

Article Adaptive Algorithm for the Generation of Superconfigurations in Hot-Plasma Opacity Calculations

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Abstract: In hot plasmas, such as the ones encountered in astrophysics or laser-fusion studies, the number of ionic excited states may become huge, and the relevant electron configurations cannot always be handled individually. The Super Transition Array approach enables one to calculate the massic photo-absorption cross-section (or radiative opacity) in a statistical manner consisting of grouping configurations close in energy into superconfigurations. One of the main issues of the method, beyond its spectral resolution, is the determination of the most relevant configurations that contribute to opacity. In this work, we discuss different aspects of the generation of superconfigurations in a hot plasma and propose a new adaptive algorithm.

Keywords: radiative opacity; statistical methods; super transition arrays; superconfigurations; adaptive algorithm; master theorem



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1. Introduction

The radiative opacity is an essential quantity governing the structure and evolution of stars. In plasmas of medium to high-*Z* elements, some of the electrons remain bound to the ions even at very high temperature (this is for instance the case of iron in the center of the sun). Among the different contributions to opacity of plasmas at local thermodynamic equilibrium (LTE), the photo-excitation process (also called sometimes "line absorption" or bound–bound opacity), consisting of transitions between electronic states of the ions, is of particular importance.

The methods for the evaluation of the line absorption coefficient, in hot dense plasmas, even in non-LTE conditions, involve a compromise between the needed spectral resolution and the available computer resources. At one extremity one finds the uncompromising method of detailed line accounting (DLA), yielding a highly resolved (or detailed) spectrum, including all photo-absorption lines of all configuration-to-configuration transition arrays. For complex configurations, the numerical cost resulting from the huge number of transitions becomes prohibitive. In this case, one may turn to the unresolved transition arrays (UTA) method [1], which assumes that all lines in the spectrum of each configurationto-configuration excitation merge into a single effective (super-) line, which can be depicted by a Gaussian function. The efficiency of the UTA method comes from the fact that compact formulas are available for the three lowest energy moments (orders 0, 1 and 2) of the line-strength weighted line energies of a transition array. Such moments are expressed in terms of reduced matrix elements of the dipole operator, Slater integrals, and subshell occupation numbers. The effect of higher-order moments was also investigated, using more sophisticated distributions [2,3]. Sometimes, the number of configurations is so high that the UTA approach and its relativistic counterpart the SOSA (Spin-Orbit Split Array) approach [4] are not tractable. For that reason, Bar-Shalom et al. developed the STA model, consisting of grouping the large number transition lines between an enormous number of configurations into large assemblies, called Super Transition Arrays (STAs) [5]. The STA

moments are calculated analytically using a canonical partition function algebra, and can be split into smaller STAs until convergence (of the Rosseland mean for instance) is achieved.

The method was implemented in the SCO code, and combined to DLA calculations in the SCO-RCG code [6–9], which is used to interpret high-resolution spectra (see for instance Ref. [10]). The SCO code was developed in two versions, the first one in the Local Density Approximation [11], the second one in the statistical Hartree–Fock theory [12–14].

The STA approach was successfully applied to the interpretation of photo-absorption spectra [9,15–20], to solar physics [21–24] and equation of state [25–33]. The plasma modeling was extended to mixtures [29,34]. Much work was done on the optimization of the canonical partition functions, in the independent-particle approximation [35–41], and for a better inclusion of electron-electron interactions [42,43] in the Gibbs-Bogolyubov or Jensen-Feynman approach.

The STA formalism was recently improved by Kurzweil and Hazak within the framework of the CRSTA (Configurationally Resolved Super Transition Array) model [44–46], which enables one to refine the STAs to reveal the underlying structure. The basic idea is an adaptation of the Liouville evolution operator technique to the photo-absorption spectra.

Whatever the variant of the method that we consider, the choice of the superconfigurations that must be included in the calculation is an important issue. In order to obtain converged Rosseland mean opacities, the best completeness as possible has to be ensured. This is a difficult point because each opacity code has its own balance between accuracy (trying to use the most accurate models as possible), and completeness (including as many excited states as possible [7,47]). Since it is not realistic to calculate a full-range opacity spectrum for a trial list of superconfigurations, and then add a superconfiguration and calculate the spectrum again, etc. until convergence of the latter, one has to be predictive. In the present work, we discuss different ways of generating superconfigurations at a given temperature and plasma density, and propose in particular an adaptive "divide and conquer" algorithm.

The estimate of configuration probabilities, based on the average-atom model and/or involving correlated or uncorrelated binomial distributions, are presented in Section 2. The superconfiguration approach is described in Section 3 and the way the superconfigurations can be populated by electrons is described in Section 4. Our adaptive algorithm is presented in Section 5, and results are analyzed in Section 6. Finally, two alternative methods are briefly mentioned and discussed in Section 7—a first one consisting of generating superconfiguration using the correlated Gaussian approximation for configurations and the algorithm used in the SCROLL model—emphasizing the novelty of our approach.

2. Estimating Configuration Probabilities

2.1. Configuration Probabilities Based on the Average-Atom Model

The real ions in the plasma are in various multi-electron configurations, each one corresponding to a specific set of integer occupation numbers in the bound subshells. Starting from the average-atom picture, it is possible to build a law for the abundance of such ionic species, assuming that

- The configurations are statistically independent,
- A configuration *C* is entirely defined by the integer occupation numbers *q_i* in each subshell *i*, 1 ≤ *i* ≤ *N*.
- The total energy of *C* in terms of the occupation numbers can be expressed using quantities provided by the average-atom calculation.

In the grand canonical ensemble, knowing the form of the configuration energy $E(q_1, \dots, q_N)$ with $0 \le q_i \le g_i$, $1 \le i \le N$ (g_i is the degeneracy of subshell *i*), the probability law of the configurations reads:

$$\mathscr{P}(q_1,\cdots,q_N) = \frac{1}{\mathcal{U}}\left[\prod_{i=1}^N \binom{g_i}{q_i}\right] \exp\left[-\beta\left(E(q_1,\cdots,q_N) - \mu\sum_{i=1}^N q_i\right)\right],\tag{1}$$

where \mathcal{U} is the partition function and μ the chemical potential; we also set $\beta = 1/(k_BT)$, where k_B denotes Boltzmann's constant and T the temperature. $\begin{pmatrix} g_i \\ q_i \end{pmatrix} = g_i!/q_i!/(g_i - q_i)!$ represents the usual binomial coefficient. The direct summation over all the configurations can become intractable when the number of subshells increases, in particular for large atomic numbers. It is, therefore, essential to make approximations to perform such summations. The energy can be formulated as a quadratic form of the subshell occupation numbers:

$$E(q_1, \cdots, q_N) = E_0 + \sum_{i=1}^N x_i \epsilon_i + \frac{1}{2} \sum_{i,j=1}^N x_i V_{ij} x_j,$$
(2)

with $x_i = q_i - \langle q_i \rangle$ the deviation of the integer q_i with respect to its average-atom average value $\langle q_i \rangle = g_i f_i$, where f_i denotes the Fermi-Dirac factor:

$$f_i = \frac{1}{1 + e^{\beta(\epsilon_i - \mu)}}.$$
(3)

The quantity V_{ij} is an interaction matrix element including the dominant Coulomb interaction between states *i* and *j* and an exchange-correlation contribution [48]. All the quantities entering Equation (2), except the occupation numbers q_i , are given by the average-atom calculation.

