, we have (using the non-LTE energy levels E_n, E_m)

$$K(m,n) = \frac{P_n^O Q_m^O}{P_m^O Q_n^O} K(n,m), \quad (6.8)$$

which gives

$$T_{nm}^{CU} = P_n Q_m R_{nm}^{CU}, R_{nm}^{CU} = N \sum K(n, m); \quad (6.9a, b)$$

$$T_{nm}^{CD} = P_m Q_n R_{nm}^{CD}, R_{nm}^{CD} = N \sum \frac{P_n^0 Q_m^0}{P_m^0 Q_n^0} K(n, m). \quad (6.10a, b)$$

The collisional rates are given by prescriptions derived by B. Tarter⁷ based on results found in the literature, as follows:

$$K(n, c) = 3.45 \times 10^{-11} \theta^{1/2} \frac{e^{-u_n}}{E_n^2} \Gamma_n \text{ cm}^3/\text{sec}, \quad (6.11)$$

$$K(n, m) = 4.99 \times 10^{-10} \frac{f(n, m)}{(E_n - E_m)} \frac{e^{-u_{nm}}}{\theta^{1/2}} g_{nm} \text{ cm}^3/\text{sec}, \quad (6.12)$$

where $f(n, m)$ is the hydrogenic oscillator strength (see Appendix B), $u_n = E_n/\theta$, and θ , E_n , E_m are in keV. The factors Γ_n and g_{nm} are given by

$$\Gamma_n = 12.18 e^{-n/(n+5)} (1 + 0.0335 n) \left(1 - \frac{0.622}{Z} - \frac{0.0745}{Z^2} \right) (1 - e^{-u_n}) f(y),$$

$$f(y) = 0.23 + 0.046 y + 0.1074 y^2 - 0.0459 y^3 - 0.01505 y^4,$$

$$y = \log_{10}(u_n/4),$$

$$g_{nm} = 0.19 \left\{ 1 + 0.9 \left[1 + \frac{m(m-n)}{20} \right] (1 - (1 - 2/Z) u_{nm}) \right\} e^{u_{nm}} \epsilon_1(u_{nm}).$$

Here ϵ_1 is the exponential integral given by Eq. (8.3b).

In analogy to the radiative case, these rate coefficients are to be evaluated by using the current non-LTE values of energy levels.

7. Radiative Line Rate Approximation

An accurate treatment of the line transition rate requires a fairly precise determination of the radiation field within the line. Often such a determination is not practical because of the large number of lines, complications arising from the shifting of lines, etc. Fortunately, there are two limiting cases in which the radiation field within a line need not be determined by solving the equation of transfer. When the radiation field is negligible, the *optically thin case* is valid. The second case occurs when the line is optically thick over most of the line so that the radiation field is determined by local conditions. (Of course the time for local conditions to change significantly must be long compared to the time for light to travel across the local region of the line.) The second case is called the *optically thick case*, and this report assumes its validity. The change to the optically thin case is easily made. Therefore, we assume that the total absorption in the line is large enough that the radiation field in the vicinity of a line is as if it were in a steady state in an infinite medium. This is likely to be true at or near the center of all opaque lines, and we will assume it true over the entire line shape.

If we ignore scattering, then the steady-state radiation field, J_v^∞ , is given by the balance of total emission and total absorption. We will once again assume that the continuous emission and absorption coefficients do not change appreciably over the line width. With these assumptions plus the approximation that lines do not overlap, we have

$$(\kappa^C + \kappa_v^{nm}) J_v^\infty = (H^C + H_v^{nm}) e^{-u_{nm}} (B_o E_{nm}^3 + J_v^\infty), \quad (7.1)$$

where, by using the definition of H given in Eq. (2.17), and using E_i in the ratio P_i^o/Q_i^o ,

$$\kappa^C = \left(D^{ff} g_{nm}^{ff} + \sum_{i=n+1}^{n \max} F(i, c) P_i g_{i, nm}^{bf} \right) (E_{nm})^{-3}, \quad (7.2)$$

$$H^C = \left(D^{ff} g_{nm}^{ff} + \frac{Z}{Z_o} \sum_{i=n+1}^{n \max} F(i, c) \frac{P_i^o}{Q_i^o} Q_i g_{i, nm}^{bf} \right) (E_{nm})^{-3}, \quad (7.3)$$

$$\kappa_{\nu}^{nm} = F(n, m) P_n Q_m \psi_{\nu}^{nm}, \quad (7.4)$$

$$H_{\nu}^{nm} = F(n, m) P_m Q_n \psi_{\nu}^{nm} \frac{n^2}{m^2} e^{u_{nm}^0}. \quad (7.5)$$

Define

$$\bar{\kappa}^C = \kappa^C - H^C e^{-u_{nm}}, \quad (7.6)$$

$$\bar{\kappa}_{\nu}^{nm} = \kappa_{\nu}^{nm} - H_{\nu}^{nm} e^{-u_{nm}} = \kappa_{\nu}^{nm} \left(1 - \frac{P_m Q_n}{P_n Q_m} \frac{n^2}{m^2} \right), \quad (7.7a)$$

where we have again assumed the line center is near its LTE value. If we let $\bar{\kappa}^{nm}$ represent the line opacity of the line center, then we can write

$$\bar{\kappa}_{\nu}^{nm} = \bar{\kappa}^{nm} \psi_{\nu}^{nm}. \quad (7.7b)$$

Using these expressions, we have

$$J_{\nu}^{\infty} = \frac{(H^C + H_{\nu}^{nm} \psi_{\nu}^{nm}) e^{-u_{nm}} B_o E_{nm}^3}{(\bar{\kappa}^C + \bar{\kappa}^{nm} \psi_{\nu}^{nm})}. \quad (7.8)$$

If we define the line and continuous source functions at the line center as

$$S^{nm} = \frac{B_o E_{nm}^3}{\frac{P_n Q_m}{P_m Q_n} \frac{n^2}{m^2} - 1}, \quad (7.9a)$$

$$S^C = \frac{B_o E_{nm}^3}{\frac{\kappa^C}{H^C} e^{u_{nm}} - 1}, \quad (7.9b)$$

then Eq. (7.8) can be written as

$$J_v^\infty = \frac{s^{nm} + s^c \frac{\bar{\kappa}^c}{\bar{\kappa}^{nm} \psi_v^{nm}}}{1 + \frac{\bar{\kappa}^c}{\bar{\kappa}^{nm} \psi_v^{nm}}} . \quad (7.10)$$

Note that when the level populations take on their equilibrium values, both source functions become Planck functions. The value of Eq. (7.10) is then just B_v . For the general case, we insert Eq. (7.10) for J_v in Eqs. (5.9b) and (5.10b).

