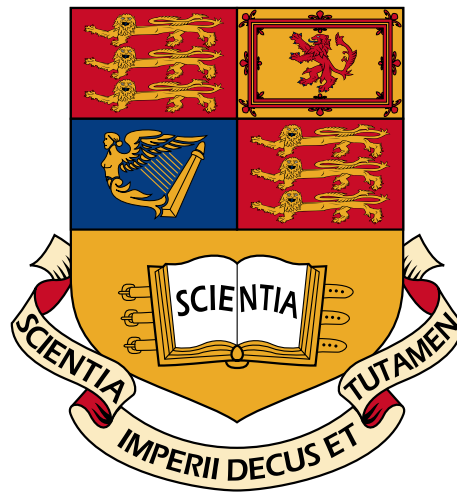


Development of a Pseudo Non-LTE model for Z-pinch simulations

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Submitted in partial fulfilment of the requirements for the degree of Doctor of
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Declaration

I hereby certify that the material in this thesis, which I submit for the degree of Doctor of Philosophy, is entirely original unless otherwise cited or acknowledged in the text.

Nicolas-Pierre Louis Niasse

27 September 2011

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DÉDIÉ À CEUX QUI S'ACCROCHENT AU PINCEAU
LORSQU'ON LEUR RETIRE L'ÉCHELLE

Abstract

Predicting the energetic and spectral characteristics of Z-pinch sources is a very delicate task. Z-pinch plasmas conditions are spread across a wide range of parameter space and often far from Local Thermodynamic Equilibrium (LTE). In addition, the increasing optical depth of the plasma at stagnation can have a strong influence on its own dynamics, suggesting that simultaneous solution of both the magnetohydrodynamic (MHD) and radiative response is required. Unfortunately, the estimation of the frequency and time dependent radiative properties of Z-pinch is computationally challenging and the recent improvements made to the parallel architecture of the 3D resistive Eulerian MHD code GORGON have only reinforced the strong emphasis already placed on optimizing the physics solvers used in Z-pinch simulations.

To address these issues, we have developed a simple and fast pseudo NLTE code based on a Screened Hydrogenic Model (SHM) that can be run in-line with GORGON or as a post processing tool with synthetic spectra capabilities. Making use of a computationally inexpensive modification of the Saha equation, this highly optimized code has demonstrated a good ability to represent Non-LTE plasma conditions. In order to handle the amount of data generated by the spectral treatment of the billions of numerical cells constituting the simulation grids, an original data structure derived from a self-balancing binary search tree has been developed, enabling the use of Non-LTE DCA calculations in a large scale three dimensional environment for the first time.

The implementation of this model is described in detail and comparisons with a commercial package are offered. Results from Z-pinch simulations performed with the new code are discussed and possible future improvements are presented.

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Thesis Outline

The following work is divided into six parts.

The first Chapter is a general introduction to Z-pinch physics and presents the main concepts related to wire array dynamics, design and limitations.

In Chapter 2, the current numerical methods developed in order to model the evolution of Z-pinch plasmas are described and the requirements of the new radiation model are outlined.

In Chapter 3, we recall the basic atomic physics concepts related to plasma simulations and make a quick review of some of the existing theoretical approaches.

In Chapter 4, we introduce the inline version of the new atomic solver in details, outlining some of the methods employed to optimize the calculations.

Chapter 5 focus on the specificities of the offline implementation and compares the results obtained with a commercial package.

Finally, in Chapter 6, we presents and discuss the results of several three-dimensional Z-pinch simulations incorporating the new model.

Chapter 1

The Z-pinch approach to fusion

Nuclear fusion is a process in which atomic nuclei merge or “fuse” together to form a heavier single nucleus. In the case of light elements, this process is accompanied by the release of a very large amount of energy (under the form of radiation and kinetic energy given to the reaction products) and unlike fission, does not generate long-lived radioactive waste.

For the last 50 years, tremendous efforts have been invested in controlled nuclear fusion research. The quest for a new energy source that could advantageously replace the fossil and conventional/current nuclear fuels has led to the study of a large variety of reactor concepts. The vast majority of these designs are aimed to achieve thermonuclear conditions in a plasma of hydrogen isotopes.

