Daniel Bouche, Alain Decoster, Laurent Desvillettes & Valeria Ricci
A Coherent Derivation of an Average Ion Model Including the Evolution of Correlations Between Different Shells

A Coherent Derivation of an Average Ion Model Including the Evolution of Correlations Between Different Shells

Daniel Bouche [*]
Alain Decoster [**]
Laurent Desvillettes [***]
Valeria Ricci [†]

[*] ENS Cachan, CMLA, CNRS 61 Av. du President Wilson 94235 Cachan Cedex and
CEA/DIF Bruyères-Le-Châtel, 91297 Arpajon Cedex, FRANCE
E-mail address: daniel.bouche@cmla.ens-cachan.fr
[**] ENS Cachan, CMLA, CNRS 61 Av. du President Wilson 94235 Cachan Cedex and
CEA/DIF Bruyères-Le-Châtel, 91297 Arpajon Cedex, FRANCE
E-mail address: alain.decoster@cmla.ens-cachan.fr
[***] ENS Cachan, CMLA, CNRS 61 Av. du President Wilson 94235 Cachan Cedex, FRANCE
E-mail address: desville@cmla.ens-cachan.fr
[†] Dipartimento di Matematica e Informatica, Università degli Studi di Palermo Via Archirafi
34, I90123 Palermo, ITALY
E-mail address: valeria.ricci@unipa.it.

Abstract

We propose in this short note a method enabling to write in a systematic way a set of refined equations for average ion models in which correlations between populations are taken into account, starting from a microscopic model for the evolution of the electronic configuration probabilities. Numerical simulations illustrating the improvements with respect to standard average ion models are presented at the end of the paper.

1. Introduction

In the last years, the extension of average-ion models to the modeling of plasmas in off-equilibrium conditions has been considered (cf. [3, 2]). Those models give a simplified macroscopic statistical description of a large set of ions, by calculating the populations of N "levels". This is an alternative to the more complex detailed description based on evolution equations for the probabilities of the many states through microscopic processes in the plasma. If more detail about the distribution of states (for example the $N(N+1)/2$ correlations between level populations) is needed in an average-ion model, this will be calculated afterwards (cf. [2]). In a previous paper (cf. [1]), it was provided a study about the conditions under which the average ion model can rigorously be derived as a limit of the detailed models.

In this paper, we provide a model which is more complicated than the average ion model (it basically requires the resolution of $N(N+3)/2$ ordinary differential equations (ODEs) when the average ion model requires N ODEs) but still much simpler than the microscopic models (which may require the resolution of a number of ODEs of the order of $2^N (N!)^2$). This model is derived from the microscopic detailed description of the plasma by using a systematic procedure of moment closure.

We recall the setting and notations used in [1] and [2]: we consider a set of ions which belong to the same species of atoms in a bath of particles (electrons) at Maxwellian equilibrium at a given temperature T. We denote by Z the charge of the nucleus of the considered atomic species.

We consider the set of bound electrons in each ion and we collect the electrons in subsets which we shall call levels.

Levels are defined by grouping electrons with about the same energy, and usually the grouping is built in such a way that the number N of levels for bound electrons is finite: in our simulations, the levels will be indexed according to the principal quantum number n (up to the number N which is a priori fixed), so that they will correspond to the atomic shells, and we shall use indifferently both words (shells or levels) to denote the same object.

A configuration $\vec{k} = (k_1, \ldots, k_N)$ of an ion is specified by the occupation number (i.e. the integer number of electrons) $k_i \in \mathbb{N}$ of each level i in the ionic configuration.

Each bound electron shell i can accommodate a finite number of electrons D_i ($D_i = 2\,i^2$ in the numerical examples that we present). We shall denote as $\mathcal{C}$ the set of all allowed ($0 \leq k_i \leq D_i$) ionic configurations $\vec{k}$.

At the microscopic level, the set of ions is described by the probability to find an ion in the configuration $\vec{k}$ at time t, which we denote by $g_{\vec{k}}(t)$. We have of course $\sum_{\vec{k} \in \mathcal{C}} g_{\vec{k}}(t) = 1$, and the evolution equation for $g_{\vec{k}}(t)$ is

$$\frac{d}{dt} g_{\vec{k}}(t) = \sum_{\vec{k}' \in \mathcal{C}} B_{\vec{k}' \to \vec{k}}\, g_{\vec{k}'}(t) - \sum_{\vec{k}' \in \mathcal{C}} B_{\vec{k} \to \vec{k}'}\, g_{\vec{k}}(t) \, , \qquad (1.1)$$

where $B_{\vec{k}' \to \vec{k}}$ is the rate of the transition from configuration $\vec{k}'$ to configuration $\vec{k}$. Here and later, we assume that only allowed configurations are included in the sums.

The average populations of the shells $\vec{f}(t) = (f_1(t), \ldots, f_N(t))$ are defined for $h = 1, \ldots, N$ by

$$f_h(t) = \sum_{\vec{k} \in \mathcal{C}} k_h\, g_{\vec{k}}(t) \, , \qquad (1.2)$$

where $g_{\vec{k}}$ satisfies eq.(1.1).

The number of significant configurations in the plasma is often so large that a detailed model (1.1) is unpractical. The description of the system can be simplified thanks to the use of a macroscopic model in which the set of ions in different electronic configurations is replaced by a set of ions all in the same electronic configuration (*average ion*). The electronic configuration of each (and all) ion in this last system is such that the occupation number of each shell of the average ion is the average (1.2) of the occupation numbers of the corresponding shell of the ions in the original system.