The modeling of occupation-number fluctuations in a hot plasma, based on averageatom results and determination of correlations, has a long history [49–53]. An interesting approach consists of handling the sums over all configurations at once [48,54]. It allows one to calculate the statistical properties of a whole transition array representing a monoelectronic jump. The determination of such statistical properties relies on knowing the correlations between the subshell occupation numbers. In this method, the Gaussian approximation to the binomial coefficients of the configuration degeneracy

$$g_C = \prod_{i=1}^N \begin{pmatrix} g_i \\ q_i \end{pmatrix} \tag{4}$$

is used to gather the binomial coefficients and the Boltzmann factor in a single exponential. Using elementary matrix algebra on the argument of this exponential, the problem of finding the correlations reduces to the inversion of a matrix. This boils down to expressions of the configuration free energy, which are quadratic forms of the occupation numbers.

2.1.1. Uncorrelated Probability Law

The simplest possible approximation amounts to neglect the interaction terms in the energy. The consequence is that the probability reduces to a product of independent binomial laws, which presents the following advantages:

- The average occupation number of each subshell is a direct result of the average-atom calculation,
- The probability can be factorized shell by shell, making the calculation of averages simple. For instance, the variance of the total number of bound electrons $Z_B = \sum_{i=1}^{N} q_i$ is

$$\mathscr{V}_B = \langle Z_B^2 \rangle - \langle Z_B \rangle^2 = \sum_{i=1}^N \mathscr{V}_i, \tag{5}$$

 \mathcal{V}_i being the uncorrelated variance of the number of electrons in shell *i*:

$$\mathscr{V}_i = \langle q_i \rangle (1 - f_i). \tag{6}$$

The latter approximation (Equations (5) and (6)) tends to overestimate the variance \mathscr{V}_B , leading to erroneous distribution widths, with a dramatic impact on Rosseland mean opac-

ities. Better approximations must account for the quadratic interaction terms (correlations) in the energy.

2.1.2. Correlated Probability Law: Integral Transformation and High Temperature Limit

To deal with the statistical mechanics of systems associated with the quadratic energy in Equation (2), a clever method was proposed, making use of an integral transformation [55,56]. The quadratic term in the Boltzmann factor in Equation (1) is replaced with a linear one, at the cost of a multiple integration over auxiliary variables y_i , $1 \le i \le N$. The consequence is that the Boltzmann factor has the same form as in the uncorrelated case, and the probability can be written as a product of factors, each one corresponding to one subshell. However, the method can thus be useful if the multiple integral is easily approximated, but reaches its numerical limits when accurate results are needed. Green proposed a treatment of the interacting system applicable to high temperatures when $\beta V_{ij} \ll 1$ [57,58], consisting of computing the correlation factors up to second order in βV_{ij} . The technique, rather cumbersome to implement, can lead to serious practical issues since the accuracy of the obtained expressions decreases as the electron correlations increase. If the temperature is too low, the occupation-number variances can even become negative, which of course makes the method inapplicable.

2.1.3. Correlated Gaussian Approximations

The correlated Gaussian approximations avoid the difficulties of the previous approaches. They treat the occupation-number deviations x_i as continuous variables, which is equivalent to replace the binomial law by its Gaussian continuous limit, an approximation justified when the degeneracies of the electron subshells are large and if the number of electrons in a subshell is neither too close to zero nor to its degeneracy (in virtue of the central-limit theorem [59]). In that case, the probability law of Equation (1) becomes

$$\mathscr{P}(q_1,\cdots,q_N) = \frac{1}{\mathcal{U}} \exp\left[-\frac{1}{2}\mathbf{x}^T \mathbf{M} \mathbf{x}\right],\tag{7}$$

where **x** is the vector with components x_i and **M** the $N \times N$ correlation matrix. The elements of the positive definite matrix **M** are [48,56]:

$$M_{ij} = \beta V_{ij} + \frac{1}{\gamma_i} \delta_{ij},\tag{8}$$

and its eigenvalues are noted ω_i^{-2} . Equation (7) becomes

$$\mathscr{P}(q_1,\cdots,q_N)d^N x = \prod_{i=1}^N \frac{1}{\sqrt{2\pi\omega_i}} \exp\left[-\frac{y_i^2}{2\omega_i^2}\right] dy_i,$$
(9)

where **y** is defined as $\mathbf{x} = \mathbf{S}\mathbf{y}$, **S** being the unitary transformation diagonalizing **M**. The equivalent of Equation (5) then reads

$$\Sigma_B^2 = \sum_{ij} \langle x_i x_j \rangle = \sum_{i,j} \left(\mathbf{M}^{-1} \right)_{ij}.$$
 (10)

The correlated Gaussian approximation described above is very easy to implement. Its results are in excellent agreement with the exact calculation. For instance, in the case of a plasma at an electronic temperature $T_e = 100 \text{ eV}$ and solid density, Wilson found that it is accurate to better than 1% [55]. We confirmed such an estimate, and found that in most usual situations encountered in laser-fusion experiments or stellar physics, the accuracy is usually of the order of a few percent. The method can be improved by combining the discrete variation of integer occupation numbers in a small number of subshells (the active

ones and spectator subshells strongly coupled to them) and the continuous variation of occupation numbers in the other (spectator) subshells.

3. The Superconfiguration Method

3.1. Subshells, Configurations

Let us consider the ensemble \mathcal{E} of potential bound subshells (n_i, ℓ_i) for electronic configurations of ions in LTE conditions. The occupation numbers of the subshells satisfy $0 \le q_i \le g_i$ and $\sum_{i \in \mathcal{E}} q_i \le Z$. We define

$$Z_{\mathsf{C}}^* = Z - \sum_{i \in \mathcal{E}} q_i,\tag{11}$$

the ionization corresponding to that configuration.

3.2. Supershells, Superconfigurations

Let $\mathcal{B} = \{\sigma\}$ be a partition of the ensemble of bound states \mathcal{E} into $n_{\mathcal{B}}$ supershells:

$$\bigcup (\sigma \in \mathcal{B}) = \bigcup_{i=1}^{n_{\mathcal{B}}} \sigma_i = \mathcal{E}$$
(12)

with $\sigma_i \in \mathcal{B}$, $\sigma_j \in \mathcal{B}$, $\sigma_i \neq \sigma_j$, $\sigma_i \cap \sigma_j = 0$, $i, j = 1, \dots, n_{\mathcal{B}}$. A supershell $\sigma \in \mathcal{B}$ gathers an ensemble of subshells satisfying a given criterion. For instance, two subshells *i* and *j* belong to the same supershell σ if their energies are sufficiently (to be precisely defined) close: $i, j \in \sigma$ if $\beta |\epsilon_i - \epsilon_{\sigma}| \leq \eta_{\sigma}$ and $\beta |\epsilon_j - \epsilon_{\sigma}| \leq \eta_{\sigma}$, where ϵ_i and ϵ_j are the energies of subshells *i* and j, and η_{σ} is the "width" (in reduced energy, i.e., energy divided by $k_B T$ or multiplied by β) of the supershell σ of median energy ϵ_{σ} .

A superconfiguration is defined by a set of integer occupation numbers $\{Q_{\sigma}\}$ of the supershells. The occupation numbers satisfy $0 \le Q_{\sigma} \le G_{\sigma}$, where $G_{\sigma} = \sum_{i \in \sigma} g_i$ represents the degeneracy of supershell σ and

$$\sum_{\sigma \in \mathcal{B}} Q_{\sigma} \le Z.$$
(13)

We write

$$Z_{\Xi}^{*} = Z - \sum_{\sigma \in \mathcal{B}} Q_{\sigma}, \tag{14}$$

the ionization corresponding to that superconfiguration Ξ .