Indeed, in order to fuse, particles have to overcome the mutual electrostatic repulsion of their nuclei and get close enough to merge by means of the strong nuclear force. The probability for a given fusion reaction to occur is a function of the particles relative velocity and admits a maximum depending on the reaction considered. Therefore, by heating up a gas of reactants (thus increasing the velocity of its particles) to the temperature of interest, one can expect the formation of a thermal plasma in which some ions would have acquired sufficient kinetic energy to overcome the previously mentioned “Coulomb barrier”.

For an energy production device based on this principle to be economically efficient, it has to be designed to minimize at maximum the amount of power required to keep the plasma in thermonuclear conditions, which in turn implies keeping the various losses as small as possible. This idea of confining the energy in the plasma is the key feature that led to the division of the fusion energy research into two branches.

The Magnetic Confinement Fusion (MCF) approach to this problem is, as the name suggests, to use magnetic fields to confine the hot mixture of reactants. This concept relies on the ability to create a thermonuclear plasma and maintain it in a steady state for a relatively long time (several seconds) using the magnetic pressure created by a special configuration of solenoids, the mixture being kept hot by ohmic and radio frequency heating. In the Inertial Confinement Fusion (ICF) scheme, on the other hand, fusion conditions are only upheld for a very short time (few ns) and the energy confinement is mainly ensured by the fuel high density and inertia. Most of the ICF concepts are aimed to uniformly compress and heat a target (generally a small spherical capsule filled with deuterium/tritium) up to its ignition point. Typically, by directly or indirectly subjecting the low Z materials constituting the surface of the capsule to a high incident X-ray flux, the multiple beams of a high power laser produce an outward ablation flow that conversely exerts an inward thrust driving the target compression. A great deal of the challenge lies in the difficulty of controlling the multiple instabilities occurring during the compression process while delivering the right amount of heating power at the very right moment. This last condition justifies in itself the initial use of lasers for ICF research.

Nevertheless, for many years now, it has been shown that Z-pinches were also very intense and reliable sources of X-ray power. Being one of the most efficient way of converting magnetic energy into radiative energy, modified Z-pinch configurations have further demonstrated the possibility of pulse shaping, thus opening

the door to ICF applications.

Developing and optimizing targets and pulsed power devices that could lead to Z-pinch fusion reactors demands a deep understanding of the physics involved. Unfortunately, the many complexities and nonlinearities of these systems leave little room for analytical solutions. As a matter of fact, it appears that a better comprehension of the Z-pinch dynamics requires to perform large scale numerical simulations combining a great number of methods and models borrowed from various branches of physics (Plasma Physics, Radiative and Resistive Magnetohydrodynamic (MHD), Quantum Equation Of States (QEoS), etc...) with a good amount of supercomputing power.

This work by no means pretends to embrace all the aspects of this formidable task. It constitutes an attempt to address one part of the problem, laying down the basis of a simple pseudo Non-LTE model suitable for Z-pinch simulations.

1.1 Motivations for Cylindrical Wire Array

Z pinches studies

Laboratory Z-pinches are a very old concept dating back to the end of the 18th century when a Dutch scientist named Martin van Marum[21] made use of a 100 Leyden jars¹ to discharge 1 kJ of energy into a 1 meter long metallic wire, making it explode. The causes of this explosion remained unknown until the beginning of the 19th century when studies on crushed lightning rods performed by Pollock and Barraclough[33] in Australia led to the understanding of the magnetic field - current interaction process responsible of the phenomenon. Subsequently, in 1934, Bennettwill derive the important relation describing the pressure balance for a stable Z-pinch.

Investigations on Z-pinches for fusion related applications started in the 50s'

¹early type of capacitor made of a glass jar.

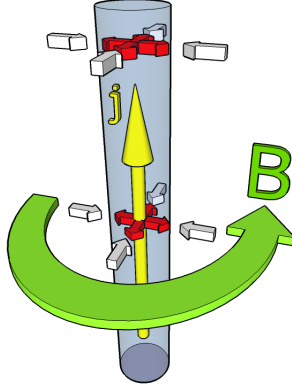


Figure 1.1: Schematic of a Z-pinch equilibrium, where the thermal pressure (red arrows) created by the axial flow of current j (in yellow) balances the magnetic pressure (white arrows) associated with the azimuthal magnetic field B (in green).

in conjunction with other thermonuclear fusion studies. The initial idea was to ohmically heat deuterium-tritium gas mixture using high current and to keep the resulting plasma in equilibrium, self-constricted in the axial (Z) direction, the magnetic energy balancing the internal one (fig 1.1) (Pease and Braginskii[30] will later predict that pinches can be subjected to radiative collapse for sufficient current).