At this macroscopic level, the set of ions is described by the collection of populations of levels for the average ion, which we shall denote by $\{f_h\}_{h \geq 1}$ or $\vec{f} = (f_1, \ldots, f_N)$, where $f_h \in [0, D_h]$ denotes the (non necessarily integer) population of the h-th level of the average ion.

In the average ion description, $\vec{f}$ satisfies the following evolution equation (for $n = 1, \ldots, N$):

$$\frac{d}{dt} f_n = \sum_{m \neq n} (A_{m \to n} - B_{n \to m}) + A_{c \to n} - B_{n \to c} \, , \qquad (1.3)$$

where we denote by $A_{m \to n}$ and $A_{c \to n}$ the transition rates to the level n from other levels m and the continuum c, and by $B_{n \to m}$ and $B_{n \to c}$ the transition rates from level n to other levels or the continuum. In general, the rates A and B are functions of the populations of the levels.

In [1], an equation of the form (1.3) was obtained as a consequence (in a certain asymptotics) of an evolution equation for the probability $g_{\vec{k}}$ of the form (1.1). It was also described there the situations in which one can expect the average ion eq.(1.3) to reasonably mimic the microscopic eq.(1.1).

Our goal in this paper is to introduce (following a coherent closure procedure) an *intermediary model* between (1.1) and (1.3), which is hopefully closer to the microscopic eq.(1.1) than the average ion model, but is still tractable (that is, not too many ODEs have to be solved). In this

model, the state of the system will be described not only by average populations (1.2), but also by second order moments $\chi_{hl} = \sum_{\vec{k} \in \mathcal{C}} k_h k_l \; g_{\vec{k}}$, or correlations

$$f_{hl} = \sum_{\vec{k} \in \mathcal{C}} (k_h - f_h)(k_l - f_l) \; g_{\vec{k}} = \chi_{hl} - f_h f_l \;. \tag{1.4}$$

In section 2, we describe in detail the microscopic model that we shall study, and we write a non closed equation for the moments of order 1 and 2 of the probabilities $g_{\vec{k}}$ of the shells. In the next section, we introduce the closure assumptions and deduce our intermediary model. Numerical illustrations are finally provided in section 4.

2. **The microscopic model and the equations for its moments**

2.1. **Description of the microscopic model**

We shall use in the sequel the following notation for sums of vectors:

$$\begin{cases} \vec{k} + (h,l)_{ij} = (k_1, \ldots, k_i + h, \ldots, k_j + l, \ldots, k_N) & 1 \leq i < j \leq N \;, \\[2mm] \vec{k} + (h,l)_{ij} = (k_1, \ldots, k_j + l, \ldots, k_i + h, \ldots, k_N) & 1 \leq j < i \leq N \;, \\[2mm] \vec{k} + (h)_i = (k_1, \ldots, k_i + h, \ldots, k_N) & 1 \leq i \leq N \;. \end{cases}$$

In order to keep things as simple as possible, we consider the evolution of the level populations in ions where the only transition processes between levels are one-electron transitions (excitation and de-excitation, ionization and recombination) which are due to collisions with particles in the bath. As a consequence, we do not take into account here radiative transitions nor two-electron transitions. We notice that, because we included among the allowed transitions the processes of ionization and recombination, the transition $\vec{k} \to \vec{k}''$ does not necessarily preserve the total number of electrons in the configuration $\vec{k}$.

According to the above assumptions, the transition probabilities $B_{\vec{k}' \to \vec{k}}$ in (1.1) will be nonzero only when $\vec{k}' = \vec{k} + (\pm 1, \mp 1)_{ij}$ for some $i, j \in \{1, .., N\}$, or $\vec{k}' = \vec{k} + (\pm 1)_i$ for some $i \in \{1, .., N\}$. Then the evolution equation (1.1) of the probability $g_{\vec{k}}(t)$ can be written as

$$\tag{2.1}$$

$$\frac{d}{dt} g_{\vec{k}} = \sum_{j=1}^{N} \sum_{m=1}^{N} \left[(T_{jm} \; g)_{\vec{k}+(1,-1)_{jm}} - (T_{mj} \; g)_{\vec{k}} \right]$$

$$+ \sum_{j=1}^{N} \left[(T_{jc} \; g)_{\vec{k}+(1)_j} + (T_{cj} \; g)_{\vec{k}+(-1)_j} - (T_{jc} \; g)_{\vec{k}} - (T_{cj} \; g)_{\vec{k}} \right] \;,$$

with bound-bound transition rates T_{jm} and bound-free transition rates T_{jc} (ionization) and T_{cj} (recombination). The rates T are written as functions of the *initial* configuration of the transition and of course $T_{jm} = 0$ when $j = m$.

The number of electrons k_j in the departure level and the number of holes $D_m - f_m$ in the arrival level can be factored out:

$$T_{jm} = k_j (D_m - k_m) R_{jm} \;, \; T_{jc} = k_j R_{jc} \;, \; T_{cj} = (D_j - k_j) R_{cj}$$

(where, as before, $R_{jm} = 0$ when $j = m$).

This writing recalls that there is no transition starting from an empty level, or going to a full level. Moreover, it allows to introduce one essential approximation in our model: the reduced rates R are assumed not to be functions of configurations, but to depend on the average populations $\vec{f}$ only. This is the "macroscopically screened model" of [1].

