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The Calculation of Ionization in Hydrodynamics Codes

I: Theory

los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87544

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ABSTRACT

A formalism is developed for calculating ionization in laser driven hydrodynamics codes. Starting from equations for collisional ionization and radiative recombination, approximations are made to allow their easier solution. Steady-state solutions are assumed to be of most importance to the extent that transient solutions to the rate equations are ignored. Free-bound radiation is also treated in an hydrogenic approximation.

I. INTRODUCTION

One of the objectives of this research was to produce a hydrodynamics code which would follow the motion of a pellet in the field of an intense laser beam. Since energies on the order of joules, instead of kilojerks, are available in prepulses, ionization may not always be assumed to be instantaneous and complete. This is especially true if some of the heavier elements are to be treated. In this case the ionization energy may form an important part of the equation of state. Additionally, radiative processes depend on knowledge of the density of free electrons and the distribution of ionic states.

The goals we describe here are quite modest. No attempt is made to solve the rate equations in their time-dependent form. A steady-state model is assumed. Relaxation times are found to be on the order of tenths of a nanosecond for ionization-recombination equilibrium. This may be too slow for some processes to be described by a steady-state model but it was felt that solving the full set of rate equations every cycle, in every cell, was too costly. It was also felt that obtaining effective charge from the Thomas-Fermi-Dirac[1] (TFD) model would not be an improvement. (For example: Carbon has an experimental electron binding energy of 1 keV. Thomas-Fermi-Dirac predicts 1.5 keV. Furthermore, the statistical processes assumed by TFD are not valid under all conditions of density and temperature.)

Another approximation is that we ignore the radiation due to bound-bound transitions. While this is not a bad assumption for Carbon, it is a very bad assumption for Aluminum at standard density and 1 keV temperature. The model, however, is a great simplification which easily lends itself to future additions.

II. THE RATE EQUATIONS

Suppose we consider the ions of an element having Z electrons in the neutral state. Let the total number density, in cm^{-3}, of this element be n_i. There are now Z + 1 ions corresponding to having stripped the original atom 0, 1, . . . , Z times. If f_j is the fraction of atoms ionized j times then we may write the rate equations at a point in the material

$$\frac{\partial f_0}{\partial t} = n_e[-S_0 f_0 + (\alpha_0 + \beta_0 n_e) f_1], \tag{1a}$$

$$\frac{\partial f_1}{\partial t} = n_e[S_0 f_0 - (\alpha_0 + \beta_0 n_e + S_1) f_1 + (\alpha_1 + \beta_1 n_e) f_2], \tag{1b}$$

$$\vdots$$

$$\frac{\partial f_j}{\partial t} = n_e[S_{j-1} f_{j-1} - (\alpha_{j-1} + \beta_{j-1} n_e + S_j) f_j + (\alpha_j + \beta_j n_e) f_{j+1}], \tag{1c}$$

$$\vdots$$

$$\frac{\partial f_z}{\partial t} = n_e[S_{z-1} f_{z-1} - (\alpha_{z-1} + \beta_{z-1} n_e) f_z]. \tag{1d}$$

In Eqs. (1a-1d) we have the following definitions:

α_j is the radiative (2-body) recombination coefficient from state j + 1 to state j,

β_j is the three-body recombination coeffi- from state j + 1 to state j,

S_j is the collisional ionization coefficient from state j to j + 1,

n_e is the number density of electrons.

In Eqs. (1) it is assumed that only single-electron processes are taking place. It should also be noted that we have unnaturally split the recombination rate into a 2-body and a 3-body part, whereas recombination should be considered as a "collisional-radiative" process.[2]

Although we are working on models in which Eqs. (1) are solved as a function of time, our present working model assumes that our system is always in a quasi-steady state. That is, all the left-hand sides of Eqs. (1) are assumed to be negligible. The equations may then be solved for the steady state, obtaining

$$f_j/f_{j+1} = (\alpha_j + n_e\beta_j)/S_j \quad . \tag{2}$$

This determines the f_j's when one remembers that

$$\sum_{j=0}^{z} f_j = 1 \quad . \tag{3}$$

The coefficients α_j, β_j, and S_j are functions of temperature, in general. Although other methods of calculating and approximating ionization and recombination rates exist we have chosen to use McWhirter's analytic fits for the 2-body processes.[2] These are

$$S_j = 7.68 \times 10^{-19} \, \frac{\zeta_j T_e^{1/4} e^{-X_j/T_e}}{X_j^{1/4}} \, \text{cm}^3/\text{shake}, \tag{4}$$

$$\alpha_j = 6.02 \times 10^{-21} \, X_j/T_e^{1/2} \text{cm}^3/\text{shake}. \tag{5}$$

In Eqs. (4) and (5);

ζ_j is the number of electrons in the outer shell of the j-times ionized element (A_j)

X_j is the ground-state binding energy of A_j in keV

T_e is the electron temperature in keV.