Experiments were carried out that seemed to exhibit the production of neutrons. Unfortunately, it was found that these neutrons were not of thermonuclear nature but sub-products of accelerated deuterons. Instabilities in the plasma column were causing current disruptions introducing high electric field which, in turn, were accelerating the ionised deuterium atoms. The discovery of this latest phenomenon dismissed the Z-pinches from the fusion research field for decades.

In the beginning of the 1960s', some annular gas shell experiments were also conducted by Linhart and Massonier et al.[19]. In this special configuration, the acceleration of the gas "liner" toward the central axis is taking the major part of the current pulse width. Therefore, when the plasma reaches the axis, the magnetic pressure has already dropped and the shell simply bounces back, converting a major part of its kinetic energy into x-ray radiation but preventing the pinch

from reaching the equilibrium state[35]. Although less perturbed by equilibrium instabilities, gas shells are more sensitive to Rayleigh-Taylor ones. Furthermore, this kind of set up is originally nonconducting when the current is switched on. This last point leads to multiple breakdowns in the material causing unpredictable initial states of discharges.

The interest for Z-pinches was revived in 1976 when Stallings et al.[41] made use of wire array loads for the first time. Replacing the gas shells, these metallic "liners" were conducting the current by default and therefore represented the assurance of a better control on the initial state and implosion symmetry. Although the number of wires was limited at that time, this original approach resulted in a considerable sharpening of the x-ray pulse. Nevertheless, the first concepts of fusion targets radiatively driven by Z-pinches will not be published before 1991 (Smirnov[39]).

In the middle of the 90s', technological progress allowed the use of loads made of hundreds of very fine metallic wires assembled together into symmetrical cylindrical configurations. Sanford et al.[36] demonstrated in 1996 that by reducing the gap between the wires, the x-ray production could be dramatically improved. Later on, the introduction of nested concentric arrays by Davis et al.[14] on the Z facility at Sandia National Laboratories will further increase the radiative performance.

1.2 Description of the dynamics

As it was briefly mentioned in the previous part, a cylindrical wire array Z-pinch consists of two electrodes linked together axially by very thin metallic wires (few μm $\varnothing$) arranged in cylinder (fig 1.2a). These electrodes are themselves connected to a pulse-power generator providing a current of several mega-amperes in a very short time ($\sim 100ns$).

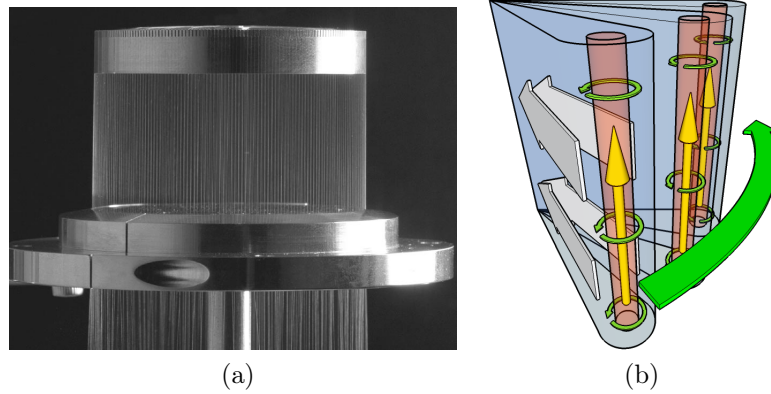


Figure 1.2: (a) A photograph of a 4 cm diam tungsten wire array at Sandia National Laboratories. The array has 240, $7.5 \mu\text{m}$ diameter wires[40]. (b) Schematic of the magnetic field topology around the wires (in red) of a cylindrical array with the local (little green arrows) and global (big green arrow) azimuthal fields associated with the current (yellow) sweep the coronal plasma (in blue) to the axis.