A superconfiguration is then an ensemble of configurations that are close in energy. In practice, a good choice is to group configurations *C* with energies differing by less than k_BT . The superconfigurations are made of supershells σ containing several ordinary shells. The total occupation number of each supershell is fixed. For instance

$$1s^{2}, 2s^{2}, 2p^{5}, (3s, 3p, 3d)^{7}, (4s, 4p, 4d)^{3}, (4f, 5s, 5p)^{1}$$
(15)

is a superconfiguration for which the first three supershells coincide with the normal lowest shells while each one of the others contains three shells supposed to be close in energy. The choice of the shells to group in a supershell is done on the basis of the average-atom eigenvalues. In each supershell of Ξ , the total number of electrons is fixed. For instance, $(3s, 3p, 3d)^7$ contains 20 configurations, corresponding to the number of possibilities to distribute seven electrons in subshells 3*s*, 3*p* and 3*d*, i.e.,

$$\sum_{p_1=0}^{2} \sum_{p_2=0}^{6} \sum_{p_3=0}^{10} \delta_{p_1+p_2+p_3,7} = 20$$
(16)

and $\binom{18}{7} = 31,824$ micro-states. The total number of configurations represented by the superconfiguration in Equation (15) is 3960 and the total number of micro-states 3,427,826,688!

3.3. Linearization of the Energy of a Superconfiguration

In Section 2, the energy of any configuration of the plasma was written as a quadratic form of the occupation numbers, its coefficients being obtained from a single self-consistent average-atom calculation. The difficulty relied on the statistical description of the system, while the electronic structure was obtained at a low numerical cost. The superconfiguration method relies on another choice: instead of keeping a unique quadratic expression for the total energy of any configuration, it uses several linear expressions, each one being valid for a superconfiguration (an ensemble of configurations), for which the electronic structure is computed independently. With this assumption, the statistical mechanics of the problem is simpler, thanks to the partition function algebra, but calculating the electronic structure becomes much more expensive, especially if a self-consistent calculation (similar to the average-atom one but with integer occupation numbers) is performed for each superconfiguration. An advantage of the method is that the refinement of the electronic structure description also improves the accuracy of the spectral opacity.

3.4. Number of Configurations, Weight of a Superconfiguration

A superconfiguration $\Xi = \{Q_{\sigma}\}$ gathers all the possible configurations $C = \{q_i\}$. The total number of micro-states (i.e., nondegenerate ion states), noted $\mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma})$, satisfies, for each supershell σ (and using Vandermonde identity for the second equality):

$$\mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \sum_{\substack{\{q_i\}\\\sum_{i \in \sigma} q_i = Q_{\sigma}}} \prod_{i \in \sigma} \binom{g_i}{q_i} = \binom{G_{\sigma}}{Q_{\sigma}},$$
(17)

where $\{g\}_{\sigma}$ represents the list of degeneracies of the subshells belonging to the supershell σ . Therefore, the total number of micro-states in that superconfiguration is equal to

$$\mathcal{M}_{\Xi} = \prod_{\sigma \in \mathcal{B}} \mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}).$$
(18)

The probability that a superconfiguration Ξ takes into account the thermodynamics at LTE can be expressed through the Boltzmann factors $X_i = e^{-\beta \epsilon_i}$ of the subshells. Its statistical weight is proportional to the quantity

$$\mathcal{U}_{\Xi} = \prod_{\sigma \in \mathcal{B}} \mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}), \tag{19}$$

where the partition functions are defined by the relation

$$\mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \sum_{\substack{\{q_i\}\\\sum_{i \in \sigma} q_i = Q_{\sigma}}} \prod_{i \in \sigma} {\binom{g_i}{q_i}} X_i^{q_i}.$$
 (20)

The number of configurations contained in $(\sigma)^{Q_{\sigma}}$, where σ contains N_{σ} subshells of respective degeneracies $g_1, g_2, \ldots, g_{\sigma}$, is (see Ref. [60]):

$$\mathcal{C}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \sum_{i=0}^{Q_{\sigma}} \binom{i+N_{\sigma}-1}{i} \times \sum_{\substack{\vec{\alpha} \\ \sum_{j=1}^{N_{\sigma}} \alpha_{j} = Q_{\sigma}-i}}^{\sum_{i=0}^{n}} \frac{1}{\alpha_{1}!\alpha_{2}!\dots\alpha_{N_{\sigma}}!} \times \prod_{j=1}^{N_{\sigma}} \left(\delta_{\alpha_{j},0} - (g_{j}+1)!\delta_{\alpha_{j},g_{j}+1}\right).$$
(21)

Let us consider the case where σ is made of n_1 orbitals with the same degeneracy g_1 and n_2 orbitals with the same degeneracy g_2 , with $N_{\sigma} = n_1 + n_2$. For instance $(2p_3p_4p_3d_4d)^{10}$ correspond to $g_1 = 6$, $g_2 = 10$, $n_1 = 3$, $n_2 = 2$ and N = 10. One has

$$\mathcal{C}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \sum_{i_{1}=0}^{n_{1}} \sum_{i_{2}=0}^{n_{2}} (-1)^{i_{1}+i_{2}} {n_{1} \choose i_{1}} {n_{2} \choose i_{2}} \times {n_{1}+n_{2}-1+Q_{\sigma}-i_{1}(g_{1}+1)-i_{2}(g_{2}+1) \choose n_{1}+n_{2}-1}.$$
(22)

If we generalize and gather the n_1 subshells of degeneracy g_1 , the n_2 subshells of degeneracy g_2 , ..., the n_s subshells of degeneracy g_s (with therefore $n_1 + n_2 + \cdots + n_s = N_\sigma$) [60], we obtain

$$\mathcal{C}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \sum_{i_{1}=0}^{n_{1}} \sum_{i_{2}=0}^{n_{2}} \cdots \sum_{i_{s}=0}^{n_{s}} (-1)^{i_{1}+i_{2}+\cdots n_{s}} {n_{1} \choose i_{1}} {n_{2} \choose i_{2}} \cdots {n_{s} \choose i_{s}} \times {n_{1}+n_{2}-1+Q_{\sigma}-i_{1}(g_{1}+1)-i_{2}(g_{2}+1)-\cdots -i_{s}(g_{s}+1) \choose n_{1}+n_{2}-1}}$$

$$(23)$$

The latter Formulas (21)–(23) show that it is possible to resort to an explicit formula for the number of configurations, avoiding the multiple nested summations (see Equation (16)) which become numerically costly for a large number of supershells containing many subshells. The most efficient way to compute the number of configurations consists of resorting to recurrence relations (see for instance Ref. [60]). Although the combinatoric number of configurations can be huge even for mid-*Z* elements, the number of configurations which have non-negligible occupation numbers is much lower and depends on temperature and density. Krief recently published two useful methods for the estimation of the number of populated configurations: the first one relies on an exact calculation of the total combinatoric number of configurations within superconfigurations in a converged STA calculation, and the second one involves an estimate for the multidimensional width of the probability distribution for electronic occupation number over bound subshells [61]. The latter work presents a detailed discussion about the effects of temperature and density on the number of populated configurations.