We shall use the centimeter-gram-shake (10^{-8} sec) system throughout this work.

To find the three-body coefficient β_j we shall make use of detail balance. Referring back to Eq. (2), note that if n_e were very large, local thermodynamic equilibrium would obtain.[3] In that case the Saha equation[4] is valid:

$$f_j/f_{j+1} = 2\left(\frac{2\pi m T_e}{n^2}\right)^{3/2} \frac{1}{n_e} \, \frac{u_j}{u_{j+1}} \, e^{X_j/T_e} \tag{6}$$

where h is Planck's constant,

u_j is the partition function for state j.

$$u_j = \sum_i g_{ij} e^{X_{ij}/T_e} \quad . \tag{7}$$

As approximations we ignore all but the first term in u_j as well as pressure and degeneracy effects. In Eq. (7), g_{ij} and X_{ij} are the degeneracy and binding energy of the <u>ith</u> bound state of ionic state j. Thus, in the limit of high densities using Eqs. (2) and (6)

$$S_j = 1.91 \times 10^{26} \, \frac{g_{ij}}{g_{ij+1}} \, T_e^{3/2} \, \beta_j \, e^{X_j/T_e}, \tag{8}$$

or

$$\beta_j = 4.01 \times 10^{-45} \, \frac{\zeta_j}{X_j^{1/4} T_e^{5/4}} \, \frac{g_{ij+1}}{g_{ij}} \quad . \tag{9}$$

At our present state of development, Eqs. (4), (5), and (9) are regarded as only approximate rates, to be improved on later.

III. SOLVING THE STEADY-STATE EQUATIONS

We now analyze the system implied by Eqs. (2) and (3). Let's rewrite Eq. (2) as

$$f_{j+1}/f_j = A_j + \bar{Z}B_j, \tag{10}$$

where

$$A_j = \alpha_j/S_j, \tag{11}$$

$$B_j = n_i\beta_j/S_j, \tag{12}$$

$$\bar{Z} = n_e/n_i. \tag{13}$$

In the above equations, n_i is the total ionic density. Since $\bar{Z}$ may also be expressed as

$$\bar{Z} = \sum j f_j, \tag{14}$$

the equations represented by Eq. (10) are not linear.

If we were to solve the system (10) and (2) we would obtain

$$\bar{Z} = \bar{Z}_0, \tag{15}$$

$$f_j/f_{j+1} = (f_j/f_{j+1})_o. \tag{16}$$

For any arbitrary $\overline{Z}$, now,

$$f_j/f_{j+1} = (f_j/f_{j+1})_o + (\overline{Z}-\overline{Z}_o)B_j. \tag{17}$$

We shall assume that none of the ratios $(f_{j+1}/f_j)_o$ are equal to 1.0. In that case, there exists a largest f, say f_k. It follows then that

$$r_j = (f_j/f_{j+1}) = \begin{cases} >1 \text{ if } j < k \\ <1 \text{ if } j \geq k \end{cases} \tag{18}$$

because the values of X_j monotically increase as j increases. Note also that B_j is positive. It follows then that

$$f_j/f_{j+1} \leq (f_j/f_{j+1})_o \text{ if } \overline{Z} \leq \overline{Z}_o, \tag{19a}$$

$$f_j/f_{j+1} \geq (f_j/f_{j+1})_o \text{ if } \overline{Z} \geq \overline{Z}_o. \tag{19b}$$

We now assume that no more than three values of j contribute to the sums in Eqs. (3) and (14), i.e., f_{j-1}, f_j, f_{j+1} are the only important f's. Using Eqs. (18) and (19), $\overline{Z}_o$ may be calculated very quickly.

To see this, let

$$q_j(\overline{Z}) = f_j/f_{j+1} \tag{20}$$

for any value of $\overline{Z}$. Now calculate $q_j(j) + q_j(j+1)$. If this quantity is greater (less) than two then r_j is greater (less) than two. This follows from Eqs. (17) and (18). This is very important because it says that if

$$q_j(\overline{Z}) \lesseqgtr 1 \text{ for } j \leq \overline{Z} \leq j+1 \tag{21a}$$

then

$$r_j \lesseqgtr 1. \tag{21b}$$

Several cases now arise near the value of j for the maximum f_j.