Following Grasberger,⁴ we now redefine the line rate terms so that they represent the net electron flow. This is done to reduce round-off errors. We have for the change in population of level n , caused by transitions to and from level m ,

$$\frac{dP_n^{nm}}{dt} = P_m Q_n R_{mn}^{RD} - P_n Q_m R_{nm}^{RU} . \quad (7.11)$$

By using Eqs. (5.9b) and (5.10b) and the steady-state radiation field assumption,

$$\begin{aligned} \frac{dP_n^{nm}}{dt} &= 4\pi \frac{\rho}{N} \frac{F(n,m)}{E_{nm}} \\ &\times \left[\frac{n^2}{m^2} P_m Q_n \int_0^\infty \psi_v^{nm} \left(B_0 E_{nm}^3 + J_v^\infty \right) d(h\nu) - P_n Q_m \int_0^\infty \psi_v^{nm} J_v^\infty d(h\nu) \right] \\ &= 4\pi \frac{\rho}{N} F(n,m) B_0 E_{nm}^2 \frac{n^2}{m^2} P_m Q_n \int_0^\infty \psi_v^{nm} \left(1 - \frac{\frac{m^2}{n^2} \frac{P_n Q_m}{P_m Q_n} - 1}{B_0 E_{nm}^3} J_v^\infty \right) d(h\nu) \\ &= 4\pi \frac{\rho}{N} F(n,m) B_0 E_{nm}^2 \frac{n^2}{m^2} P_m Q_n \int_0^\infty \psi_v^{nm} \left(1 - \frac{J_v^\infty}{E_{nm}} \right) d(h\nu) . \end{aligned} \quad (7.12)$$

If we compare Eq. (7.12) with the definition of J_v^∞ as given in Eq. (7.10), we note that for frequencies at which the line is much stronger than the continuum, the net change in P_n caused by this line transition is zero. This is

a consequence of the assumption that the radiation field is in steady-state and holds for any set of populations. A net imbalance between rates (n,m) and (m,n) is possible only at frequencies at which the line strength has fallen to values comparable to the continuous. At these frequencies, in the wings of the line, any non-equilibrium level populations will give a net flow of electrons. Because of the breakdown of the assumption that the line is optically thick in the far wings, our calculated net flow of electrons is subject to possible error, which is the price we must pay to avoid solving the equation of transfer over the line.

Using Eq. (7.9a) for the line source function and Eq. (7.8) for J_v^∞ , the integral in Eq. (7.12) becomes

$$\int_0^\infty \psi_v^{nm} \left(1 - \frac{J_v^\infty}{S^{nm}} \right) d(h\nu) = \left(\kappa^C - H^C e^{-u_{nm}} \frac{P_n Q_m m^2}{P_m Q_n n^2} \right) \int_0^\infty \frac{\psi_v^{nm} d(h\nu)}{(\kappa^C + \kappa^{nm} \psi_v^{nm})}. \quad (7.13)$$

Recalling the form for ψ_v^{nm} in Eq. (3.13)

$$\psi_v^{nm} = \exp \left(-\frac{1}{2} \frac{(h\nu - E_{nm})^2}{W_{nm}^2} \right), \quad (7.14)$$

we have

$$\int_0^\infty \psi_v^{nm} \left(1 - \frac{J_v^\infty}{S^{nm}} \right) d(h\nu) = \left(\frac{\kappa^C}{\kappa^{nm}} - \frac{H^C e^{-u_{nm}}}{\kappa^{nm}} \frac{P_n Q_m m^2}{P_m Q_n n^2} \right) W_{nm} L(y), \quad (7.15)$$

with

$$L(y) = \int_{-\infty}^{\infty} \left(1 + y e^{x^2/2} \right)^{-1} dx, \quad (7.16)$$

where x and the parameter y are given as

$$x = \frac{h\nu - E_{nm}}{W_{nm}}, \quad y = \frac{\kappa^C}{\kappa^{nm}}. \quad (7.17a,b)$$

A good fit for $L(y)$ for the range $10^{-9} < y < \infty$ is given by

$$L(y) = \frac{a_0 + a_1 y}{b_0 + b_1 y + b_2 y^2} + \frac{0.00248 + 3.86 y}{0.000235 + 0.7 y + 1.54 y^2}. \quad (7.18)$$

Figure 7-1 shows both the function and the fit.

Inserting the expression derived in Eq. (7.15) for the reduced integral of Eq. (7.12) and collecting terms, we have for the redefined net rates per electron

$$R_{nm}^{RD} = 4\pi \frac{\rho}{N} F(n,m) B_o E_{nm}^2 W_{nm} \frac{n^2}{m} \frac{K^C}{K_{nm}} L(y), \quad (7.19)$$

$$R_{nm}^{RU} = 4\pi \frac{\rho}{N} F(n,m) B_o E_{nm}^2 W_{nm} \frac{H^C}{K_{nm}} \frac{e^{-u_{nm}}}{K_{nm}} L(y). \quad (7.20)$$

As desired, these approximate reduced line rates now do not depend explicitly on the radiation field.

Fig. 7-1. The function $L(y)$ given by Eq. (7.16).

8. Radiative Continuous Rate Approximation

In practice, the integrals required for R_{nc}^{RU} and R_{cn}^{RD} must be replaced by sums over groups in photon energy. The integrals must be approximated carefully both for accuracy and so that the rate terms will cancel when the gas approaches equilibrium.

First, we rewrite Eqs. (5.15b) and (5.14b) as, with k max energy groups and boundaries $h\nu_k$,

$$R_{nc}^{RU} = 4\pi \frac{\rho}{N} F(n, c) \left(\int_{E_n}^{h\nu_a} J_\nu g_n^{bf} \frac{d(h\nu)}{(h\nu)^4} + \sum_{k=a+1}^{k \max} \int_{h\nu_{k-1}}^{h\nu_k} J_\nu g_n^{bf} \frac{d(h\nu)}{(h\nu)^4} \right), \quad (8.1)$$

$$\begin{aligned} R_{cn}^{RD} = 4\pi \frac{\rho}{N} F(n, c) \frac{P_n^O}{Z_n^O Q_n^O} & \left[B_0 \int_{E_n}^{h\nu_a} g_{n\nu}^{bf} e^{-u} \frac{d(h\nu)}{h\nu} \right. \\ & + B_0 \sum_{k=a+1}^{k \max} \int_{h\nu_{k-1}}^{h\nu_k} g_{n\nu}^{bf} e^{-u} \frac{d(h\nu)}{(h\nu)} \\ & \left. + \int_{E_n}^{h\nu_a} e^{-u} J_\nu g_{n\nu}^{bf} \frac{d(h\nu)}{(h\nu)^4} + \sum_{k=a+1}^{k \max} \int_{h\nu_{k-1}}^{h\nu_k} e^{-u} J_\nu g_{n\nu}^{bf} \frac{d(h\nu)}{(h\nu)^4} \right] \quad (8.2) \end{aligned}$$

where $h\nu_a$ is the lowest boundary energy greater than the binding energy of level n , E_n . Remember, P_n^O/Q_n^O should use the non-LTE energy level E_n .