The ion charge is given by the formula

$$Z^* = Z^*(\vec{f}) = Z - \sum_{h=1}^{N} f_h \; , \tag{2.2}$$

and to each level j is associated an energy $E_j(\vec{f})$ which is also assumed to be a function of the average populations $\vec{f}$.

2.2. Equilibrium solution of the microscopic model

Since we consider here only transitions due to collisions with particles in the bath, the stationary solution of the model is the thermodynamical equilibrium with free electrons. We want the equilibrium solution of eqs.(2.1) to be the (factorized) binomial distribution

$$g_{\vec{k}}^{eq} = \prod_{h=1}^{N} \binom{D_h}{k_h} \left(\frac{f_h^{eq}}{D_h} \right)^{k_h} \left(\frac{D_h - f_h^{eq}}{D_h} \right)^{D_h - k_h} \; . \tag{2.3}$$

with the equilibrium average populations given implicitly by the Fermi-Dirac formula:

$$f_h^{eq} = \frac{D_h}{1 + \exp\left(-E_h(\vec{f^{eq}})/T \right) / Z^*(\vec{f^{eq}}) \; C_T} \; , \tag{2.4}$$

where C_T is a positive constant (depending only on T).

For this, we tell that, as a consequence of the microreversibility, the reduced transition rates must satisfy the "*detailed balance*" relations: each rate of transition is related to the rate of the inverse transition so that the equilibrium (2.3-2.4) is possible. For $n, m = 1, \ldots, N$,

$$R_{mn} = \exp\left(\frac{E_n - E_m}{T} \right) \; R_{nm} \; ,$$

and for $n = 1, \ldots, N$

$$R_{cn} = Z^* C_T \; \exp\left(\frac{E_n}{T} \right) \; R_{nc} \; .$$

2.3. Non closed equations for moments

It is possible to write an equation for the averages f_h defined in (1.2) (first moments of $g_{\vec{k}}$), starting from eq.(2.1) and making suitable changes of indices, as a sum over all possible configurations. It reads

$$\tag{2.5}$$

$$\begin{aligned}
\frac{d}{dt} f_h &= \sum_{\vec{k}} \left[\sum_{j=1}^{N} (T_{jh} - T_{hj}) + T_{ch} - T_{hc} \right] g_{\vec{k}} \\
&= \sum_{\vec{k}} \left\{ \sum_{j=1}^{N} \left[k_j (D_h - k_h) R_{jh}(\vec{f}) - k_h (D_j - k_j) R_{hj}(\vec{f}) \right] \right. \\
&\quad \left. + (D_h - k_h) R_{ch}(\vec{f}) - k_h R_{hc}(\vec{f}) \right\} g_{\vec{k}} \; .
\end{aligned}$$

We observe that the r.h.s. of eq.(2.5) can be expressed in terms of the first and second moments of $g_{\vec{k}}$, or as well the average populations (1.2) and the correlations f_{hl} (1.4). Eq.(2.5) becomes

$$(2.6)$$

$$
\frac{d}{dt} f_h = \sum_{j=1}^{N} \left[f_j (D_h - f_h) R_{jh}(\vec{f}) - f_h (D_j - f_j) R_{hj}(\vec{f}) \right]
$$

$$
+ (D_h - f_h) R_{ch}(\vec{f}) - f_h R_{hc}(\vec{f}) + \sum_{j=1}^{N} f_{hj} \left[R_{hj}(\vec{f}) - R_{jh}(\vec{f}) \right].
$$

In the same way, starting from eq.(2.1) and making suitable changes of indices, we can write an equation for the evolution of the $\chi_{hl} = \sum_{\vec{k}} k_h k_l \, g_{\vec{k}}$ (second moments of $g_{\vec{k}}$) as a sum over configurations:

$$(2.7)$$

$$
\frac{d}{dt} \chi_{hl} = \sum_{\vec{k}} \left\{ k_h \left[\sum_{j=1}^{N} (T_{jl} - T_{lj}) + T_{cl} - T_{lc} \right] \right.
$$

$$
+ k_l \left[\sum_{j=1}^{N} (T_{jh} - T_{hj}) + T_{ch} - T_{hc} \right]
$$

$$
\left. - T_{hl} - T_{lh} + \delta_{hl} \left[\sum_{j=1}^{N} (T_{jh} + T_{hj}) + T_{ch} + T_{hc} \right] \right\} g_{\vec{k}} \; .
$$

The r.h.s. of eq.(2.7) can be expressed in terms of the first, second and third moments of $g_{\vec{k}}$, or as well the average populations (1.2), the correlations (1.2), and the triple correlations

$$
f_{hlm} = \sum_{\vec{k}} (k_h - f_h)(k_l - f_l)(k_m - f_m) \, g_{\vec{k}} \; .
$$

We obtain thus an equation for the evolution of correlations:

$$(2.8)$$

$$
\frac{d}{dt} f_{hl} = B_{hl}(\vec{f}) + \sum_{j=1}^{N} \left[A_{hj}(\vec{f}) f_{jl} + A_{lj}(\vec{f}) f_{jh} \right]
$$

$$
+ \left[R_{hl}(\vec{f}) + R_{lh}(\vec{f}) \right] f_{hl} - \delta_{hl} \sum_{j=1}^{N} \left[R_{hj}(\vec{f}) + R_{jh}(\vec{f}) \right] f_{hj}
$$

$$
+ \sum_{j=1}^{N} \left[R_{hj}(\vec{f}) - R_{jh}(\vec{f}) + R_{lj}(\vec{f}) - R_{jl}(\vec{f}) \right] f_{jhl} \; ,
$$

where

$$
A_{hj} = f_h R_{hj} + (D_h - f_h) R_{jh}
$$

$$
- \delta_{hj} \left\{ \sum_{l=1}^{N} [(D_l - f_l) R_{hl} + f_l R_{lh}] + R_{ch} + R_{hc} \right\},
$$

and

$$
\begin{aligned}
B_{hl} &= -f_h(D_l - f_l)R_{hl} - f_l(D_h - f_h)R_{lh} \\
&\quad + \delta_{hl}\left\{\sum_{j=1}^{N}\left[f_h(D_j - f_j)R_{hj} + f_j(D_h - f_h)R_{jh}\right]\right. \\
&\quad \left. + (D_h - f_h)R_{ch} + f_h R_{hc}\right\} \; .
\end{aligned}
$$