Case I:

$$q_j(\overline{Z}) < 1,\ j \leq Z \leq 1 \tag{22a}$$

$$q_{j+1}(\overline{Z}) > 1,\ j+1 \leq \overline{Z} \leq j+2 \tag{22b}$$

Case II:

$$q_j(\overline{Z}) \leq 1 \quad j \leq Z \leq j+\varepsilon, \tag{23a}$$

$$q_j(\overline{Z}) > 1 \quad j+\varepsilon < Z < j+1 \tag{23b}$$

$$q_{j+1}(\overline{Z}) > 1 \tag{23c}$$

Case III:

$$q_j(\overline{Z}) < 1 \quad j \leq \overline{Z} \leq j+1 \tag{24a}$$

$$q_{j+1}(\overline{Z}) \leq 1 \quad j+1 \leq \overline{Z} \leq j+1+y \tag{24b}$$

$$q_{j+1}(\overline{Z}) > 1 \quad j+1+y < \overline{Z} \leq j+2. \tag{24c}$$

In Case I it is clear that f_{j+1} is the largest f. Cases II and III are not so clear cut. Either f_j or f_{j+1} may be dominant in Case II. To determine which f is the largest we calculate $q_j(j + 1/2)$. If $q_j(j + 1/2)$ is less than 1, f_j is taken to be dominant. Otherwise f_{j+1} is dominant. Similar reasoning applies to Case III, where $q_{j+1}(j + 3/2)$ would be used to decide between f_{j+1} and f_{j+2}.

Now given a dominant f_k we will assume that only f_{k-1}, f_k, and f_{k+1} will enter into the calculations. Including only three states is an approximation, but a good one in practice. When done as above one always includes the largest two states in the calculation. An algebraic equation may now be written for $\overline{Z}$. From the relations

$$\overline{Z} = k + f_{k+1} - f_{k-1} \tag{25a}$$

$$1 = f_{k-1} + f_k + f_{k+1} \tag{25b}$$

$$f_{k-1} = (A_k + B_k\overline{Z})f_k \tag{25c}$$

$$f_k = (A_{k+1} + B_{k+1}\overline{Z})f_{k+1} \tag{25d}$$

$$f_{k-1} = (A_k + B_k\overline{Z})(A_{k+1} + B_{k+1}\overline{Z})f_{k+1} \tag{25e}$$

we get

$$f_{k+1} = \left[1 + (A_{k+1} + B_{k+1}\overline{Z}) + (A_k + B_k\overline{Z})(A_{k+1} + B_{k+1}\overline{Z})\right]^{-1} \tag{26}$$

by combining Eqs. (25b), (25c), and (25d). From (25a) and (25e) we get

$$\overline{Z} = k + \left[1 - (A_k + B_k\overline{Z})(A_{k+1} + B_{k+1}\overline{Z})\right]f_{k+1}. \tag{27}$$

Combining Eqs. (26) and (27) we get

$$\overline{Z} = k - 1 + [2 + (A_{k+1} + B_{k+1}\overline{Z})][1 + (A_{k+1} + B_{k+1}\overline{Z}) + (A_k + B_k\overline{Z})(A_{k+1} + B_{k+1}\overline{Z})]^{-1} \tag{28}$$

Although Eq. (28) is a cubic for $\overline{Z}$ we solve it presently by iterations. Old values of $\overline{Z}$ are used on the right side and the new of $\overline{Z}$ is then the left side.

As for all iterative procedures, an initial value for $\overline{Z}$ is needed. We obtain this with the use of Eq. (25e), using $\overline{Z} = k$. If $f_{k-1} < f_k$ then $\overline{Z} = k - 1/2$. Otherwise $\overline{Z} = k + 1/2$.

A more sophisticated model with time dependence based on Eqs. (1) is also under consideration at present. It, too, neglects all but three f's. In this model quickly arising and quickly dying states may be followed. No more will be said about this model except that the time constants for collisionally ionizing atoms near equilibrium is found to be about .1 ns (in Carbon, found from the steady-state runs[5]). For processes taking less than .1 ns, ionization will be incomplete and rate equations should be used.