Next, assume the Gaunt factor, $g_{n,k-1/2}^{bf}$, to be constant over a group $h\nu_{k-1}$ to $h\nu_k$. Then the first part of Eq. (8.2) becomes

$$\begin{aligned} B_0 g_{n,a-1/2}^{bf} [\epsilon_1(u_n) - \epsilon_1(u_a)] + B_0 \sum_{k=a+1}^{k \max} g_{n,k-1/2}^{bf} \\ \times [\epsilon_1(u_{k-1}) - \epsilon_1(u_k)], \quad (8.3a) \end{aligned}$$

where $\epsilon_1(u)$ is the exponential integral,

$$\epsilon_1(u_k) \equiv \int_{u_k}^{\infty} \frac{e^{-u}}{u} du = \int_{h\nu_k}^{\infty} \frac{e^{-u}}{h\nu} d(h\nu). \quad (8.3b)$$

A good fit to the exponential integral must be used because of the rapid decay of the integral. Approximating the integral over the interval by a simple trapezoidal area could result in a very inaccurate value for the spontaneous emission rate.

We use the Cody and Thacher⁸ fit, which is a set of ratios of polynomials:

$$\epsilon_1(u) = \ln(u) + R_a(u) \quad 0 \leq u < 1, \quad (8.4a)$$

$$\epsilon_1(u) = e^{-u} R_b(u^{-1}) \quad 1 \leq u < 4, \quad (8.4b)$$

$$\epsilon_1(u) = \frac{e^{-u}}{u} \left[1 + u^{-1} R_c(u^{-1}) \right] \quad 4 \leq u < \infty, \quad (8.4c)$$

where

$$R_a(u) = \sum_{q=0}^3 \alpha_i^a u^i / \sum_{i=0}^3 \beta_i^a u^i, \quad (8.5a)$$

$$R_b(u^{-1}) = \sum_{i=0}^4 \alpha_i^b u^{-i} / \sum_{i=0}^4 \beta_i^b u^{-i}, \quad (8.5b)$$

$$R_c(u^{-1}) = \sum_{i=0}^3 \alpha_i^c u^{-i} / \sum_{i=0}^3 \beta_i^c u^{-i}. \quad (8.5c)$$

The coefficients (α_i , β_i) given in Cody's paper give a fit accurate to about 10 decimal places.

Recall that the integration of J_ν over a photon energy range is related to the energy density of the radiation field. In particular,

$$e_{k-1/2} = \frac{4\pi}{c} \int_{h\nu_{k-1}}^{h\nu_k} J_\nu d(h\nu). \quad (8.6)$$

Let this be the quantity provided by the transport code.

Now the variation of J_ν across the interval needs to be specified. In an early version, J_ν was assumed to have a quadratic variation in the interval. The coefficients were chosen so that the energy density, as given by the integral in Eq. (8.6), would be as specified by the transport code, and so that J_ν would be everywhere continuous. The fitting technique was thus a cubic spline in $e_{k-1/2}$. This method came to grief, however, for cases in which a group with a small $e_{k-1/2}$ was sandwiched between two groups with large values of $e_{k-1/2}$. The J_ν fit for the middle group would have to become negative, both to give the correct area ($e_{k-1/2}$) and to be continuous at the boundaries. Since the integrations can begin anywhere (E_n changes in time), and since the integrals decay rapidly, the rate terms could be so inaccurate as to actually be negative.

In the current code, we assume that the factors of J_ν in the integrals can be evaluated at an average photon energy. This leaves the integral of j_ν itself, which is replaced by $e_{k-1/2}$. For example, using the constant Gaunt factor assumption, we can write the second term of Eq. (8.1) and the fourth term of Eq. (8.2) as

$$\begin{aligned} \sum_{k=a+1}^k \max \quad g_{n,k-1/2}^{bf} \int_{h\nu_{k-1}}^{h\nu_k} J_\nu \frac{d(h\nu)}{(h\nu)^4} &\cong \sum_{k=a+1}^k \max \frac{g_{n,k-1/2}^{bf}}{(h\bar{\nu}_{k-1/2})^4} \int_{h\nu_{k-1}}^{h\nu_k} J_\nu d(h\nu) \\ &= \frac{c}{4\pi} \sum_{k=a+1}^k \max \frac{g_{n,k-1/2}^{bf}}{(h\bar{\nu}_{k-1/2})^4} e_{k-1/2}, \end{aligned} \quad (8.7)$$

and

$$\begin{aligned} \sum_{k=a+1}^k \max \quad g_{n,k-1/2}^{bf} \int_{h\nu_{k-1}}^{h\nu_k} e^{-u} J_\nu \frac{d(h\nu)}{(h\nu)^4} &\cong \\ \frac{c}{4\pi} \sum_{k=a+1}^k \max \quad g_{n,k-1/2}^{bf} e_{k-1/2} \frac{e^{-\bar{u}_{k-1/2}}}{(h\bar{\nu}_{k-1/2})^4} \end{aligned} \quad (8.8)$$

The average photon energy, $h\bar{\nu}_{k-1/2}$, is determined such that if the gas were in equilibrium, the radiative continuous rate terms, T_{nc}^{RU} and T_{cn}^{RD} , would cancel each other in each group.

This means that, using Eqs. (8.3a), (8.7) and (8.8), we can write for each group in equilibrium,

$$T_{nc}^{RU} = T_{cn}^{RD},$$

or

$$\frac{\epsilon_{k-1/2}^0}{(h\bar{\nu}_{k-1/2})^4} = \frac{4\pi B_0}{c} [\epsilon_1(u_{k-1}) - \epsilon_1(u_k)] + \frac{e^{-u_{k-1/2}}}{(h\bar{\nu}_{k-1/2})^4} \epsilon_{k-1/2}^0, \quad (8.9)$$

where $\epsilon_{k-1/2}^0$ is the integral over the group of the black body energy density at the local temperature. A Newton's method solution for $h\bar{\nu}_{k-1/2}$ converges rapidly and has proven reliable. The solutions for a range of u_k and u_{k-1}/u_k (the equation scales with θ) are shown in Fig. 8-1.

Fig. 8-1. Solution of Eq. (8.9).

Fig. 8-2. Energy density of the first group above the bound-free edge.

For the first integral of Eq. (8.2), we assume the energy density scales as the fraction of the group to be integrated (Fig. 8-2). Thus, the energy density of the cross hatched region is given by $\delta_n e_{a-1/2}$, where

$$\delta_n = \frac{h\nu_a - E_n}{h\nu_a - h\nu_{a-1}}. \quad (8.10)$$

In determining $h\bar{\nu}_{a-1/2}$, we use E_n as the lower bound in finding the integrated black body energy density. (However, to guarantee that the rate terms cancel as equilibrium is approached, δ_n must be defined as the ratio of the black body integrals.)