1.2.1 Ablation phase

In the early stages of a Z-pinch experiment, current flow starts and the wires are heated ohmically. Hot plasma is then ablated from the material and forms a coronal layer around each wire. The majority of the current is subsequently conducted through this coronal plasma, as it has much lower resistance than the wire core (Spitzer like resistivity $\eta \propto T^{-3/2}$). This large current forms a local poloidal magnetic field around each wire and a more global poloidal field around the whole array (fig 1.2b). The Lorentz force therefore sweeps the coronal plasma towards the axis where it forms a precursor column.

For many years, it had been assumed that the dynamics of the array at this point could be described by the simple analytical model of a thin shell of plasma imploding on the axis (0D model). Indeed, it was suggested that the small fraction of the wires mass represented by the precursor plasma was converging to the axis letting the wire cores exposed to the strong axial electric field. This latter was supposed to ionise the total mass of remaining material, which in turn would have converged following the equation of radial motion:

$$m_0 \frac{d^2 r}{dt^2} = -\frac{\mu_0 I^2}{4\pi r} \quad (1.1)$$

where m_0 is the total mass (per unit length) of the shell and $I = I(t)$ the pinch current.

However, the radiographs of the experiments showed that the wire cores were surviving at their initial position for as long as 80 % of the implosion time (given by the 0D model). Thus, it became obvious that the dynamic would be better represented by an equation describing the ablation rate at a fixed radius:

$$V_a \frac{dm}{dt} = -\frac{\mu_0 I^2}{4\pi R_0} \quad (1.2)$$

where m is the mass per unit length, R_0 the initial radius of the pinch and V_a the ablation velocity. This is the so-called rocket model[26]. The velocity V_a is in general measured but can be treated as a parameter depends weakly on a number of variables such as the diameter, the interwire gap or the wire diameter[13]. Integrating 1.2, we can find the mass already ablated from the wires at some moment t :

$$\delta m(t) = \frac{\mu_0}{4\pi V R_0} \int_0^t I^2 dt \quad (1.3)$$

Typically, with V_a experimentally measured for different materials, taking $t = 0.8 t_{implosion}$ in the equation above gives $\delta m/m_0 \sim 0.5 - 0.6$. Without taking a closer look to the radiographs, the fact that $\sim 50\% - 60\%$ of the wire material is ablated at 80% of the implosion time does not explain by itself the change of dynamic and the start of the radial motion at that time.

In fact, these radiographs also reveals the existence of periodic axial modulations in the coronal plasma flow. These instabilities form "bulges" and "necks" in the ablated plasma along the wires, modulating the radial streams with a spa-

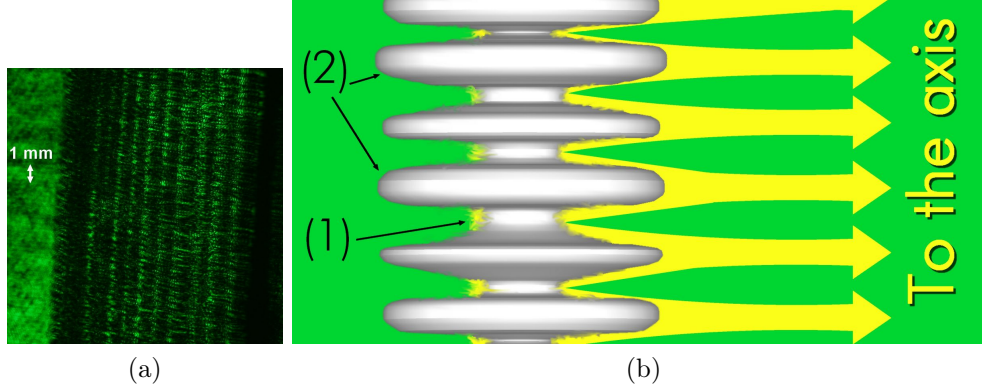


Figure 1.3: (a) Lasers images of shot 0718_06 on MAGPIE ($32 \times 10 \mu\text{m}$ Al), short wavelength instabilities are observed along the wires. (b) Schematic of axial modulation with plasma tranfers from the "neck" (1) to the "bulges" (2) before being streamed (yellow arrows) to the axis.

tial periodicity similar to the core size (~ 0.5 mm for Al, ~ 0.25 mm for W)(fig 1.3a). Although the plasma streams are seemingly produced by the "bulges", wire gaps open at the "neck" positions after 80% of the implosion time. We can infer from this last point that the plasma is ablated from half of the wires length (in the "neck" zones), transfers axially by MHD instabilities to the "bulges" and streamed to the axis (fig 1.3b). Consequently, the average ablation of 50% of the mass given by equation 1.3 appears to match the complete ablation of the wires half-length.