3.5. Number of Superconfigurations Associated with a Partition \mathcal{B}

For a given partition \mathcal{B} in fixed supershells, the number of possible superconfigurations is

$$N_{\mathcal{B},\text{tot}} = \prod_{\sigma \in \mathcal{B}} \min(Z, G_{\sigma}).$$
(24)

4. Populating a Partition in Superconfigurations Ξ from the Average-Atom Results

For a fixed partition $\mathcal{B} = \{\sigma\}$, we estimate $N_{\mathcal{B}}$ from the average-atom results, obtained *a priori*. We assume that the ensemble of possible subshells \mathcal{E} for any configuration is included in the average-atom one. The average-atom calculation consists of a self-consistent computation of the energies of the subshells ϵ_i , the average (fractional) occupation num-

bers $\langle q_i \rangle$ of the subshells and their associated variances \mathscr{V}_i and the chemical potential μ , connected to each other by the relations

$$\langle q_i \rangle = g_i f_i \quad \text{and} \quad \mathscr{V}_i = g_i f_i (1 - f_i),$$
(25)

where f_i depends only on ϵ_i and μ (see Equation (3)).

4.1. Calculation of N_B

For each subshell σ of the partition \mathcal{B} , we define, for the average atom, the degeneracy, the average occupation number and the variance, by summing over the subshells it contains:

$$\begin{cases}
G_{\sigma} = \sum_{i \in \sigma} g_{i} \\
\langle Q_{\sigma} \rangle = \sum_{i \in \sigma} \langle q_{i} \rangle \\
\mathscr{V}_{\sigma} = \sum_{i \in \sigma} \mathscr{V}_{i}.
\end{cases}$$
(26)

We try to generate the possible (integer) occupation numbers Q_{σ} under the constraints $0 \leq Q_{\sigma} \leq G_{\sigma}$ and $\sum_{\sigma \in \Xi} Q_{\sigma} \leq Z$. Since the superconfigurations to generate are at local thermodynamic equilibrium, one can restricts the first constraint to an interval around the average occupation number $\langle Q_{\sigma} \rangle$ of the average atom, characterized by an integer number of standard deviations n_{σ} :

$$\max\left(\langle Q_{\sigma}\rangle - n_{\sigma}\sqrt{\mathscr{V}_{\sigma}}, 0\right) \le Q_{\sigma} \le \min\left(\langle Q_{\sigma}\rangle + n_{\sigma}\sqrt{\mathscr{V}_{\sigma}}, G_{\sigma}\right).$$
(27)

In practice, one defines

$$\begin{cases} m_{\sigma} = \max(\langle Q_{\sigma} \rangle - n_{\sigma} \sqrt{\mathcal{V}_{\sigma}}, 0), \\ M_{\sigma} = \min(\langle Q_{\sigma} \rangle + n_{\sigma} \sqrt{\mathcal{V}_{\sigma}}, G_{\sigma}, Z - \sum_{r < \sigma} m_{r}), \\ Y_{\sigma} = M_{\sigma} - m_{\sigma} + 1, \end{cases}$$
(28)

where Y_{σ} is the total number of ways to choose Q_{σ} integer satisfying $m_{\sigma} \leq Q_{\sigma} \leq M_{\sigma}$, and the total number of possible superconfigurations for the partition \mathcal{B} is

$$N_{\mathcal{B}} = \prod_{\sigma \in \mathcal{B}} Y_{\sigma}.$$
 (29)

The quantity $N_{\mathcal{B}}$ in Equation (29) represents the number of essentially populated superconfigurations, while the quantity $N_{\mathcal{B}}$ in Equation (24) denotes the total number of superconfigurations, irrelevant to their populations. It is important to note that the number of superconfigurations accounted according to Equations (28) and (29) is excessive. If the occupation numbers of several supershells are simultaneously close to m_{σ} or M_{σ} determined from Equation (28), the populations of corresponding superconfigurations are negligible and the latter can be safely disregarded.

4.2. Estimating Statistical Weights

In each superconfiguration calculated self-consistently, the energy is accurately approximated by the linear form

$$E_{\Xi}(q_1, \cdots, q_N) = E_0^{(\Xi)} + \sum_{i=1}^N q_i \epsilon_i^{(\Xi)}.$$
(30)

 $E_0^{(\Xi)}$ is an average energy independent of the occupation numbers, and $\epsilon_i^{(\Xi)}$ is the selfconsistent one-electron energy in subshell *i* of Ξ . In the grand canonical ensemble, the probability law takes the form

$$\mathscr{P}(q_1,\cdots,q_N) = \frac{1}{\mathcal{U}}\sum_{\Xi} \exp\left[-\beta E_0^{(\Xi)}\right] \mathscr{P}_{\Xi}(q_1,\cdots,q_N)$$
(31)

where \mathscr{P}_{Ξ} is an uncorrelated probability relative to a specific superconfiguration Ξ . In analogy with the ideal electron gas partition functions, Bar-Shalom et al. have derived recurrence relations for calculating analytically all the sums required in the averages needed [5]. Hole counting is used instead of electron counting in order to avoid loss of accuracy when the number of electrons is larger than half the total degeneracy of the supershell [12].

One of the limitations of the superconfiguration method is that every non-linear term in the configuration free energy has to be averaged over all configurations belonging to the same superconfiguration. Another limitation is that depending on the supershells that are considered, the superconfiguration set resulting from that choice can still be large.

The N_B superconfigurations are generated by covering all the possible partitions of electrons in the supershells. For each superconfiguration $\Xi = \{Q_\sigma\}$, its statistical weight is estimated using

$$\mathscr{P}_{\Xi} \propto \mathcal{U}_{\Xi} \ e^{-\beta \Lambda_{\Xi}} \tag{32}$$

where

$$\mathcal{U}_{\Xi} = \prod_{\sigma \in \Xi} \mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma})$$
(33)

is the partition function for the set of occupation numbers of that superconfiguration. Λ_{Ξ} is an estimate of the free energy of that superconfiguration. A rigorous calculation of the statistical weight implies a self-consistent computation of the electronic structure of each superconfiguration, what we precisely wish to avoid at this stage. It is satisfactory to take an estimate of the statistical weight making the following assumptions:

- In the calculation of the statistical sum U_{Ξ} , the one-electron energies (and subsequently the Boltzmann factors $X_i = e^{-\beta \epsilon_i}$) are approximated by the ones of the average atom.
- The free energy of the superconfiguration is estimated by the relation $\Lambda_{\Xi} \approx \mu Z_{\Xi}^*$, $Z_{\Xi}^* = Z - \sum_{\sigma \in \Xi} Q_{\sigma}$ being its ionization and μ the average-atom chemical potential.

The N_B superconfigurations are then sorted by decreasing weights. Finally, the list can be truncated by eliminating the superconfigurations with a weak weight, either using a criterion based on a maximum number, or on a minimum weight.

5. Adaptive Algorithm

5.1. Algorithm "Divide and Conquer"

We are looking for a partition \mathscr{B} of the ensemble of bound states in supershells, providing a compromise between constraints on the energies of the subshells of the kind: $\beta|\epsilon_i - \epsilon_j| \leq \eta$, for $i, j \in \sigma$ while generating a reasonable number of superconfigurations. We are looking for \mathscr{B} such as η be minimum under the constraint $N_{\Xi} \leq N_{\text{max}}$, where N_{max} is the maximum number that we do not want to override. For a fixed partition $\mathscr{B} = \{\sigma\}$, let us define

$$\begin{aligned}
\epsilon^{\sigma}_{\min} &= \min_{i \in \sigma} \epsilon_{i} \\
\epsilon^{\sigma}_{\max} &= \max_{i \in \sigma} \epsilon_{i} \\
\Delta \epsilon_{\sigma} &= \epsilon^{\sigma}_{\max} - \epsilon^{\sigma}_{\min}
\end{aligned} (34)$$

where ϵ_i are the energies of the average-atom model. For a fixed value of η , we try to find a partition \mathscr{B} such that

$$\beta(\epsilon_{\max}^{\sigma} - \epsilon_{\min}^{\sigma}) = \beta \Delta \epsilon_{\sigma} \le \eta.$$
(35)