To save computer time, we wish to approximate the calculation of $h\bar{\nu}_{a-1/2}^{-1}$ for succeeding iterations. Assuming $h\bar{\nu}_{a-1/2}^{-1}$ for the i^{th} iterate scales with the variation in E_n^i shown as follows:

$$h\bar{\nu}_{a-1/2}^{-1} = h^i (1 - \alpha_n) + \alpha_n E_n^i, \quad (8.11)$$

where

$$\alpha_n = \frac{h\nu_a - h\nu_{a-1/2}^{-1}}{h\nu_a - E_n^1}, \quad (8.12)$$

and $h\nu_{a-1/2}^{-1}$ is the correct solution to Eq. (8.9) with the initial energy level, E_n^1 , as the lower bound. This energy, E_n^1 , is calculated by using the first estimates of P_n .

9. Newton's Method Solution of Rate Equations

Combining the results of the above sections, we can now list the reduced transition rates with their coefficients evaluated (units are in number/second/occupation number/atom, with $h\nu$, E_n , θ in keV).

$$\begin{aligned} \bullet \quad R_{nc}^{RU} = 1.30 \times 10^{-14} F(n,c) A \left(\frac{c}{4\pi} \right) & \left[g_{n,a-1/2}^{bf} \frac{\delta_n e_{a-1/2}}{(h\nu_{a-1/2})^4} \right. \\ & \left. + \sum_{k=a+1}^{k \max} g_{n,k-1/2}^{bf} \frac{e_{k-1/2}}{(h\nu_{k-1/2})^4} \right]. \end{aligned} \quad (9.1)$$

$$\begin{aligned} \bullet \quad R_{cn}^{kD} = 1.30 \times 10^{-14} F(n,c) A \frac{P_n^0}{Z Q_n^0} & \left(g_{n,a-1/2}^{bf} \left\{ B_o \left[\varepsilon_1(u_n) - \varepsilon_1(u_a) \right] \right. \right. \\ & + \left. \frac{c}{4\pi} \frac{e^{-u_{a-1/2}}}{(h\nu_{a-1/2})^4} \delta_n e_{a-1/2} \right\} \\ & + \sum_{k=a+1}^{k \max} g_{n,k-1/2}^{bf} \left\{ B_o \left[\varepsilon_1(u_{k-1}) - \varepsilon_1(u_k) \right] \right. \\ & \left. \left. + \left(\frac{c}{4\pi} \right) \frac{e^{-u_{k-1/2}}}{(h\nu_{k-1/2})^4} e_{k-1/2} \right\} \right). \end{aligned} \quad (9.2)$$

$$\bullet \quad R_{cn}^{CU} = 2.08 \times 10^{13} \frac{\rho}{A} \frac{Z^*}{E_n^2} \theta^{1/2} e^{-u_n} \Gamma_n. \quad (9.3)$$

$$\bullet \quad R_{cn}^{CD} = 2.08 \times 10^{13} \frac{\rho}{A} \frac{Z^*}{Z^0} \frac{\theta^{1/2} e^{-u_n} P_n^0}{E_n^2 Q_n^0} \Gamma_n. \quad (9.4)$$

$$\bullet \quad R_{nm}^{RU} = 1.73 \times 10^{13} f_{nm} E_{nm}^2 \frac{H^C e^{-u_{nm}}}{\kappa_{nm}} L(y), \quad (9.5)$$

$$\bullet \quad R_{nm}^{RD} = 1.73 \times 10^{13} f_{nm} E_{nm}^2 \frac{n^2}{m^2} \frac{\kappa^C}{\kappa_{nm}} L(y), \quad (9.6)$$

$$\bullet \quad R_{nm}^{CU} = 3.01 \times 10^{14} f_{nm} \frac{\rho}{A} \frac{Z^*}{Z} \frac{e^{-u_{nm}}}{E_{nm} \theta^{1/2}} g_{nm}, \quad (9.7)$$

$$\bullet \quad R_{nm}^{CD} = 3.01 \times 10^{14} f_{nm} \frac{\rho}{A} \frac{Z^*}{Z} \frac{P_n^0 Q_n^0}{P_m^0 Q_n^0} \frac{e^{-u_{nm}}}{E_{nm} \theta^{1/2}} g_{nm}, \quad (9.8)$$

with f_{nm} the absorption oscillator strength. For large n values, we have

$$f_{nm} = 1.960 \frac{nm^3}{(m^2 - n^2)^3}. \quad (9.9)$$

Equation (4.1), giving the rate of change of level n population, can be written as

$$\frac{dP_n}{dt} = A_n Q_n - B_n P_n, \quad (9.10)$$

where

$$\text{into level } n: \quad A_n = \sum_{m=1}^{n-1} P_m R_{mn}^U + \sum_{m=n+1}^{n \max} P_m R_{mn}^D + Z R_{cn}^D \quad (9.11)$$

$$\text{out of level } n: B_n = \sum_{m=1}^{n-1} Q_m R_{nm}^D + \sum_{m=n+1}^{n \text{ max}} Q_m R_{nm}^U + R_{nc}^U \quad (9.12)$$

The single superscript means both the radiative and collisional rates so defined are included. The coefficients A_n and B_n are functions of the populations. However, we shall assume that if our time interval is $\Delta t = t_1 - t_0$, then if A_n and B_n are evaluated at $t = t_1$, a reasonable approximation is given by the solution,

$$P_n^{(1)} = \frac{P_n^{(0)} + A_n \Delta t}{1 + \left(\frac{A_n}{2n^2} + B_n \right) \Delta t} \quad (9.13)$$

We do not give proof that Eq. (9.13) is a good approximation to Eq. (9.10). Furthermore, one must solve even this equation by successive calculations, where

$$P_n^{(1)} = \tilde{P}_n^{(1)} + \delta P_n \quad (9.14)$$

Here $\tilde{P}_n^{(1)}$ is our last approximation substituted into the calculation of the coefficients A_n , B_n , and δP_n represents the unknown correction. To solve for the δP_n 's, we use Newton's method. Let

$$F_n(P) = -P_n^{(1)} + \frac{P_n^{(0)} + A_n \Delta t}{1 + \left(\frac{A_n}{2n^2} + B_n \right) \Delta t} = 0. \quad (9.15)$$

Expanding $F_n(P)$ in a Taylor series and neglecting all but the first two terms, one obtains

$$F_n(\tilde{P}) = F_n(\tilde{P}) + \sum_m \left(\frac{\partial F_n}{\partial P_m} \right) \delta P_m = 0. \quad (9.16)$$