IV. THE ENERGY EQUATIONS

Assuming that, at any time, the f_j's in Eqs. (1) are known it is now required to use this information in the energy balance equations. The processes of importance are assumed to be collisional ionization, collisional recombination, and radiative recombination. Referring back to Eq. (1c) we may write

$$\frac{\partial E_j}{\partial t} = \left\{\left[-S_j f_j + (\alpha_j + \beta_j n_e) f_{j+1}\right] X_j \right\} - n_i \alpha_j f_{j+1} (\overline{E}_{j+1} + X_j - \overline{X}) \qquad (29)$$

In Eq. (29) $\frac{\partial E_j}{\partial t}$ is the time rate of change of the energy of the free electron gas with respect to ionic state j. $\overline{E}_{j+1,j}$ is the average energy of each photon emitted in recombining with ionic state j + 1 to form state j. $\overline{X}$ may be interpreted as an average binding energy for recombination.

The first term in curly brackets represents the negative of the rate of change of ionic energy due to state j. The second term is the rate of energy lost by the free electrons due to recombinations to state j. Equation (29) may be partially integrated when one notices that Eqs. (1) can be rewritten in the form

$$\dot{f}_o = \left[-S_o f_o + (\alpha_o + \beta_o n_e) f_1\right] n_e \qquad (30a)$$

$$\dot{f}_1 = \left[-S_1 f_1 + (\alpha_1 + \beta_1 f_2) n_e\right] - f_o \qquad (30b)$$

$$\vdots$$

$$\dot{f}_j = \left[-S_j f_j + (\alpha_j + \beta_j n_e) f_{j+1}\right] n_e - {}_{i=0}^{j-1} f_i \qquad (30c)$$

$$\vdots$$

$$\dot{f}_z = -\sum_{i=0}^{z-1} f_i, \qquad (30d)$$

where the dots mean differentiation with respect to t.

Letting

$$\overline{F}_{j+1,j} = \overline{E}_{j+1,j} + X_j - \overline{X}, \qquad (31a)$$

$$E_a = \sum_{i=0}^{z} E_i \qquad (31b)$$

we obtain

$$E_a = n_{ion} \sum_{j=0}^{z-1} f_j \sum_{i-j}^{z-1} X_i - n_e \sum_{j=0}^{z-1} \int \alpha_j f_{j+1} \overline{F}_{j+1,j} \, dt + q, \qquad (32)$$

where q is a constant of integration. Despite its formidable appearance Eq. (32) is easily understood on an intuitive basis when one realizes that f_o represents a state whose total binding energy is $\sum_{j=0}^{z-1} X_j$. The integral term says that state i + 1 is continually recombining to state i. When the electron temperature, T_e, is zero the classical assumption is made that the number density of electrons n_e is practically zero. Thus $f_o = 1$ and

$$E_a = n_{ion} \sum_{j=0}^{z-1} X_j + q \qquad (33)$$

Since the value of q can be arbitrary without affecting any physical results we let

$$q = -n_{ion} \sum_{j=0}^{z-1} X_j \qquad (34)$$

The total energy of the free electrons E_e, then, is equal to a sum of three terms:

$$E_e = 3/2 n_e k T_e + n_{ion} \sum_{j=0}^{z} f_j \sum_{i=j}^{z-1} X_i - n_e \sum_{j=0}^{z-1} \int \overline{F}_{j+1,j} d_j f_{j+1} dt - n_{ion} \sum_{j=0}^{z-1} X_j \qquad (35)$$

We can interpret the terms in order as kinetic energy, potential energy, and radiated energy.

We now need an approximation to the quanity $E_{j+1,j}$. Stratton[6] gives a formula for the energy spectrum of the photons emitted by electrons recombining into the nth shell of a hydrogenlike ion corresponding to our ionic state j =

$$\frac{dE_{bf}^{jn}}{d\nu} = c n_e n_i f_{j+1} \left(\frac{.0136}{T_e}\right)^{3/2} \left(\frac{X_{j,n}}{.0136}\right)^2 \frac{\delta_n}{n} g_{bf} \exp (X_{j,n} - h\nu)/T_e \qquad (36)$$

where δ_n is the number of states available in the nth shell, $c = 1.7 \times 10^{-40}$ erg cm^3, $X_{j,n}$ is the binding energy of the nth shell in the jth ion. Integrating Eq. (38) overall ν we finally get

$$E_{bf}^{jn} = 3.5 \times 10^{-46} X^2_{j,n} n_e n_i \frac{\delta_n}{n} f_{j+1} (T_e)^{-1/2} \frac{\text{jerks}}{\text{cm}^3\text{shake}}. \tag{37}$$

Thus recombination energy is being produced at the rate $\sum_{n=n_o}^{\infty} E_{bf}^{jn}$. If the average energy of these photons is $\overline{E}_{j+1,j}$ then

$$\sum_{n=n_o}^{\infty} E_{bf} = \alpha_j f_{j+1} n_e n_i (\overline{E}_{j+1,j} + X_j - \overline{X}) \tag{38}$$

Using Eq. (5) for α_i we get

$$\overline{E}_{j+1,j} = .58 \times 10^{-25} \sum_{n=n_o}^{\infty} (X_{jn}^2/X_j)\frac{\delta_n}{n}. \tag{39}$$

To be more useful we must make some assumptions and approximations on the right-hand-side of Eq. (40).