1.2.2 Snowplow implosion

As it was mentioned before, the full ablation at some points leads to the wires breakage. The opening of these gaps is the trigger to the second phase of the dynamic, the "snowplow" implosion. Driven by the magnetic "piston", the remaining plasma is push toward the central axis, accumulating on its front the precursor and leaving behind the rest of the wire cores. This compression converts the kinetic energy of the plasma (previously contained inside the Poynting flux) into internal energy which will be in part released as radiation (a radiative cooling mechanism allowing further compression). We can make an estimation of

the power increase during the snowplow, assuming that the density profile of the plasma inside the array (averaged in the axial and azimuthal directions) can be integrated from the equation . The "retarded density" is given by:

$$\rho(r, t) = \frac{\mu_0}{8\pi^2 V_a^2 R_0 r} \left(I \left(t - \frac{R - r}{V_a} \right) \right)^2 \quad (1.4)$$

Taking the variation of the kinetic energy, we obtain the power increase :

$$P(t) = \frac{1}{2} \frac{dm}{dt} \left(\frac{dr}{dt} - V_a \right)^2 \propto \frac{1}{2} \rho(r, t) (V_p - V_a)^3 \quad (1.5)$$

With V_p the pinch (radially imploding edge) velocity. The values given by this equation are in good agreement with the experiments.

1.2.3 Stagnation phase

Unfortunately, the radial implosion is not endless and the "snowplow" finally stops when the thermal pressure balances the magnetic one. During this stagnation phase, the ion kinetic energy is initially thermalized by ion-ion collisions before heating up the electron by equipartition. This increase of the electron temperature leads to further ionization in the plasma and the release of strong x-ray radiation. The resulting smaller thermal pressure related to the loss of some internal energy can no longer sustain the external magnetic one: the compression is resumed and the cycle is repeated. This process is the essence of the radiative cooling mechanism.

If the density has reached such a level that the plasma becomes optically thick, radiation losses are not substantial enough to extract the thermal energy from the pinch . In that extreme case, the "black body limit" prevents any additional compression.

1.3 Applications to ICF and limitations

For many years, it has been shown that cylindrical wire array Z-pinches are a very efficient way to convert electrical energy into thermal X-ray energy, which makes them attractive drivers for Inertial Confinement Fusion (ICF). The impressive results achieved on the Z-facility at Sandia National Laboratories of 1.8 MJ energy and 220 TW x-ray power give a strong impetus to this possibility.

1.3.1 The hohlraum concept

The hohlraum approach is a concept well-known by the ICF community. It consists in employing a cavity coated with a high Z material (for example gold) in order to get energy densification and spatial homogenisation of the radiation emitted by a primary source (laser, Z-pinch, etc...) (fig 1.4). This smoothed radiation is therefore used to drive a plastic capsule containing a mixture of deuterium and tritium to fusion conditions.

Let's consider that the hohlraum volume has been filled with some radiation stemming from the source. The cavity delivers a certain amount of radiant energy flux to the walls of the hohlraum. A part of this incident flux is in general re-emitted by the walls in the form of thermal radiation $\sigma_{SB}T^4$ (see A.1), while another part is lost in the body. Assuming that the walls behave like a black body, the radiative temperature inside can be estimated considering the following equilibrium: at each instant, the power from the primary source balances the power losses from the diagnostic holes and the absorption in the hohlraum walls. These last considerations give [22]:

$$P_{rad} = \sigma_{SB}T_r^4(A_{diags} + (1 - \alpha)A_{walls}) \quad (1.6)$$

with P_{rad} power of the source, σ_{SB} the Stefan-Boltzmann, T_r the radiative temperature, α the albedo of the cavity (fraction of the incident energy that is reemitted