Write

$$A_n = P_n^{(0)} + A_n \Delta t, \quad (9.17)$$

$$g_n = 1 + \left(\frac{A_n}{2n^2} + B_n \right) \Delta t. \quad (9.18)$$

Then, after some cancellation of terms, one obtains

$$\frac{\partial F_n}{\partial P_m} = -\delta_{nm} + \frac{\Delta t}{g_n^2} \left(\mathcal{N}'_n \frac{\partial A_n}{\partial P_m} - \mathcal{N}_n \frac{\partial B_n}{\partial P_m} \right), \quad (9.19)$$

where

$$\delta_{nm} = 0 \text{ if } n \neq m \text{ and } = 1 \text{ if } n = m, \text{ and}$$

$$\mathcal{N}'_n = 1 - \frac{P_n^{(0)}}{2n^2} + B_n \Delta t. \quad (9.20)$$

Eq. (9.16) is a set of linearized equations in the unknowns δP_m , which only approximately satisfy our solution given by Eq. (9.13). However, it is expected that after a few iterations, Eq. (9.16) will converge. To solve these equations, one needs the derivatives $\partial A_n / \partial P_m$ and $\partial B_n / \partial P_m$. From Eqs. (9.11) and (9.12), one obtains

$$\frac{\partial A_n}{\partial P_m} = \frac{\partial A_n^*}{\partial P_m} + R_{nm}^U (m < n) + R_{nm}^D (m > n), \quad (9.21)$$

$$\frac{\partial B_n}{\partial P_m} = \frac{\partial B_n^*}{\partial P_m} - \frac{R_{nm}^D (m < n)}{2m^2} - \frac{R_{nm}^U (m > n)}{2m^2}. \quad (9.22)$$

Here, $R_{nm}^U (m < n)$ stands for R_{nm}^U if $m < n$ and zero, if $m > n$, etc. We evaluate the starred derivatives by differencing:

$$\frac{\partial A_n^*}{\partial P_m} \approx \frac{A_n - A_n^*}{\epsilon P_m}, \quad (9.23)$$

$$\frac{\partial B_n^*}{\partial P_m} \approx \frac{B_n - B_n^*}{\epsilon P_m}. \quad (9.24)$$

We evaluate A_n^* and B_n^* :

$$A_n^* = \sum_{m=1}^{n-1} P_m (R_{mn}^U)' + \sum_{m=n+1}^{n \max} P_m (R_{mn}^D)' + (Z_{cn}^D)', \quad (9.25)$$

$$B_n^* = \sum_{m=1}^{n-1} Q_m (R_{nm}^D)' + \sum_{m=n+1}^{n \max} Q_m (R_{nm}^U)' + (R_{nc}^U)'. \quad (9.26)$$

All unprimed quantities are evaluated by using populations $\tilde{P}_m$. Primed quantities use

$$\left. \begin{aligned} P_m' &= (1 - \varepsilon) P_m \quad (n=m) \\ &= P_m \quad (m \neq n). \end{aligned} \right\} \quad (9.27)$$

Here, ε is a small positive number. This method of evaluating the derivatives by using part 11 explicit differentiation is superior to an older method used in XSNQ where complete differencing was applied.

10. Non-LTE Radiative Transport

Having calculated a set of time-advanced non-LTE occupation numbers based on a specified radiation field, we now use these values to calculate emission and absorption in the transport and energy equations.

Using the results of Eqs. (2.15) and (2.18) for emission and absorption, we can write the equation of transfer as

$$\frac{1}{\rho c} \frac{\partial I_\nu}{\partial t} + \frac{1}{\rho} \vec{\omega} \cdot \vec{\nabla} I_\nu = e^{-u} H_\nu \left[B_0 (h\nu)^3 + I_\nu \right] - \kappa_\nu I_\nu, \quad (10.1)$$

where H_ν and κ_ν are the total mass emission and absorption coefficients at frequency ν . They are given as

$$e^{-u} H_{\nu} = e^{-u} H_{\nu}^c + \sum_t F(n, m) P_n Q_m \left(\frac{n}{m} \right)^{2'} \psi_{\nu}^{nm}, \quad (10.2)$$

$$\kappa_{\nu} = \kappa_{\nu}^c + \sum_t F(n, m) P_n Q_m \psi_{\nu}^{nm}, \quad (10.3)$$

where H_{ν}^c and κ_{ν}^c are given as

$$H_{\nu}^c = \left[D^{ff} g_{\nu}^{ff} + \frac{Z}{Z_0} \sum_{i=1}^{n \max} F(i, c) \frac{P_i^0}{Q_i^0} Q_i g_{i, \nu}^{bf} \right] (h\nu)^{-2}, \quad (10.4)$$

$$\kappa_{\nu}^c = \left[D^{ff} g_{\nu}^{ff} + \sum_{i=n+1}^{n \max} F(i, c) P_i g_{i, \nu}^{bf} \right] (h\nu)^{-3}, \quad (10.5)$$

and the sum $\sum_t$ indicates all lines contributing at frequency ν should be included. The ratio P_i^0/Q_i^0 is evaluated by using the non-LTE energy level E_n .

We wish to make the form of the non-LTE transfer equation as similar as possible to the LTE version. This is to minimize the problem of incorporating non-LTE effects into any existing LTE transport code. Therefore, we define

$$\bar{\kappa}_{\nu} = \kappa_{\nu} - e^{-u} H_{\nu}, \quad (10.6)$$

and

$$\bar{H}_{\nu} = e^{-u} H_{\nu} (e^u - 1), \quad (10.7)$$

and Eq. (10.1) becomes

$$\frac{1}{\rho c} \frac{\partial I_{\nu}}{\partial t} + \frac{1}{\rho} \vec{\omega} \cdot \vec{\nabla} I_{\nu} = \bar{H}_{\nu} B_{\nu} - \bar{\kappa}_{\nu} I_{\nu}. \quad (10.8)$$

The material temperature cannot, of course, be determined from standard specific heat tables, as in Eq. (2.23), because the level of ionization is not solely determined by the electron temperature. Instead, changes in the number of bound electrons and the binding energy of each level (the potential energy)

must be followed separately from the change in average Maxwellian velocities of the gas (thermal or kinetic energy). The sum of these changes would then equal the variation in material energy. Thus, by using (2.1b) and assuming a partially ionized perfect gas in units of ergs/g/sec,

$$\begin{aligned} \frac{\partial E_m}{\partial t} &= \frac{1.44 \times 10^{23}}{A} \frac{\partial[(\bar{Z} + 1) \bar{\theta}]}{\partial t} + \frac{9.6 \times 10^{22}}{A} \frac{\partial \left(\sum_{n=1}^{n \max} P_n E_n \right)}{\partial t} \\ &= \dot{S} - \int_0^\infty \left(4\pi \bar{H}_\nu B_\nu - \int_{4\pi} \bar{\kappa}_\nu I_\nu d\Omega \right) d(h\nu). \end{aligned} \quad (10.9)$$

In general, then, a transport code using XSNQ would send values of J_ν for a specified group structure to the subroutine after each transport time step. The quantities $\bar{\kappa}_\nu$ and $\bar{H}_\nu$ would then be calculated, averaged over the group structure, and used in Eqs. (10.8) and (10.9) to solve for the next time step's values of I_ν and material temperature.

11. Numerical Examples

An infinite medium model with no scattering, has been constructed to test the method described above.