2.4. **Equilibrium solution of the moment equations**

Since the equilibrium solution of the microscopic equations (2.1) is the (factorized) binomial distribution (2.3), the r.h.s of equations (2.6) and (2.8) vanishes if the average populations are the Fermi-Dirac ones (2.4), and the correlations are those of a binomial distribution, i.e.

$$
f_{hl}^{eq} = \delta_{hl}\,\frac{f_h^{eq}(D_h - f_h^{eq})}{D_h}, \tag{2.9}
$$

and

$$
f_{jhl}^{eq} = \delta_{jh}\,\delta_{hl}\,\frac{f_h^{eq}(D_h - f_h^{eq})(D_h - 2f_h^{eq})}{D_h^2} \; .
$$

An interesting property is that the r.h.s of equations (2.8) vanishes as well if the triple correlations are only auto-correlations ($f_{jhl} \neq 0$ only if $j = h = l$), in particular if they are null.

3. **The intermediary model**

We propose to use as a refined average ion model a closed set of ODEs consisting of $N\,(N+3)/2$ equations for the quantities $(f_h)_{h=1..N}$ and
$(f_{hl})_{h,l=1..N}$. This model is defined in a systematic way by neglecting the triple correlations f_{jhl} in eq.(2.8):

$$
\tag{3.1}
$$

$$
\begin{aligned}
\frac{d}{dt}f_{hl} &= B_{hl}(\vec{f}) + \sum_{j=1}^{N}\left[A_{hj}(\vec{f})f_{jl} + A_{lj}(\vec{f})f_{jh}\right] \\
&\quad + \left[R_{hl}(\vec{f}) + R_{lh}(\vec{f})\right]f_{hl} - \delta_{hl}\sum_{j=1}^{N}\left[R_{hj}(\vec{f}) + R_{jh}(\vec{f})\right]f_{hj} \; .
\end{aligned}
$$

From what we just said, the equilibrium solution of our model set of equations (2.6) and (3.1) is the Fermi-Dirac one (2.4) and (2.9).

Comparing the set of equations of our intermediary model with previous average-ion ones,

- the equation (2.6) for the averages has additional terms depending on correlations;

- the evolution equation for correlations (3.1) has new terms depending on correlations (second line) in addition to those (first line) already present in [2] and well-known references in statistics (see [4], Sec.5, especially eq.5.17).

The interest of this model is two-fold. First, we think that its validity goes beyond that of standard average ion models. We recall that in [1], it was established the validity of such models in various situations:

- When the plasma is close to equilibrium;

- For high temperatures;

- When each shell is either almost full or almost empty.

For contexts far from the above situation, we think that our model with $N(N + 3)/2$ ODEs gives results closer to the microscopic model than the average ion model with N equations. We provide in the next section experiments which sustain this point of view.

A second interest of this model is the control of the error in the average ion model. Indeed, as soon as the off-diagonal correlations f_{hl}, $h \neq l$ become significant, there is a strong suspicion that the results obtained with the average ion model are far from what is obtained with the microscopic (detailed) model.

Before presenting the numerical simulations which sustain our modeling choices, we briefly indicate which rigorous mathematical results are already or could in the future be proven. Note first that the standard average ion model, as indicated above, was rigorously proven in [1] to be valid (asymptotically) in three cases (close to equilibrium, for high temperatures, and when each shell is either almost full or almost empty). We think that arguments quite similar to those used in [1] could also be used for our intermediary model with $N(N+3)/2$ ODEs for the same cases (close to equilibrium, etc.). The corresponding computations would be more involved but we do not think that any new idea would be necessary.

It looks to us in fact far more interesting to investigate the cases in which one is far from those situations (for example when one of the shell is initially almost empty and becomes almost full during the evolution). Then, our feeling is that retaining from the microscopic eq. (2.1) an equation for the n-th order correlations and assuming that the $n + 1$-th order correlations (other than autocorrelations) vanish constitutes an approximation which, for a given n, cannot be proven to be valid (except close to equilibrium, etc.).

What could nevertheless be done at the rigorous level would be to show that when $n \to +\infty$, one recovers the initial microscopic model. Indeed, such a result would not be surprising and maybe not very difficult to show (it is also expected when one considers e.g. n-th order moments of the Boltzmann equation), but it would not really reinforce the conviction that the $N(N+3)/2$ ODEs intermediary model (which corresponds to taking $n = 2$) is a better approximation of the microscopic model than the standard average ion model.

This conviction can from our point of view only come from numerical simulations, such as the ones that we present in next section.

4. Numerical Simulations

We present in this section some figures in order to illustrate the advantages and the drawbacks of our new intermediary model.