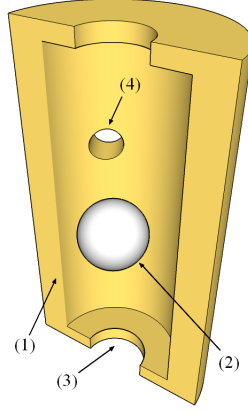


Figure 1.4: Cross section of a typical hohlraum. (1) High Z material walls (2) Target capsule (3) Entry hole (4) Diagnostic hole.

by the walls), A_{diags} the area of the diagnostic holes and A_{walls} the area of the cavity walls. Thus, it becomes possible to evaluate the power enhancement allowed by a given hohlraum (neglecting the diagnostic losses):

$$\frac{P_{rad}}{1 - \alpha} = \sigma_{SB} T^4 A_{walls} \quad (1.7)$$

with α typically ~ 0.8 , an enhancement of ~ 5 is expected. It appears that optimizing the cavity efficiency comes to increase the walls albedo and the source power per unit area (P_{rad}/A_{walls}).

Vacuum hohlraum

For the Z-pinch configuration, fulfilling the last condition led to place the cylindrical arrays inside the hohlraum, the latter performing the role of return current path at the same time. Driving a capsule to ignition requires a fine control of the radiation shape and timing, necessities incompatible with the presence of the target inside the primary chamber. For symmetry requirements, a concept of double-ended hohlraum (DEH) using two compact nested Z-pinches to drive a secondary cavity has been proposed (fig 1.5). In this configuration, a large pulse power generator[42] will provided the current needed to drive 2 PW in the sec-

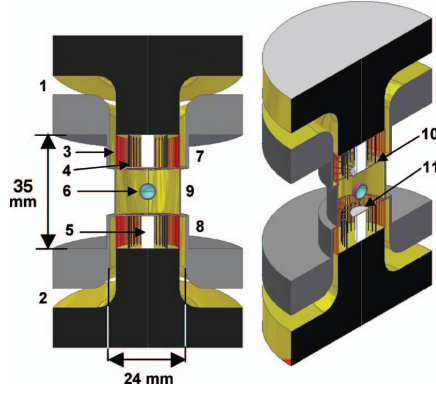


Figure 1.5: (Color) This is the conceptual layout of the double z-pinch driven hohlraum ICF concept . The design is symmetric about the midplane. Shown here are the (1) upper MITL power feed, (2) lower MITL power feed, (3) outer wire array, (4) inner wire array, (5) foam pulse shaping target, (6) high-yield scale cryogenic fusion capsule, (7) upper primary hohlraum, (8) lower primary hohlraum, (9) secondary hohlraum, (10) beryllium spokes for coupling to secondary , and (11) axial shine shield to prevent pole hot capsule drive. (see [42])

ondary chamber and reach the 220 eV required for ICF.

Dynamic hohlraum

Setting up cylindrical arrays inside the cavities implies designing relatively large diameter hohlraums ($\sim 20\text{mm } \varnothing$) which will therefore be limited in temperature. A solution to this problem consists in using the imploding array itself as a radiative cavity (fig 1.6).

Embedded in a low opacity foam liner, the fusion capsule is placed on the axis at the center of the array. During the implosion phase, the array impacts the outer layer of the foam, radiating a consequent part of its kinetic energy. Diffusing through the optically thin liner, this radiation is trapped and thermalized by the high-Z imploding wall constituted by the array material. In this configuration, the constant decrease of the hohlraum surface area with the magnetic compression of the liner ensures a high radiation temperature and a substantial power enhancement in the cavity. In addition, the energy coupling between the source and the target is facilitated by their mutual proximity.