For $i, j \in \sigma$, we have therefore $\beta |\epsilon_i - \epsilon_j| \leq \eta$. It is worth mentioning that the condition

$$\frac{|X_i - X_j|}{X_i} = \left|1 - e^{\beta(\epsilon_i - \epsilon_j)}\right| \le \eta \tag{36}$$

is equivalent, at first order, to $\beta |\epsilon_i - \epsilon_j| \le \eta$. We set two mechanisms:

 A procedure consisting of splitting ("Split") of a supershell *σ* into two supershells *σ*₁ and *σ*₂:

$$\sigma \to \sigma_1, \sigma_2 \quad \text{with} \quad \sigma_1 \bigcup \sigma_2 = \sigma.$$
 (37)

Such a mechanism will be activated if $\Delta \epsilon_{\sigma} > \eta$ (unverified energy criterion). Its effect is to reduce the energy differences, but it increases by one the size of the partition. The number of superconfigurations to generate is multiplied by

$$\frac{N_{\sigma_1}N_{\sigma_2}}{N_{\sigma}}.$$
(38)

• A concatenation (gathering) mechanism of consecutive σ_1 and σ_2 supershells ("Merge")

$$\sigma_1, \sigma_2 \to \sigma \quad \text{with} \quad \sigma_1 \bigcup \sigma_2 = \sigma.$$
 (39)

Such a mechanism will be activated if $N_{\mathscr{B}} > N_{\text{max}}$. Its effect is to reduce by one the size of the partition and the number of superconfigurations to generate is divided by the factor (38), but increases the energy differences inside the resulting supershell:

$$\begin{cases} \epsilon_{\min}^{\sigma} = \epsilon_{\min}^{\nu_1} \\ \epsilon_{\max}^{\sigma} = \epsilon_{\max}^{\nu_2} \\ \Delta \epsilon_{\sigma} = \Delta \epsilon_{\sigma_1} + \Delta \epsilon_{\sigma_2} + \epsilon_{\min}^{\sigma_2} - \epsilon_{\max}^{\sigma_1} \approx \Delta \epsilon_{\sigma_1} + \Delta \epsilon_{\sigma_2}. \end{cases}$$
(40)

5.2. Algorithm "Divide and Conquer": General Procedure

• <u>Phase 1:</u> gathering the supershells. As far as the number of superconfigurations to generate $N_{\mathscr{B}}$ is larger than an imposed maximal value N_{max} , we try to reduce the number of supershells $n_{\mathscr{B}}$ of the partition. More precisely, we look for two consecutive supershells such that the energy dispersion (spread) $\epsilon_{\text{max}}^{\sigma+1} - \epsilon_{\text{min}}^{\sigma} = \Delta \epsilon_{\sigma} + \Delta \epsilon_{\sigma+1} + \epsilon_{\min}^{\sigma+1} - \epsilon_{\max}^{\sigma} \approx \Delta \epsilon_{\sigma_1} + \Delta \epsilon_{\sigma_2}$ be minimal, i.e.,

$$\epsilon_{\max}^{\sigma+1} - \epsilon_{\min}^{\sigma} = \min_{r=1,\cdots,n_{\mathscr{B}}-1} \left\{ \epsilon_{\max}^{r+1} - \epsilon_{\min}^{r} \right\}.$$
 (41)

If $\beta(\Delta \epsilon_{\sigma} + \Delta \epsilon_{\sigma+1}) \leq \eta$, we gather the states of these two supershells into a unique supershell $\tilde{\sigma}$, with characteristics

$$\begin{cases}
G_{\tilde{\sigma}} = G_{\sigma} + G_{\sigma+1} \\
\langle Q_{\tilde{\sigma}} \rangle = \langle Q_{\sigma} \rangle + \langle Q_{\sigma+1} \rangle \\
\mathscr{V}_{\tilde{\sigma}} = \mathscr{V}_{\sigma} + \mathscr{V}_{\sigma+1}
\end{cases}$$
(42)

or

$$\begin{cases} \epsilon_{\min}^{\tilde{\sigma}} = \epsilon_{\min}^{\sigma} \\ \epsilon_{\max}^{\tilde{\sigma}} = \epsilon_{\max}^{\sigma+1} \\ \Delta \epsilon_{\tilde{\sigma}} = \Delta \epsilon_{\sigma} + \Delta \epsilon_{\sigma+1} + \epsilon_{\min}^{\sigma+1} - \epsilon_{\max}^{\sigma} \approx \Delta \epsilon_{\sigma} + \Delta \epsilon_{\sigma+1}. \end{cases}$$
(43)

Otherwise, end of phase 1.

• <u>Phase 2</u>: splitting the supershells. As far as there are supershells such that $\beta \Delta \epsilon_s > \eta$, and that the number of supershells $n_{\mathscr{B}}$ remains smaller than an imposed maximum value n_{\max} , we look for the supershell such that the energy dispersion $\Delta \epsilon_s$ be maximum:

$$\Delta \epsilon_{\sigma} = \max_{r \in 1, \cdots, n_{\mathscr{B}}} \{\Delta \epsilon_r\}.$$
(44)

The supershell is then split into two supershells, each one containing half of the states. <u>Phase 3:</u> relaxation of criterion: $\eta \rightarrow \eta + \delta \eta$. This phase is necessary if there is no

Phase 3: relaxation of criterion: $\eta \rightarrow \eta + \delta \eta$. This phase is necessary if there is no partition of the subshells that ensures several superconfigurations (but less than the critical value N_{max}).

5.3. Energy Criterion

It is possible to define an alternative criterion to replace Equation (35). The partition function reads

$$\mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \sum_{\substack{\{q_i\}\\ \sum_{i \in \sigma} q_i = Q_{\sigma}}} \prod_{i \in \sigma} {g_i \choose q_i} X_i^{q_i}$$

$$= \sum_{\substack{\{q_i\}\\ \sum_{i \in \sigma} q_i = Q_{\sigma}}} \prod_{i \in \sigma} {g_i \choose q_i} e^{-\beta [\sum_{i \in \sigma} q_i(\epsilon_i - \epsilon_{\sigma})]} e^{-\beta Q_{\sigma} \epsilon_{\sigma}}.$$
(45)

Linearizing

$$e^{-\beta\sum_{i\in\sigma}q_i(\epsilon_i-\epsilon_{\sigma})},\tag{46}$$

we obtain

$$e^{\beta Q_{\sigma} \epsilon_{\sigma}} \mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \sum_{\substack{\{q_i\}\\\sum_{i \in \sigma} q_i = Q_{\sigma}}} \prod_{i \in \sigma} {g_i \choose q_i} \left[1 - \beta \sum_{j \in \sigma} q_j (\epsilon_j - \epsilon_{\sigma}) \right], \tag{47}$$

which can be put in the form

$$e^{\beta Q_{\sigma} \epsilon_{\sigma}} \mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) - \beta \sum_{j \in \sigma} (\epsilon_{j} - \epsilon_{\sigma}) \times \sum_{\substack{\{q_{i}\}\\ \sum_{i \in \sigma} q_{i} = Q_{\sigma}}} q_{j} \prod_{i \in \sigma} {g_{i} \choose q_{i}}, \qquad (48)$$

where $\mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma})$ represents the number of micro-states introduced in Equation (17):

$$\mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \begin{pmatrix} G_{\sigma} \\ Q_{\sigma} \end{pmatrix}.$$
(49)