For each figure, we represent (for some level h) the functions f_h (obtained by solving the microscopic equations), $P_h^{(1)}$ obtained by solving the average ion model (in the form introduced in [1]), and $P_h^{(2)}$, obtained by solving the intermediary model. In one typical case (that is, the one which from our point of view is most interesting, since at least one shell is neither empty nor full during the time evolution), we compare also the most relevant correlations f_{hl} and triple correlations f_{hlm}, showing that assuming (3.1) gives a good approximation of the microscopic model.

The results have been obtained thanks to the use of a standard second order explicit scheme for ODEs (16929 ODEs are solved in the microscopic model, 5 in the model of average ion, and 15 in the intermediary model)

The values of the functions and parameters used in the simulations are the same as in [1]:

The shells are built according to the first quantum number, so that $D_n = 2\,n^2$. Only $N = 4$ shells (plus the continuum) are introduced.

The screening effect (that, is, the effective charge of the nucleus seen by an electron) is modeled by

$$Z_n^*(\vec{f}) = Z - \sum_{h<n} f_h - \frac{1}{3} f_n .$$

Then the energy of each level is that of the hydrogenic atom corrected by the screening effect defined above:

$$E_n(\vec{f}) = 0.0136 \frac{(Z_n^*)^2}{n^2} \ keV .$$

The rates of transition (for $n < m$) are given by

$$R_{nm} = \frac{\mathcal{R}_{nm}}{E_n - E_m} e^{-\frac{E_n - E_m}{T}} ,$$

$$R_{nc} = \mathcal{R}_{nc} \frac{[1 - e^{-\frac{E_n}{T}}]}{E_n^2} e^{-\frac{E_n}{T}} ,$$

In those formulas, we have used the following values for $\mathcal{R}_{nm}$ (taken from [DR]):

$$\mathcal{R}_{nm} = \frac{4.99 \times 10^{-10} f(n,m) g_{nm} N_e}{\sqrt{T}} ,$$

$$\mathcal{R}_{nc} = 3.45 \times 10^{-11} N_e \sqrt{T} \, \Gamma_n ,$$

with the Gaunt factor $g_{nm} = 0.361$, and the values $f(1,2) = 0.4161$, $f(1,3) = 0.0792$, $f(1,4) = 0.029$, $f(2,3) = 0.637$, $f(2,4) = 0.119$, $f(3,4) = 0.8408$. Moreover, we take

$$\Gamma_n = 2.8014 \, e^{-\frac{n}{n+5}} ,$$

and for the electron number density:

$$N_e = \frac{6.02 \times 10^{23} \rho}{M} Z^* ,$$

where ρ is the plasma mass density (taken as $5 \times 10^{-2} g \, cm^{-3}$), Z^* is given by formula (2.2), Z is the atomic number of the atom (taken as 50) and M is the mass number of the atom (taken as 120).

Finally, the constant C_T appearing in the process of ionization is taken equal to

$$C_T = \frac{\rho}{317 \, M \, T^{\frac{3}{2}}} ,$$

and the temperature T of the bath (in keV) is chosen in a different way for the different numerical simulations.

We first check the validity of the model defined in Section 3 in the validity range of the average ion model discussed in [1]: as in [1] we take as initial datum a factorized equilibrium distribution at a given temperature T_0, which differs from the temperature T of the bath. In figures 4.1 and 4.2 we show the results of simulations corresponding resp. to the high temperature limit ($T_0 = 4.3 \ keV$ and $T = 4.5 \ keV$) and to the asymptotics in which levels are all either almost full or almost empty ($T_0 = 1.7 \ keV$ and $T = 1.9 \ keV$). The curves corresponding to the microscopic model, to the average ion model and to the intermediary model are indistinguishable.

We analyze then the case where the initial datum is still given by a factorized distribution, but with $T_0 = 0.6 \ keV$ and $T = 0.9 \ keV$. For such an initial datum, the system is out of the validity range of the average ion model presented in [1]. We can see in figure 4.3 that the new model is closer to the microscopic curve than the old one.