In an infinite medium, Eq. (10.8) becomes

$$\frac{1}{\rho c} \frac{dI_\nu}{dt} = \bar{H}_\nu B_\nu - \bar{\kappa}_\nu I_\nu. \quad (11.1)$$

We integrate over solid angle and replace the intensity with the energy density,

$$e_\nu = \frac{1}{c} \int_{4\pi} I_\nu d\Omega, \quad (11.2)$$

and have

$$\frac{1}{\rho} \frac{de_\nu}{dt} = 4\pi \bar{H}_\nu B_\nu - c\bar{\kappa}_\nu e_\nu. \quad (11.3)$$

Applying an exponential time differencing, we can write

$$e_v^{n+1} = e_v^n e^{-c\rho\bar{\kappa}_v\Delta t} + 4\pi\rho\bar{H}_v e^{-c\rho\bar{\kappa}_v t^{n+1}} \int_{t^n}^{t^{n+1}} B_v e^{c\rho\bar{\kappa}_v t} dt, \quad (11.4)$$

where $\bar{\kappa}_v$ and $\bar{H}_v$ are assumed to be constant in the time interval. Let B_v vary linearly in this interval:

$$B_v = B_v^n + \frac{t - t^n}{\Delta t} (B_v^{n+1} - B_v^n). \quad (11.5)$$

Using this approximation for B_v in Eq. (11.4), we have

$$e_v^{n+1} = e_v^n e^{-x} + 4\pi\rho\bar{H}_v\Delta t (\psi_v B_v^n + \eta_v B_v^{n+1}), \quad (11.6)$$

where

$$\psi_v = \frac{1}{x} \left[\frac{1}{x} (1 - e^{-x}) - e^{-x} \right], \quad (11.7a)$$

$$\eta_v = \frac{1}{x} \left[1 - \frac{1}{x} (1 - e^{-x}) \right], \quad (11.7b)$$

with

$$x = c\rho\bar{\kappa}_v\Delta t.$$

These are the interpolaters discussed by Nelson.⁹ Photon energies for which the material is opaque ($\psi_v \approx 0$, $\eta \approx 1/x$) will be calculated by using completely forward differencing; transparent groups ($\psi_v = \eta_v = \frac{1}{2}$) will be calculated by using Crank-Nicolson differencing.

The differencing in photon energy will be done so that the variables carried are the integral of the energy density over a group:

$$e_{k-1/2} = \int_{h\nu_{k-1}}^{h\nu_k} e_v d(h\nu). \quad (11.8)$$

The terms $\bar{\kappa}_{k-1/2}$ and $\bar{H}_{k-1/2}$ are computed by taking the reciprocal mean of the function over each group. Twenty equally spaced values within a group are used to calculate the reciprocal mean.

We wish to couple the energy equation to the transfer equation and use the Newton's method to solve simultaneously for both the advanced material temperature and the new energy densities of all groups. For this, we have the matrix equation with $k_{\max} + 1$ roots:

$$\vec{G}_{k-1/2} \begin{pmatrix} \tau_{k-1/2}^{n+1} \\ \theta^{n+1} \end{pmatrix} \cong \vec{G}_{k-1/2} \begin{pmatrix} (i) \\ \tau_{k-1/2}^{n+1} \\ \theta^{n+1} \end{pmatrix} + \vec{M} \begin{pmatrix} (i) \\ \tau_{k-1/2}^{n+1} \\ \theta^{n+1} \end{pmatrix} \cdot \vec{\delta} \begin{pmatrix} (i) \\ \tau_{k-1/2}^{n+1} \\ \theta^{n+1} \end{pmatrix} = 0 \quad (11.9)$$

The first $k_{\max}$ terms of $\vec{G}_{k-1/2}$ are the $k_{\max}$ expressions of Eq. (11.6) for each energy group:

$$G_{k-1/2} = e_{k-1/2}^{n+1} - e_{k-1/2}^n e^{-c\rho\kappa_{k-1/2}\Delta t} - 4\pi\rho\tilde{H}_{k-1/2}^{n+1/2}\Delta t \left[\tilde{\psi}_{k-1/2}^{n+1/2} B_{k-1/2}^n + \tilde{H}_{k-1/2}^{n+1/2} B_{k-1/2}^{n+1} \right]. \quad (11.10)$$

The tilde quantities are obtained by offsetting in time the rate-equation calculation and the calculation of $e_{k-1/2}^{n+1}$:

where

$$\tilde{t}^{n-1/2} = \frac{1}{2} (t^n + t^{n-1}), \quad \tilde{t}^{n+1/2} = \frac{1}{2} (t^{n+1} + t^n), \text{ etc.}$$

The rate equations are advanced from time $\tilde{t}^{n-1/2}$ to $\tilde{t}^{n+1/2}$ with temperature and radiation energy values θ^n and $e_{k-1/2}^n$. The results are used to calculate $\tilde{\kappa}_{k-1/2}^{n+1/2}$ and $\tilde{H}_{k-1/2}^{n+1/2}$ which are in turn used to get θ^{n+1} and $e_{k-1/2}^{n+1}$. If necessary, the rate equations may require several time steps to advance the population successfully to $\tilde{t}^{n+1/2}$. Conversely, populations may be changing slowly enough so that the rate equation, Δt , exceeds $(\tilde{t}^{n+1/2} - \tilde{t}^{n-1/2})$ and XSNQ may be skipped.

The k max + 1 term of $\tilde{G}_{k-1/2}$ is the energy equation,

$$\frac{1.44 \times 10^{23}}{A} \frac{\partial[(\tilde{Z} + 1)\theta]}{\partial t} + \frac{9.6 \times 10^{22}}{A} \frac{\partial \left(\sum_{n=1}^{n \text{ max}} P_n E_n \right)}{\partial t} - \tilde{S} + \sum_{k=1}^{k \text{ max}} \left(4\pi \tilde{H}_{k-1/2} B_{k-1/2} - \tilde{\kappa}_{k-1/2} c e_{k-1/2} \right) = 0, \quad (11.11)$$

where $\tilde{B}_{k-1/2}$ is the integral of the Planck function over the interval $(h\nu)_{k-1}$ to $(h\nu)_{k-1}$.

For the test code, we have differenced the first two terms as

$$\frac{1.44 \times 10^{23}}{A} \left[\left(\frac{\tilde{Z}^{n+1/2}}{2} + 1 \right) \theta^{n+1} - \left(\frac{\tilde{Z}^{n-1/2}}{2} + 1 \right) \theta^n \right] \frac{1}{\Delta t},$$

and

$$\frac{9.6 \times 10^{22}}{A} \left[\sum_{n=1}^{n \text{ max}} \tilde{E}_n^n \left(\tilde{P}_n^{n-1/2} - \tilde{P}_n^{n+1/2} \right) \right] \frac{1}{\Delta t},$$

where

$$\tilde{E}_n^n = 1/2 \left(\tilde{E}_n^{n+1/2} + \tilde{E}_n^{n-1/2} \right).$$

Since the last term of Eq. (11.11), the total change in radiant energy, must be balanced by a corresponding change in the total material energy, we can insure exact energy conservation by replacing it with the direct expression for this cycle's change in radiation energy:

$$(\rho \Delta t)^{-1} \sum_k (e_{k-1/2}^{n+1} - e_{k-1/2}^n).$$

In a full transport calculation, of course, the change in $e_{k-1/2}$ is partly caused by the flux across boundaries. The energy equation must then account separately for this energy sink or source. For the infinite medium calculation, however, we can write $\vec{G}_{k \max+1}$ as

$$\begin{aligned} G_{k \max+1, \theta} = G_{\theta} = \theta^{n+1} - \frac{(\tilde{Z}^{n-1/2} + 1)}{(\tilde{Z}^{n+1/2} + 1)} \theta^n \\ + \left[\frac{1.44 \times 10^{23}}{A} (\tilde{Z}^{n+1/2} + 1) \right]^{-1} \left[\rho^{-1} \sum_k (e_{k-1/2}^{n+1} - e_{k-1/2}^n) \right. \\ \left. - \frac{9.6 \times 10^{22}}{A} \sum_n \tilde{E}_n^n (\tilde{P}_n^{n+1/2} - \tilde{P}_n^{n-1/2}) \right] \quad (11.12) \end{aligned}$$