Applying the relation

$$Q_{\sigma} \begin{pmatrix} G_{\sigma} \\ Q_{\sigma} \end{pmatrix} = G_{\sigma} \begin{pmatrix} G_{\sigma} - 1 \\ Q_{\sigma} - 1 \end{pmatrix}$$
(50)

one can write

$$e^{\beta Q_{\sigma} \epsilon_{\sigma}} \mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) - \beta \sum_{j \in \sigma} g_{j}(\epsilon_{j} - \epsilon_{\sigma}) \\ \times \sum_{\substack{\{q_{i}\}\\ \sum_{i \in \sigma} q_{i} = Q_{\sigma}}} \prod_{i \in \sigma} {g_{i} - \delta_{ij} \choose q_{i} - \delta_{ij}}$$
(51)

yielding

$$e^{\beta Q_{\sigma} \epsilon_{\sigma}} \mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) - \beta \begin{pmatrix} G_{\sigma} - 1 \\ Q_{\sigma} - 1 \end{pmatrix} \times \sum_{j \in \sigma} g_j(\epsilon_j - \epsilon_{\sigma})$$
(52)

or

$$e^{\beta Q_{\sigma} \epsilon_{\sigma}} \mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) = \mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) - \beta \frac{Q_{\sigma}}{G_{\sigma}} \mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma}) \times \sum_{i \in \sigma} g_{i}(\epsilon_{i} - \epsilon_{\sigma})$$

$$(53)$$

leading itself to

$$e^{\beta Q_{\sigma} \epsilon_{\sigma}} \frac{\mathcal{U}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma})}{\mathcal{M}_{\sigma}(Q_{\sigma}, \{g\}_{\sigma})} - 1 = -\beta \frac{Q_{\sigma}}{G_{\sigma}} \sum_{j \in \sigma} g_j (\epsilon_j - \epsilon_{\sigma}).$$
(54)

The condition becomes therefore

$$\forall j \in \sigma, \beta |\epsilon_j - \epsilon_\sigma| \le \eta \to \left| e^{\beta Q_\sigma \epsilon_\sigma} \frac{\mathcal{U}_\sigma(Q_\sigma, \{g\}_\sigma)}{\mathcal{M}_\sigma(Q_\sigma, \{g\}_\sigma)} - 1 \right| \le Q_\sigma \eta.$$
(55)

Such a formulation is interesting since it provides an insight into the way the partition function is involved in the criterion. It is also of practical interest, since ϵ_{σ} is arbitrary and can therefore help avoiding numerical problems. Finally, on the contrary to Equation (35), the subshells have to be scrolled only once.

5.4. Link to the Master Theorem

The above-mentioned procedure belongs to the class of "divide and conquer" algorithms, which structure and complexity are governed by the so-called "Master theorem" [62]. Consider a problem that can be solved using a recursive algorithm which divides the problem into several sub-problems recursively, each sub-problem being of size n/b. The master theorem always yields asymptotically tight bounds to recurrences from divide and conquer algorithms that partition an input into smaller sub-problems of equal sizes, solve the sub-problems recursively, and then combine the sub-problem solutions to give a solution to the original problem. The master theorem states that the time for such an algorithm can be expressed by adding the work that they perform at the top level of their recursion (to divide the problems into sub-problems and then combine the sub-problem solutions) together with the time made in the recursive calls of the algorithm.

If T(n) denotes the total time for the algorithm on an input of size *n*, and f(n) denotes the amount of time taken at the top level of the recurrence then the time can be expressed by a recurrence relation that has the form

$$\mathcal{T}(n) = a \, \mathcal{T}\left(\frac{n}{b}\right) + f(n). \tag{56}$$

Here *n* is the size of an input problem, *a* is the number of sub-problems in the recursion, and *b* is the factor by which the sub-problem size is reduced in each recursive call (b > 1). This equation can be successively substituted into itself and expanded to obtain an expression for the total amount of work done.

6. Examples and Results

Let us consider the case of an iron plasma at T = 100 eV and $\rho = 0.01$ g/cm³. Table 1 represents, for the initial value $\eta = 0.05$, the final supershell partition, the number of iterations, the final value of the parameter η and the number of effective superconfigurations found for different values of the maximum number of superconfigurations authorized

 N_{max} (respectively 10, 100, 500, 1000, 5000, 10,000 and 50,000), in the case where the initial value of η is 0.05 (which is our usual default value). The initial supershell partition reads

```
(1s)(2s)(2p)(3s)(3p)(3d)(4s)(4p)(4d)(4f)

(5s)(5p)

(5d5f)

(5g)

(6s \ 6p)

(6d \ \cdots \ 6h)

(7s \ 7p)

(7d \ \cdots \ 7i)

(8s \ \cdots \ 8g)

(8h \ \cdots \ 8k)

(9s \ \cdots \ 9l)

(10s \ \cdots \ 10m)

(11s \ \cdots \ 12g)

(12h)
```

yielding 28,311,552 superconfigurations.

In the way the algorithm is computed, it is important to start with a small value of η . However, if the value is too low, the number of required iterations to reach convergence will be very large. For instance, in the case of $N_{\text{max}} = 1000$, if we start with $\eta = 0.0005$, the initial supershell partition is

$$(1s)(2s)(2p)\cdots(12h) \tag{58}$$

yielding 9,223,372,036,854,775,807 superconfigurations, and the final one, obtained after 1643 iterations (and a final value of η of 0.79):

$$(1s)(2s)(2p)(3s 3p)(3d)(4s 4p 4d 4f)(5s 5p 5d 5f 5g)(6s 6p ... 12h) (59)$$

represents 864 superconfigurations. In the case of $\eta = 0.05$ (as can be seen in Table 1), the initial supershell partition (given in Equation (57)), yields 28,311,552 superconfigurations and the supershell partition (59) together the subsequent 864 superconfigurations are obtained after 31 iterations (and a final value of η of 0.80). In the case where $\eta = 0.5$, one has

)

yielding 1296 superconfigurations, reduced finally with partition (59) to the 864 superconfigurations after 2 iterations (and a final value of η of 1). If η is too big, the algorithm will stop, because the number of superconfigurations is likely to be already below the critical

(57)

$$\begin{array}{c}
(1s) \\
(2s \ 2p) \\
(3s \ 3p \ \cdots \ 12h)
\end{array}$$
(61)

and the number of superconfigurations is 15 (the final value of η being 10). The algorithm could be easily improved by introducing a threshold (minimum) value of the number of superconfigurations, or to impose the final number of superconfigurations to be sufficiently (according to a particular criterion) close to N_{max} , thus allowing η to decrease. Table 2 contains the Rosseland and Planck means obtained with the different maximum numbers N_{max} of superconfigurations asked (see Table 1) and Figure 1 shows the corresponding spectral opacities. Of course, the spectrum is not sufficiently resolved for $N_{max} = 10$, but the purpose of our algorithm is to provide the best "sampling" of superconfigurations as possible for a specific maximum authorized number of superconfigurations (and therefore a maximum authorized computation time). We can see that in that case, the convergence as concerns the Planck and Rosseland mean is achieved for 5000 superconfigurations, but that acceptable values are already obtained for 500 ones.

Table 1. Final supershell partitions, number of iterations, final value of η and number of effective superconfigurations found for different maximum numbers N_{max} , in the case where our initial value of η has its default value 0.05. The initial number of superconfigurations, obtained with the supershell partition of Equation (57), is 28,311,552.