First we assume that all levels above the ground state, i.e. $n > n_o$ have binding energies

$$X_{j,n} = .0136 j^2/n^2 \quad n > n_o \tag{40}$$

$$X_{j,n} = X_j, \; n = n_o \tag{41}$$

Next, let all the ions be in their respective ground states. Thus

$$\zeta_n = 2n^2, \; n > n_o, \tag{42}$$

$$\zeta_n = 2n^2 - \zeta_{j+1}, \; n = n_o, \tag{43}$$

where ζ_{j+1} first appeared in Eq. (4). Using Eqs. (40) - (44) we get

$$\overline{E}_{j+1,j} = .58 \times 10^{-25} \left\{ X_j \left(2n_o - \frac{\zeta_{j+1}}{n_o} \right) + \frac{(.0136 j^2)^2}{X_j} \sum_{n=n_o+1}^{\infty} \frac{1}{n^3} \right\} \tag{44a}$$

$$= .58 \times 10^{-25} \left\{ X_j \left(2n_o - \frac{\zeta_{j+1}}{n_o} \right) 3.7 \times 10^{-4} \frac{j^4}{X_j} \left(1.202 - \sum_{n=1}^{n_o} \frac{1}{n^3} \right) \right\} \tag{44b}$$

In Eq. (44b) we have used the relation

$$\sum_{n=1}^{\infty} \frac{1}{n^3} = 1.202059\ldots \tag{45}$$

Note that the entire right-hand-side of Eq. (45) can be tabulated once and for all. It is not a function of temperature in this approximation. If the entire spectrum were required then Eq. (38) would have to be used.

Many approximations have been made up to this point but the theory is not complete. The energy equation, Eq. (34), will point this out. Suppose that

$$\overline{F}_{j+1,j} = \gamma_j X_k, \; \gamma_j > 0 \tag{46}$$

Equation (29) can be written

$$\frac{\partial E_j}{\partial t} = \left\{ -S_j f_j + \alpha_j (1-\gamma_j) + \beta_j n_e f_{j+1} \right\} X_j n_i. \tag{47}$$

The term $\alpha_j(1-\gamma_j)n_j X_j$ represents the rate of change of the energy of the free electrons due to radiative recombination. The only process approximately taken into account is the first photon emitted on recombination. In particular the cascade down to the ground state from the state n is implicitly assumed to be collisional. We will deal with this point in more detail in a sequel. It will be shown there that $\overline{E}_{j+1,j}$ does have a temperature dependence if the cascade energy is included. It should be noted that $\overline{X}$ is temperature dependent. Also, Eq. (40) can't be right for all ions since it does not give the right answer for recombination energy to the ground state of hydrogen. (It gives $\overline{E}_{j+1,j} = 9.9$ev.) A rough theory where $\overline{X}_j = X_j$ would probably give reasonable results because it implies that all recombinations go directly into the ground state.

References

1. Barnes, J. F., Quantum- and Correlation-Corrected Thomas-Fermi-Dirac Equation, Phys. Rev. 140A, A721, 1965, and references therein. The above author is confident that newer FTD techniques will at least partially overcome the problem of overbinding in the innermost atomic shells.
2. Bates, D. R., A. E. Kingston and R. W. P. McWhirter, Proc. Roy. Soc. A257, 297 (1962).
3. McWhirter, R. W. P., "Spectral Intensities," in Plasma Diagnostic Techniques, Ed. by R. H. Huddlestone and S. Leonard, Academic Press, New York, 1965.
4. Bond, J. W., K. M. Watson and J. A. Welch, Jr., Atomic Gas Dynamics, Addison Wesley, New York, 1965.

5. Rockwood, S., unpublished results.
6. Stratton, T. F., "X-Ray Spectroscopy," in Plasma Diagnostic Techniques, Ed. by R. H. Huddlestone and S. Leonard, Academic Press, New York, 1965.