Indeed, in this case the size of the triple correlations (which are not autocorrelations), coherently with (3.1), is much lower than the size of the most relevant correlation in the evolution (the
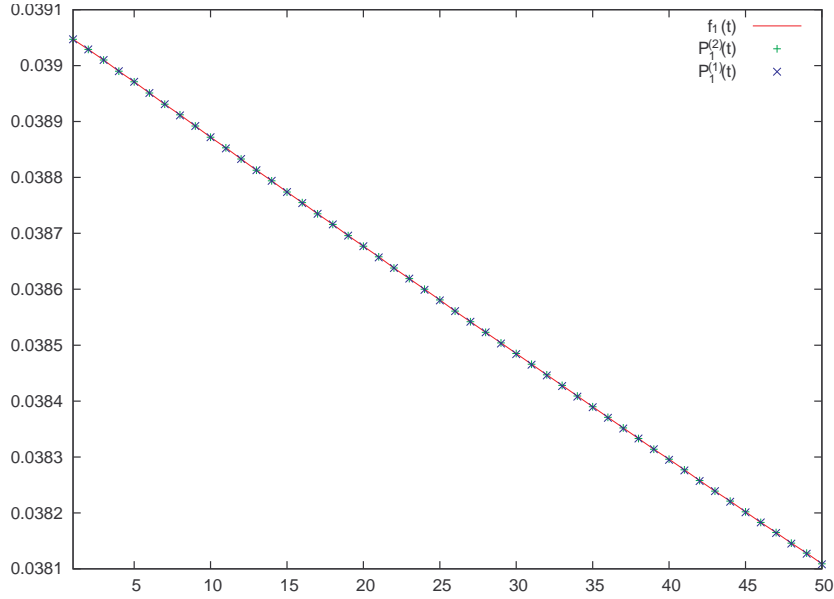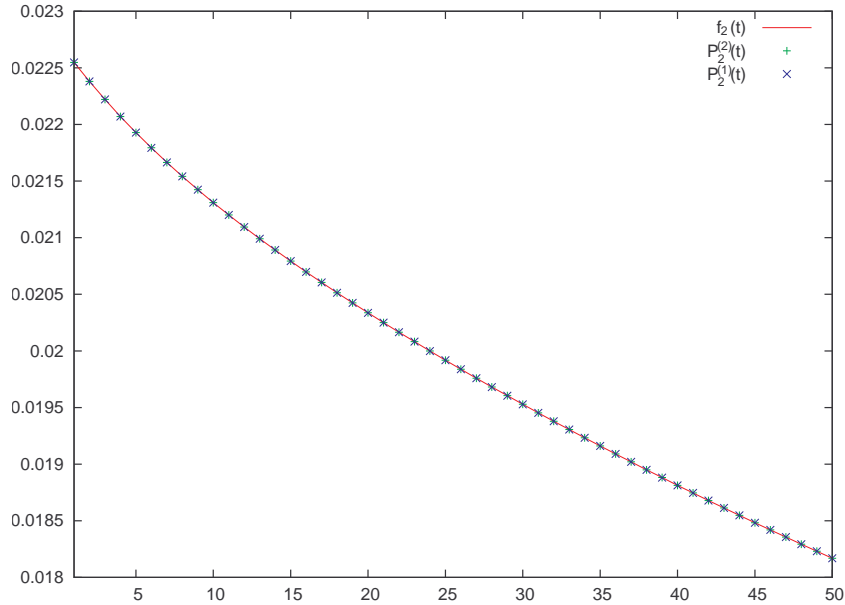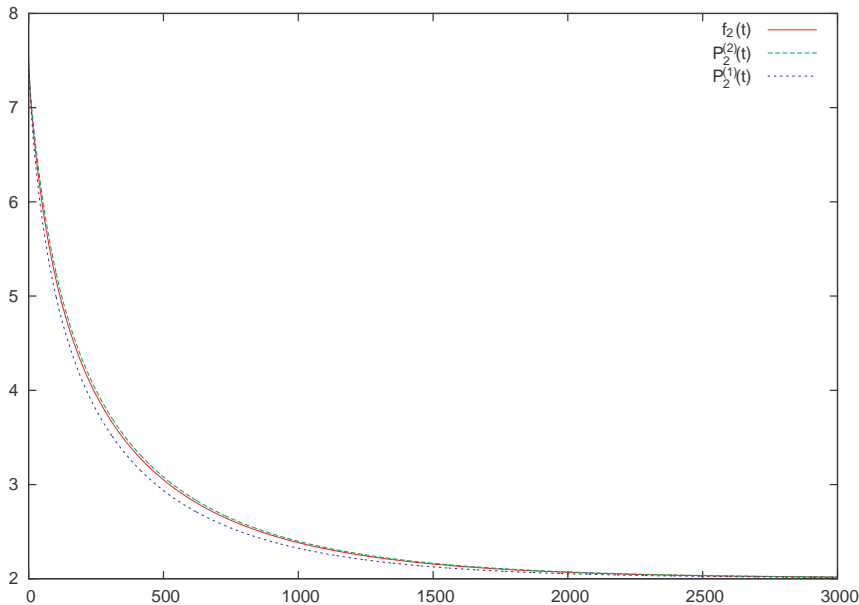
FIGURE 4.1. Occupation numbers $f_1(t)$ for the microscopic model, $P_1^{(1)}(t)$ for the average ion model, and $P_1^{(2)}(t)$ for the intermediary model in the high temperature limit, with $T_0 = 4.3\ keV$ and $T = 4.5\ keV$.

FIGURE 4.2. Occupation numbers $f_2(t)$ for the microscopic model, $P_2^{(1)}(t)$ for the average ion model, and $P_2^{(2)}(t)$ for the intermediary model in the asymptotics when all level are either almost full or almost empty, with $T_0 = 1.7\ keV$ and $T = 1.9\ keV$.

first order moments are of the same order of magnitude or bigger than the autocorrelations). We plot first in figure 4.4 the evolution of the most significant triple correlations for the microscopic model over a short time, and then we compare them in figure 4.5 with the evolution of the most relevant correlation over a longer time interval (50 times the one considered in figure 4.4). Notice
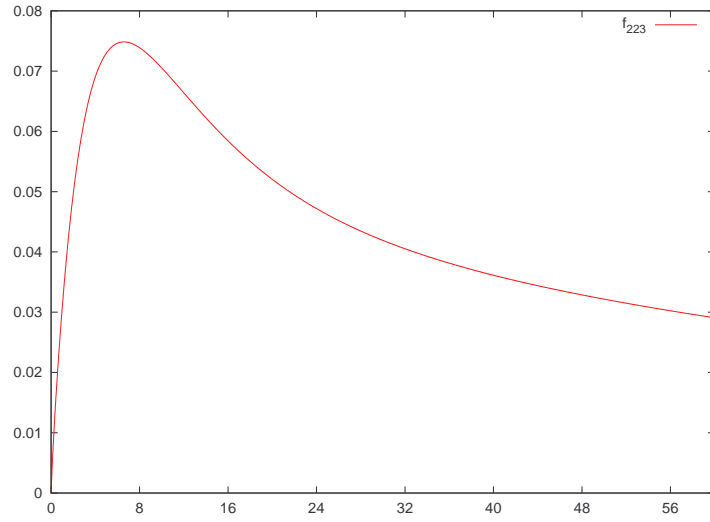
FIGURE 4.3. Occupation numbers $f_2(t)$ for the microscopic model, $P_2^{(1)}(t)$ for the average ion model, and $P_2^{(2)}(t)$ for the intermediary model, with $T_0 = 0.6 \ keV$ and $T = 0.9 \ keV$.