N _{max}	Final Partition	Number of Iterations	Final Value of η	Final Number of Superconfigurations
10	$(1s)(2s\cdots 12h)$	282	13.02	8
100	$(1s)(2s2p)(3s\ 3p\ 3d)\ (4s\cdots\ 12h)$	65	2.30	36
500	$\begin{array}{c} (1s)(2s)(2p) \\ (3s \ 3p \ 3d)(4s \cdots \ 4f) \\ (5s \cdots \ 5g)(6s \cdots \ 12h) \end{array}$	33	0.85	288
1000	$(1s)(2s)(2p) \ (3s3p)(3d) \ (4s \cdots 4f)(5s \cdots 5g) \ (6s \cdots 12h)$	31	0.80	864
5000	$(1s)(2s)(2p)(3s3p)(3d)(4s 4p)(4d 4f)(5s \cdots 5g)(6s \cdots 7i)(8s \cdots 12h)$	21	0.40	2592
10,000	$\begin{array}{c} (1s)(2s)(2p) \\ (3s3p)(3d) \\ (4s\ 4p)(4d\ 4f)(5s\ \cdots\ 5g) \\ (6s\ \cdots\ 6h)(7s\ \cdots\ 7i) \\ (8s\ \cdots\ 12h) \end{array}$	20	0.40	5184
50,000	$\begin{array}{c} (1s)(2s)(2p)(3s)(3p)(3d) \\ (4s4p)(4d4f)(5s\cdots 5g) \\ (6s\cdots 6h)(7s\cdots 7i) \\ (8s\cdots 9l)(10s\cdots 12h) \end{array}$	15	0.25	31,104

N _{max}	Planck Mean	Rosseland Mean
10	1715	321.2
100	1611	211.6
500	1616	220.1
1000	1617	215.4
5000	1621	216.7
10,000	1621	216.7
50,000	1621	216.7

Table 2. Planck and Rosseland means in the different cases displayed in Table 1. The average ionization is 15.45.



Figure 1. Total opacity of an iron plasma at T = 100 eV and $\rho = 10^{-3} \text{ g/cm}^3$ computed in the different cases $N_{\text{max}} = 10$, 100, 1000 and 10,000, which characteristics are provided in Table 1. The black ($N_{\text{max}} = 10,000$) and red ($N_{\text{max}} = 1000$) curves are almost superimposed.

Figure 2 displays a comparison between the experimental opacity deduced from an absorption-spectroscopy experiment performed on ASTERIX IV laser facility (Garching, Germany) [9,15,16] and different STA calculations, involving 3, 56, 385 and 2000 superconfigurations, respectively. The temperature is 22 eV and the density of 0.01 g/cm³. The two calculations corresponding to 385 and 2000 superconfigurations are almost superimposed. Opacity measurements are of crucial importance to test the models. However, such experiments are difficult and subject to many uncertainties [63]. Moreover, they obviously concentrate on a narrow spectral range, which is not necessarily in the vicinity of the maximum of the Planck distribution or of its derivative with respect to the temperature. Therefore, a convergence criterion focusing on the spectrum in this finite range is not equivalent to a convergence of the Rosseland mean.



Figure 2. Interpretation of an experimental spectrum measured on ASTERIX IV laser facility (Garching, Germany) by Winhart et al. [9,15,16]. The areal mass of the iron sample is $20 \ \mu g/cm^2$. The best agreement was obtained at a temperature of 22 eV and a density 0.01 g/cm³. The calculations have been carried out with 3, 56, 385 and 2000 superconfigurations, corresponding to 2, 3, 4 and 9 supershells respectively.

7. Other Possible Algorithms and Discussion

7.1. Generating Superconfigurations Using the Correlated Gaussian Approximation for Configurations

The following algorithm was suggested by Faussurier ([36] and private communication). The charge state distribution can be put in the form

$$\mathcal{P}(x) = \frac{1}{\sqrt{2\pi\mathcal{V}_B}} \exp\left[-\frac{(x-Z^*)^2}{2\mathcal{V}_B}\right] = \frac{10^{-k}}{\sqrt{2\pi\mathcal{V}_B}}$$
(62)

with $x = Z^* \pm \alpha \sqrt{V_B}$ and [48,64,65]

$$\mathscr{V}_B = \sum_{i,j} \left(\mathbf{M}^{-1} \right)_{ij}.$$
 (63)

The idea is to keep the ions between $\lfloor Z^* - \alpha \sqrt{\mathcal{V}_B} \rfloor$ and min $[Z, \lfloor Z^* + \alpha \sqrt{\mathcal{V}_B} \rfloor]$, where $\lfloor x \rfloor$ represent the integer part of *x*. For each supershell, the occupation number is allowed to vary between $Q_{\sigma,\min}$ and $Q_{\sigma,\max}$ defined as

$$Q_{\sigma,\min} = \max\left[0, \left\lfloor\sum_{i\in\sigma}\langle q_i \rangle - \alpha\sqrt{\mathscr{V}_{\sigma}}\right\rfloor\right], Q_{\sigma,\max} = \min\left[G_{\sigma}, \left\lfloor\sum_{i\in\sigma}\langle q_i \rangle + \alpha\sqrt{\mathscr{V}_{\sigma}}\right\rfloor\right],$$
(64)

where

$$\mathscr{V}_{\sigma} = \sum_{i,j\in\sigma} \left(\mathbf{M}^{-1} \right)_{ij}.$$
(65)

To define the supershells, one has to find the intersection point between the modeled energy distributions of the subshells i and i + 1:

$$\mathcal{D}_{i}(\epsilon) = \frac{1}{\sqrt{2\pi\mathcal{V}_{i}}} \exp\left[-\frac{(\epsilon - \epsilon_{i})^{2}}{2\mathcal{V}_{i}}\right]$$
(66)

and

$$\mathcal{D}_{i+1}(\epsilon) = \frac{1}{\sqrt{2\pi\mathcal{V}_{i+1}}} \exp\left[-\frac{(\epsilon - \epsilon_{i+1})^2}{2\mathcal{V}_{i+1}}\right]$$
(67)

yielding

$$\epsilon_i + \sqrt{-2\mathscr{V}_i \ln(\xi_i)} = \epsilon_{i+1} - \sqrt{-2\mathscr{V}_{i+1} \ln(\xi_i)}$$
(68)

with

$$\xi_{i} = \exp\left[-\frac{1}{2}\left(\frac{\epsilon_{i+1} - \epsilon_{i}}{\sqrt{\mathscr{V}_{i+1}} + \sqrt{\mathscr{V}_{i}}}\right)^{2}\right].$$
(69)

The physical meaning of Equations (66) and (67) may seem questionable, since they are energy distribution and the variance \mathscr{V}_i and \mathscr{V}_{i+1} are occupation-number variances. This approximation, however, can be justified considering the continuous variation of the energy of the occupied subshell as proportional to its occupation number. If $\xi_i \rightarrow 0$, the overlap tends to be weak and if $\xi_i \rightarrow 1$ it becomes difficult to distinguish between the two distributions \mathcal{D}_i and \mathcal{D}_{i+1} . The chain is broken in increasing order of the ξ_i . Let us consider that the length of link *i* is $\alpha \xi_i$. At each step, the supershell containing the largest link is cut (see Figure 3).

$$(1s - - - - 2s - - 2p - - - - - 3s - 3p - - - - 3d - - - 4s - - - 4p - - - - - 4d - - 4f)$$

$$(1s) (2s - - 2p - - - - - 3s - 3p - - - - 3d - - - 4s - - - 4p - - - - - 4d - - 4f)$$

$$(1s) (2s 2p) - - - - - 3s - 3p - - - - 3d - - - 4s - - - 4p) (4d - - 4f)$$

$$(1s) (2s 2p) (3s - 3p - - - - 3d - - - 4s) (4p) (4d - - 4f)$$

$$(1s) (2s 2p) (3s - 3p) (3d - - - 4s) (4p) (4d - - 4f)$$

$$(1s) (2s 2p) (3s - 3p) (3d) (4s) (4p) (4d - - 4f)$$

$$(1s) (2s 2p) (3s - 3p) (3d) (4s) (4p) (4d - 4f)$$

Figure 3. Illustration of the method described in Section 7.1.