For the first $k \max$ rows, all Jacobian elements are zero except the diagonal and the derivative with respect to θ^{n+1} ;

$$\frac{\partial G_{k-1/2}}{\partial e_{k-1/2}^{n+1}} = 1, \quad \frac{\partial G_{k-1/2}}{\partial \theta^{n+1}} = -4\pi \rho \tilde{H}_{k-1/2}^{n+1/2} \Delta t \eta_{k-1/2}^{n+1/2} \frac{\partial B_{k-1/2}^{n+1}}{\partial \theta}. \quad (11.13)$$

The last row of the Jacobian is

$$\frac{\partial G_{\theta}}{\partial e_{k-1/2}^{n+1}} = \left[\frac{1.44 \times 10^{23}}{A} (\tilde{Z}^{n+1/2} + 1) \right]^{-1} \quad (\text{for all } k); \quad \frac{\partial G_{\theta}}{\partial \theta^{n+1}} = 1. \quad (11.14)$$

The inversion of matrix equation (11.9) is easily obtained by the Crout method and yields

$$e_{k-1/2}^{(i+1)} = e_{k-1/2}^{(i)} + \delta e_{k-1/2}^{n+1}, \quad \theta^{(i+1)} = \theta^{n+1} + \delta \theta^{n+1}, \quad (11.15)$$

where

$$\delta e_{k-1/2}^{n+1} = -G_{k-1/2} - \left(\frac{\partial G_{k-1/2}}{\partial \theta^{n+1}} \right) \delta \theta^{n+1}, \quad (11.16)$$

and

$$\delta \theta^{n+1} = \frac{-G_\theta + \sum_k G_{k-1/2} \left(\frac{\partial G_\theta}{\partial e_{k-1/2}^{n+1}} \right)}{\frac{\partial G_\theta}{\partial \theta^{n+1}} - \sum_k \left(\frac{\partial G_{k-1/2}}{\partial \theta^{n+1}} \right) \left(\frac{\partial G_\theta}{\partial e_{k-1/2}^{n+1}} \right)}. \quad (11.17)$$

These equations are iterated until the change in the iterate is less than 10^{-6} of the function. Quadratic convergence holds well and seldom are more than four iterations required. However, occasional oscillations are encountered near the LTE limit in some runs because of the assumed time offset in the energy equation. A completely satisfactory differencing scheme for the interaction of energy and opacity calculations is yet to be found.

For the calculations reported on, the time steps in both the rate equation and transport sections were permitted to increase by at most a factor of two from cycle to cycle. A lower factor was used in the transport section if the material temperature changed by more than 3%. Also, if any occupation number changed in XSNQ by more than 5% since the last transport cycle, the rate-equation integration was halted and a transport cycle done. In both sections, the time step is reduced if more than four Newton iterations are needed. This never occurred in these runs.

The first graph (Fig. 11-1) shows the comparison of results from XSNQ and the MONTE code of W. Grasberger. The problem consisted of an infinite medium of gold at density 1 g/cc and a kinetic temperature of 1 keV. The radiation field was initially zero. The level populations were arbitrarily preset to

$$\begin{aligned} P_1 &= 2., \\ P_2 &= 8., \\ P_3 &= 17.999, \\ P_4 &= 31.99, \\ P_5 &= 8., \end{aligned}$$

and only these five levels were followed. These starting level populations are of course much higher than an equilibrium level population at 1 keV. They correspond to an equilibrium temperature of about 0.07 keV.

As Fig. 11-1 shows, the XSNQ and MONTE results are quite similar. MONTE used a combined Doppler and pressure-broadening profile called a Voigt profile while XSNQ used only a Doppler profile. The increase in level 5 population until about 3×10^{-14} seconds is due to a large value for the net collisional line transfer from level 4 to 5. This net rate becomes smaller as the gas cools. The kinetic temperature falls because energy is lost depopulating level 4 and because of the increase in free electrons. Also contributing to the rate reduction is the rise in line energy, caused again by the depopulation of level 4. The net radiative line (4-5) rate is always negative, however, and at later times it (along with the radiative and, most importantly, collisional continuous detachment processes) reverses the trend and a net depopulation of 5 levels takes place.

Figures 11-2 through 11-5 show non-LTE effects for a class of problems in which cold (0.1 keV) material at unit density is heated by an external source at a rate,

$$\dot{S} = 2.27 \times 10^{49} t^2 e^{-t^2 \times 10^{22}}.$$

This source typifies the heating of material by a laser light pulse. The source peaks at 10^{-11} seconds and is normalized to deposit 10^{16} erg/g. The problems used 63 groups to describe the radiation field. Each problem required about 250 transport cycles and 400 rate-equation cycles and used a total running time of about 1 min on the 7600.

Calculations for Z's of 26 and 92 are shown. The first graph of each pair gives the material (θ_n) and "radiation" (θ_R) temperatures as a function of time for the problem. The radiation temperature is calculated as shown on Fig. 11-1. The second graph gives the level populations versus time. Seven levels were followed in all the runs.

For $Z = 26$ at $\rho = 1$ g/cc, all but the first two levels are in or near equilibrium during the run. At times up to 10^{-11} seconds, line and collisional continuous detachment processes combine to depopulate the K shell (Fig. 11-3). As time proceeds, they are partly offset by net radiative K shell recombination caused by the high electron temperature and low radiation field above the

K shell binding energy. From 2×10^{-11} to about 10^{-10} sec, a near steady-state nonequilibrium condition is reached where the radiative recombination term is almost strong enough to prevent the line (both radiative and collisional) and collisional detachment processes from further depopulating the level. During this time, the nonequilibrium K shell population is at least a factor of 10 higher than the LTE result. As the gas cools through Bremsstrahlung and recombination to the higher levels, the net radiative recombination value for the K shell becomes less and the level population takes on its equilibrium value.