that the relevant correlations for the evolution in this context are those contributing significantly to increase the absolute value of the off-diagonal correlations in such a way that they become significant in the evolution equation (2.6) for the first moments, i.e. the autocorrelations: in the case under consideration here, the most relevant correlation is f_{22}, which is the dominant correlation involved in the evolution of the most significant off-diagonal correlation f_{23}.

We give finally in Fig. 4.6 and Fig. 4.7 the results of simulations corresponding to two initial data quite far from the validity region of the average ion model. In the simulation illustrated in Fig. 4.6, the initial datum is far from equilibrium, in the one in Fig. 4.7 the initial datum is a factorized equilibrium distribution at temperature $T_0 = 0.8 \ keV$ and the temperature of the bath is $T = 0.4 \ keV$ (the system cools down). As we can see, in the first case (Fig. 4.6), although the average ion model reproduce correctly the trend to the equilibrium of the system, the evolution described by the refined model is definitely much closer to the microscopic evolution than the standard one, while in the second case (Fig. 4.7), both the average ion model and the intermediary model fail, but the intermediary model still gives a better approximation to the microscopic evolution than the average ion model (in particular in a time interval near to $t = 0$).
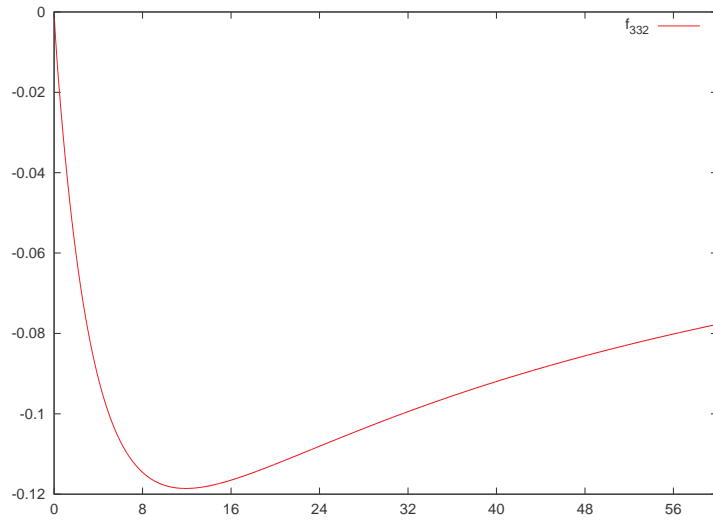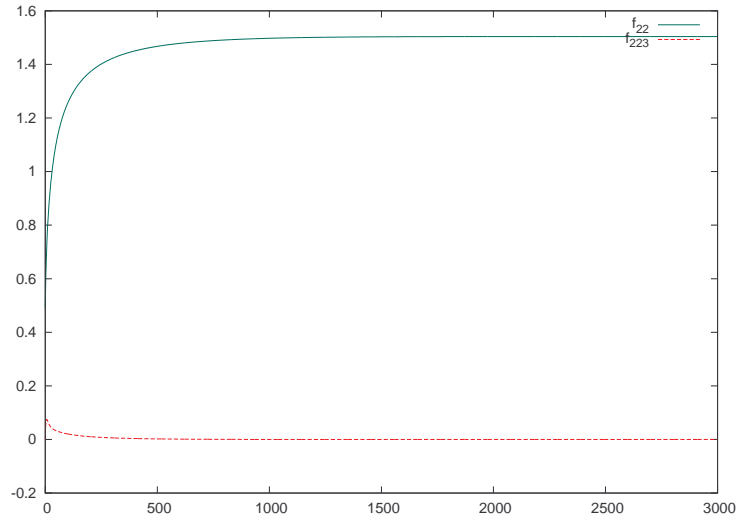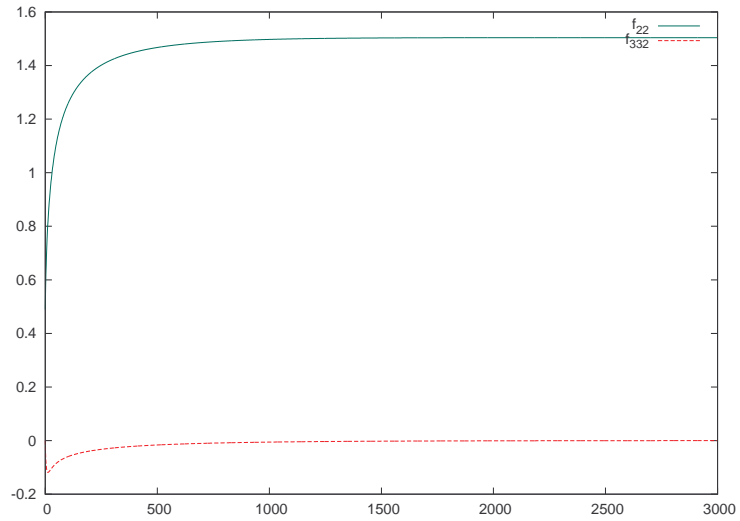
FIGURE 4.4. Triple correlations $f_{223}(t)$, Fig.4.4(a), and $f_{332}(t)$, Fig.4.4(b), for the microscopic model, with $T_0 = 0.6\ keV$ and $T = 0.9\ keV$.