The advantage of such an approach is that the average-atom model and the fluctuation theory enable one to know *a priori* the order in which the supershells will be built, as well as the number of superconfigurations obtained at each step. Therefore, a proper estimate of the electronic correlations is required in order to avoid an underestimate of the energy separation between subshells and an overestimate of the number of superconfigurations. The parameter α (typically between 1 and 10) must be chosen by the user. The relative population of a superconfiguration can be estimated by the product of Gaussian distributions such as the one of Equation (62) attributed to the different supershells. If the population is smaller than a given small parameter, then it can be disregarded, although it belongs to the initial set resulting from Equations (28) and (29).

7.2. The Scroll Algorithm

The following algorithm was proposed by Bar-Shalom et al. It was designed for the collisional-radiative superconfiguration code SCROLL (Super Configuration Radiative cOLLisional) [66–68]. The code takes into account the numerous excited and autoionizing states using superconfigurations. These are split systematically until the occupation numbers converge. The superconfigurations are refined in a stepwise manner until some convergence is reached. When the superconfiguration structure is fixed, the occupation

numbers of the superconfigurations are obtained by solving the collisional-radiative-model rate equations:

$$\frac{dN_{\Xi}}{dt} = -N_{\Xi} \sum_{\Xi'} \mathscr{R}_{\Xi\Xi'} + \sum_{\Xi'} N_{\Xi'} \mathscr{R}_{\Xi'\Xi}$$
(70)

where N_{Ξ} are the superconfiguration populations and $\mathscr{R}_{\Xi\Xi'}$ are the superconfiguration transition rates, averaged over the initial configurations $C \in \Xi$ and summed over all final configurations $C' \in \Xi'$. A basic initial assumption (relaxed in the course of the computation) in this model is that within a superconfiguration, the configuration occupation numbers N_C are estimated by a Boltzmann factor. The superconfiguration-averaged rates can thus be written as

$$\mathscr{R}_{\Xi\Xi'} = \frac{1}{\mathcal{U}_{\Xi}} \sum_{C \in \Xi, C' \in \Xi'} \mathcal{U}_C \mathscr{R}_{CC'}$$
(71)

where $\mathscr{R}_{CC'}$ are the configuration-to-configuration rates and \mathcal{U}_C the configuration partition functions. In the case of one-electron jumps, we have

$$\mathscr{R}_{CC'} \propto \frac{q_{\alpha}(g_{\beta} - q_{\beta})}{g_{\alpha}g_{\beta}} \times \mathscr{D}_{\alpha\beta}$$
(72)

where $\mathscr{D}_{\alpha\beta}$ is the radial integral associated with the transition and computed with HULLAC (Hebrew University Lawrence Livermore Atomic Code) [69]. The assumption of LTE within superconfigurations is relaxed by a convergence procedure where at each step, supershells are split, giving rise to a new set of superconfigurations in Equation (70). This splitting is done in a systematic manner following a "binary tree" algorithm. The initial occupation numbers of these new superconfigurations are taken as proportional to their partition functions. All the necessary new rates are then computed. Actually, only the occupation-number factor needs to be re-evaluated, since the $\mathcal{D}_{\alpha\beta}$ are taken from a precomputed database. Then the steady state collisional-radiative-model matrix is rebuilt and solved. A sparse matrix algorithm is used, since the superconfigurations belonging to charge states differing by more than one unit are not connected. The resulting occupation numbers are then compared to the initial ones. The superconfigurations are split in this way, repeatedly, until all N_{Ξ} converge. This convergence process eliminates gradually the explicit dependence of the rates on the LTE Boltzmann factors in \mathcal{U}_O . In the configuration limit it disappears completely. In order to accelerate the convergence of this process, the temperature assumed for the LTE occupation numbers within the superconfiguration is not the electron temperature T_e , but an effective ionization temperature T_z defined by Busquet [70].

7.2.1. Effective (Ionization) Temperature

The algorithm starts with a guess for the ionization temperature T_z . The idea behind such a concept is that the non-LTE spectrum at T_e is very close to an LTE calculation at T_z . For that guess, Busquet's model can be used [70–72], or one can simply start with T_e . With this temperature, an average-atom calculation is performed to obtain Z^* and an initial potential. The latter is used in a version of the HULLAC code with hydrogenic configurations [69], to obtain the orbital rates. At this point, a crude supershell structure is defined. A loop is described over pairs of superconfigurations and for each pair all the average rates are added to the rate matrix. A sparse matrix method is used to solve the rate equations for the occupation numbers (with the internal convergence iterations splitting supershells as mentioned above) and calculate Z^* .

The STA code is now run to find the temperature T_z that produces this average charge state Z^* in LTE. At this point, one has to go back to the calculation of rates and so on until convergence [68].

7.2.2. Binary Supershell Split Algorithm

A central point in the splitting procedure is that unlike the LTE case, it is crucial to work with the minimal matrix size. This restricts the number of supershells. The authors have therefore adopted an algorithm based on a binary tree approach.

A node represents a supershell. Starting with a single node of all bound shells, one begins splitting nodes to two daughter nodes. For each node indexed by n, the left and right daughters are indexed by 2n and 2n + 1, respectively. One goes down the tree splitting the left daughters while keeping all the other nodes fixed until convergence of that route. At this point, one must go back up the tree to the lowest unconverged parent node, take its right node and go down again splitting left daughters. We proceed in this way until all the nodes are locally converged with all other nodes fixed. At this point, the final supershell structure is constructed from all the converged nodes and a single splitting on each final node is performed separately to check the total convergence.

This algorithm, together with the one described in Section 7.1, proceeds in a unidirectional way (although the SCROLL models offer the possibility to go back in the tree, once a branch comes to its end it is not modified anymore, and other branches of the tree are explored). In other words, such algorithms consist of splitting supershells, but not gathering them. We do not pretend that our adaptive algorithm is more efficient that the above-mentioned ones. The most important points are that it is designed to ensure an optimal representation of atomic states for a given maximum authorized number of superconfigurations, and that its specificity is to rely on successive splitting and grouping.

8. Conclusions

We presented different algorithms for the generation of superconfigurations, which constitute the first step of an opacity calculation (for local thermodynamic equilibrium or non-local-thermodynamic-equilibrium plasmas) relying on the Super Transition Array approach. This is a critical issue of opacity calculations, which necessarily have to make a compromise between accuracy and completeness, which often turns out to be a real dilemma. It is difficult to assert without hesitation which algorithm is the best. Among the ones discussed above, the adaptive "divide and conquer" algorithm, which constitutes the main new result of the present work, is probably the most efficient one, since it provides the best sampling for a fixed maximal number of superconfigurations. However , the "ideal" algorithm would probably take into account the most important transitions in the plasmas, at the given temperature and density, i.e., the transitions which will contribute to the Rosseland mean.

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Abbreviations

The following abbreviations are used in this manuscript:

CRSTA	Configurationally Resolved Super Transition Array
DLA	Detailed Line Accounting
HULLAC	Hebrew University Lawrence Livermore Atomic Code
LTE	Local Thermodynamic Equilibrium
SCO	Superconfiguration Code for Opacity
SCROLL	Super Configuration Radiative cOLLisional
SOSA	Spin-Orbit Split Array
STA	Super Transition Array
UTA	Unresolved Transition Array

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