For uranium (see Fig. 11-5), a similar effect is observed in higher levels as well. At early times, upper levels usually have an additional net source of electrons from lower levels through collisional and radiative upward-line transitions. These rates can combine in complex ways. For example, in uranium the net radiative continuous process becomes negative early in the run (about 1.5×10^{-11} seconds) because of the rapid development of a radiation field above the L edge. This is offset, however, by a large radiative cascade from the next two levels.

In Figs. 11-6 through 11-9, we have plotted the same problems for Fe and U, but for a density of 10^{-3} g/cc. We see that the problems have not approached equilibrium during the 10^{-9} seconds shown.

The kinetic temperature assumption can be checked by calculating the Spitzer self-equilibration times for electrons:

$$t_{eq} \text{ (sec)} = 1.8 \times 10^{-14} \theta^{3/2} \frac{A}{Z \rho \ln \lambda}, \quad \lambda = 120 \theta \left(\frac{A}{Z\rho} \right)^{1/2}$$

This time is always less than 3×10^{-13} sec for the $\rho = 1$ g/cc runs discussed.

In Table 11-1, the ratio of non-LTE to LTE populations are listed for select times for the $\rho = 1$ g/cc problems. We see that there are large non-LTE effects during much of the gas cooling time for these problems.

Many more problems of a similar type at $\rho = 1$ g/cc are discussed in the classified report¹ where graphs of the emission and absorption coefficients at selected times are also given.

Fig. 11-1. Comparisons of results from XSNQ and MONTE codes.

Fig. 11-2. Material and radiation temperatures versus time for Fe at $\rho = 1$ g/cc.

Fig. 11-3. Level populations versus time for Fe at $\rho = 1$ g/cc.

Fig. 11-4. Material and radiation temperatures versus time for U at $\rho = 1 \text{ g/cc}$.

Fig. 11-5. Level populations versus time for U at $\rho = 1 \text{ g/cc}$.

Fig. 11-2. Material and radiation temperatures versus time for Fe at $\rho = 1$ g/cc.

Fig. 11-3. Level populations versus time for Fe at $\rho = 1$ g/cc.

Fig. 11-4. Material and radiation temperatures versus time for U at $\rho = 1$ g/cc.

Fig. 11-5. Level populations versus time for U at $\rho = 1$ g/cc.

Fig. 11-6. Material and radiation temperatures versus time for Fe at $\rho = 10^{-3}$ g/cc.

Fig. 11-7. Level populations versus time for Fe at $\rho = 10^{-3}$ g/cc.

Fig. 11-8. Material and radiation temperatures versus time for U at $\rho = 10^{-3}$ g/cc.

Fig. 11-9. Level populations versus time for U at $\rho = 10^{-3}$ g/cc.

Table 11-1: P_n/P_n^0 for Fe and U at $\rho = 1$ gm/cc.

		T_e	P_n/P_n^0				
t (seconds)		keV	n=1	n=2	n=3	n=5	n=7
Z = 26	10^{-12}	0.721	1.0	1.0	1.0	1.0	1.0
	10^{-11}	5.68	398	12	1.8	1.0	1.0
T_e peak	2×10^{-11}	11.5	329	8.8	1.5	1.0	1.0
	10^{-10}	5.87	34	2.3	1.1	1.0	1.0
	10^{-9}	3.10	3.3	1.06	1.0	1.0	1.0
Z = 92	10^{-12}	0.122	1.0	1.0	1.0	1.0	1.0
	10^{-11}	4.94	1.0	25	74	10	5
T_e peak	1.5×10^{-11}	8.27	1.0	452	117	12	6
	10^{-10}	3.25	1.0	1.6	2.3	1.5	1.3
	10^{-9}	3.06	1.0	1.2	1.5	1.2	1.1

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Appendix A Energy Levels

The isolation average atom energy levels are given either by the Dirac equation or Pauli's approximation to this equation. The Dirac formulation splits the shell of principal quantum number n into n nondegenerate sublevels. The mean of the lowest and highest energies of these sublevels is taken to represent the energy of the shell. Thus, the Dirac equation gives

$$\bar{E}_{n,k}^c = -511 \left\{ \left[1 + \frac{\alpha_n^2}{n - k + \sqrt{k^2 - \alpha_n^2}} \right]^{1/2} - 1 \right\} \quad k = 1, \dots, n$$

in keV. Here α is the fine structure constant $1/137.04$.

For low Z , the Paul approximation to $\bar{E}_{n,k}^c$ is adequate and is given by

$$\bar{E}_{n,k}^c = 0.0136 \frac{Z^2}{n^2} \left[1 + \frac{(\alpha_n^2)^2}{n} \left(\frac{1}{k} - \frac{3}{4n} \right) \right] \quad k = 1, \dots, n.$$

which is also in keV.

The lowering of the continuum is given by a prescription from Stewart and Pyatt¹⁰:

$$\Delta E = \left\{ \frac{[3(\bar{Z} + 1)K + 1]^{2/3} - 1}{2(\bar{Z} + 1)} \right\},$$

where θ and ΔE are in keV, and

$$K = 0.004767 \frac{(\bar{Z} + 1)}{\theta} \sqrt{\frac{\bar{Z}}{A} (\bar{Z} + 1) \rho}.$$

Appendix B

Oscillator Strengths and Screening Constants

The absorption oscillator strengths, or f -values, used in the average atom model for $n \rightarrow m$ transitions ($m > n$) are hydrogenic. For $n < 5$ or $m \leq 5$, the approximation

$$f(n,m) = \frac{1.960}{n^5 m^3} \left(\frac{1}{n^2} - \frac{1}{m^2} \right)^{-3}$$

is replaced by the following table for $f(n,m)$:

$f(1,2)$	= 0.4161
$f(1,3)$	= 0.0792
$f(1,4)$	= 0.0290
$f(1,5)$	= 0.0139
$f(2,3)$	= 0.6370
$f(2,4)$	= 0.1190
$f(2,5)$	= 0.0443
$f(3,4)$	= 0.8408
$f(3,5)$	= 0.1499
$f(4,5)$	= 1.037

The screening constants $\sigma_{n,m}$ used in determining the effective charge Z_n^* [see Eq. (3.5)] are given by the following table of H. Mayer¹¹:

m/n	1	2	3	4	5	6	7	8	9	10
1	0.625	0.938	0.981	0.987	0.994	0.997	0.999	1.00	1.00	1.00
2	.235	.690	.893	.940	.970	.984	.990	0.993	0.995	1.00
3	.109	.397	.702	.850	.920	.955	.970	.980	.990	1.00
4	.0617	.235	.478	.705	.830	.900	.950	.970	.980	0.990
5	.0398	.155	.331	.531	.720	.830	.900	.950	.970	.980
6	.0277	.109	.239	.400	.480	.735	.830	.900	.950	.970
7	.0204	.0808	.178	.31	.459	.610	.745	.830	.900	.950
8	.0156	.0625	.138	.243	.371	.506	.635	.750	.830	.900
9	.0123	.0494	.111	.194	.299	.431	.544	.656	.700	.830
10	0.010	0.040	0.090	0.158	0.245	0.353	0.460	0.576	0.670	0.765

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