(a)

(b)

Figure 4.5. Triple correlations $f_{223}(t)$, Fig.4.5(a), and $f_{332}(t)$, Fig.4.5(b), compared to the correlation $f_{22}(t)$ for the microscopic model, with $T_0 = 0.6\ keV$ and $T = 0.9\ keV$. The time interval considered here is 50 times the time interval considered in Fig.4.4.
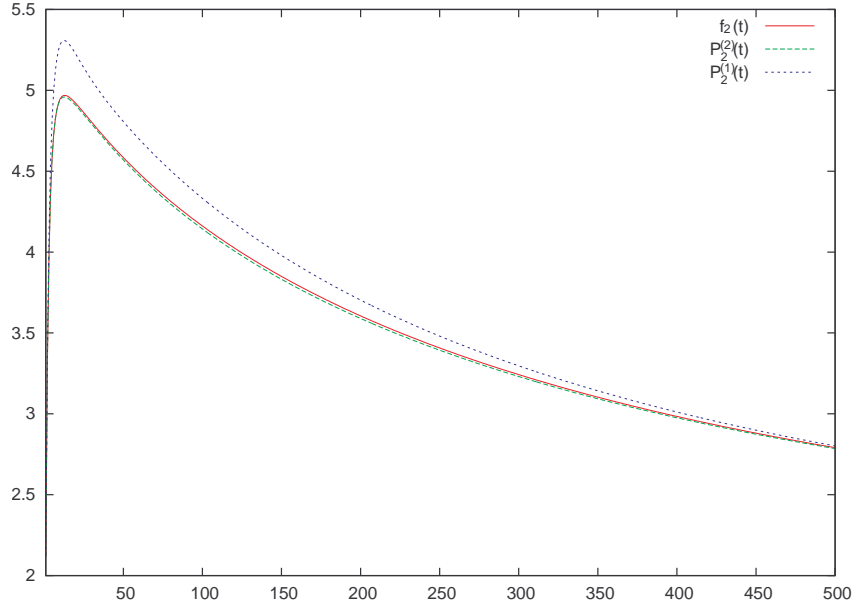
FIGURE 4.6. Occupation numbers $f_2(t)$ for the microscopic model, $P_2^{(1)}(t)$ for the average ion model, and $P_2^{(2)}(t)$ for the intermediary model for an initial datum far from equilibrium.
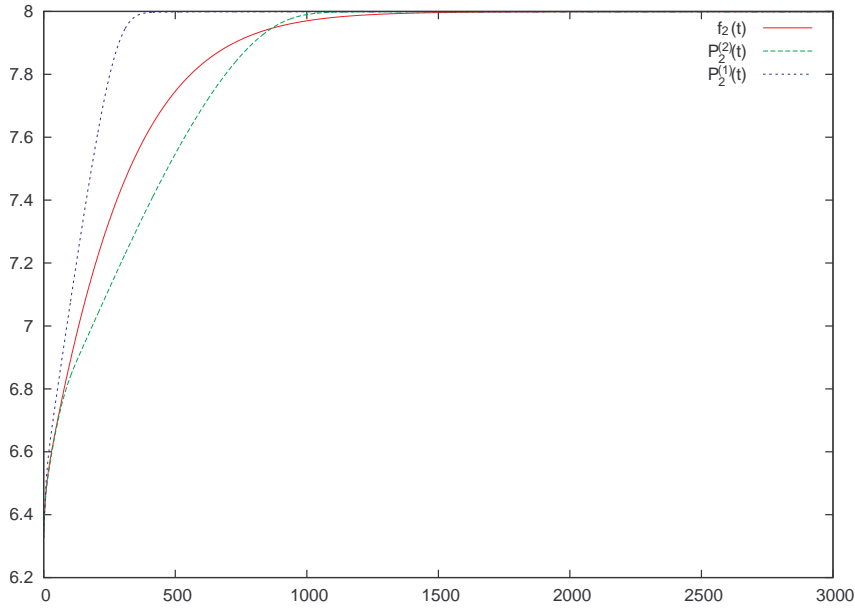

FIGURE 4.7. Occupation numbers $f_2(t)$ for the microscopic model, $P_2^{(1)}(t)$ for the average ion model, and $P_2^{(2)}(t)$ for the intermediary model for an initial factorized equilibrium distribution at temperature $T_0 = 0.8 \ keV$ and $T = 0.4 \ keV$.

References

[1] G. Cavallaro, L. Desvillettes, and V. Ricci. About the link between the detailed description of transitions in an ion and the average-ion models. *Commun. Math. Sci.*, 7(2):471–488, 2009.

[2] P. Dallot, G. Faussurier, A. Decoster, and A. Mirone. Average-ion level-population correlations in off-equilibrium plasmas. *Phys. Rev. E*, 57:1017–1028, 1998.

[3] A. Djaoui and S. J. Rose. Calculation of the time-dependent excitation and ionization in a laser-produced plasma. *J. Phys. B: At. Mol. Opt. Phys.*, 25:2745–2762, 1992.

[4] M. Lax. Fluctuations from the nonequilibrium steady state. *Rev. Mod. Phys.*, 32:25–64, 1960.