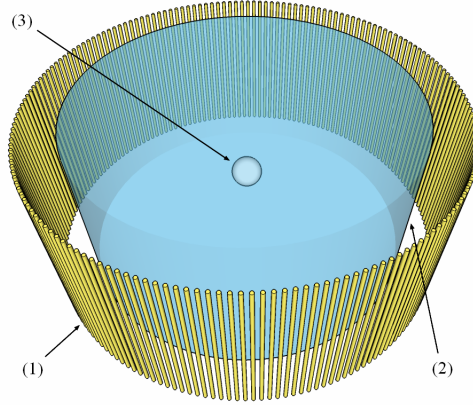


Figure 1.6: Dynamic Hohlraum. (1) High Z cylindrical array. (2) Foam. (3) Target

1.3.2 Limitations

Nevertheless, this high efficiency comes at the cost of losing illumination symmetry at the capsule poles. Moreover, the implosion phase of an ordinary cylindrical array is far from being a laminar flow.

The ideal ablation scheme previously presented is in reality strongly perturbed by the development of a global $m = 0$ instability (with a longer wavelength than the fundamental mode), making the position of the opening gaps unpredictable. Pushing its way through these gaps into the plasma, the "magnetic gas" produces Raleigh-Taylor instabilities (growing from the $m = 0$ seed) along the radii (fig 1.7b). The implosion symmetry is consequently deteriorated, so is the x-ray power.

Another interesting effect has been observed and may be caused by the electrodes themselves. On many imaging diagnostics and generator (fig 1.7a-1.7c), a curious phenomenon which will be later named "the Christmas Tree Effect" has been recorded. This effect is characterised by an early implosion of the wire parts close to the cathode, imprinting on the experimental images what looks like a Christmas tree made of plasma. One of the possible explanations is that electron emission from the cathode would result in wire hotspots leading to early breakages.

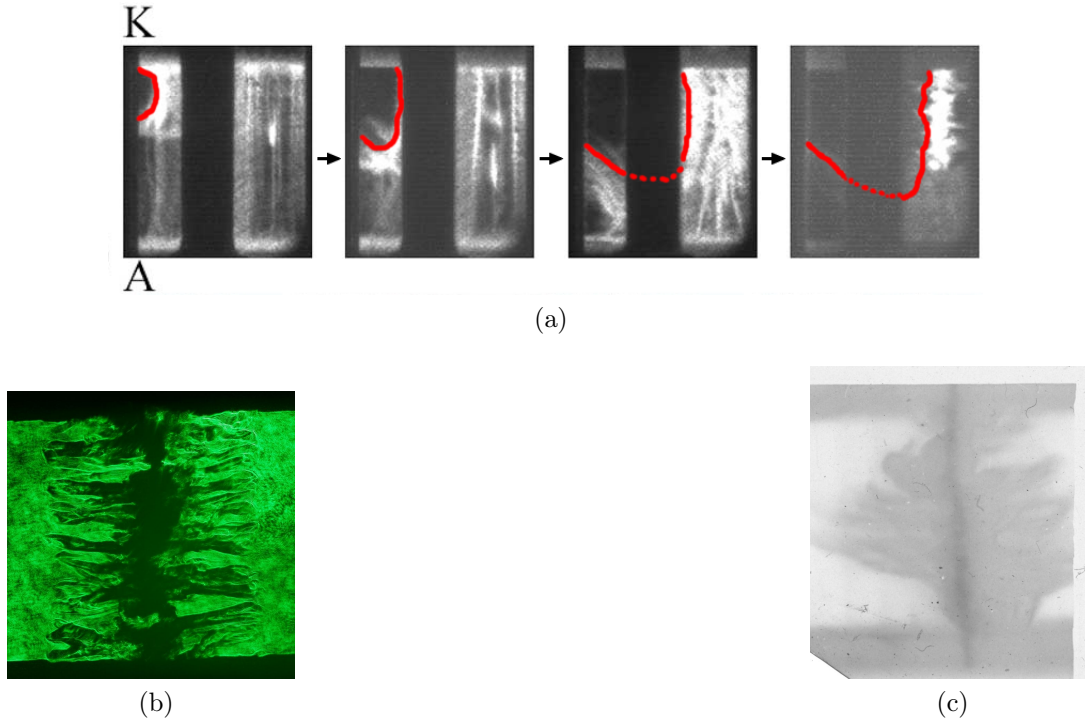


Figure 1.7: (a) Fast framing camera images of a cylindrical array on the SPHINX (4 MA, 700 ns) generator where a bubble expands and fill the entire cavity. (b) Raleigh-Taylor instabilities observed on laser images for the shot s0516 on MAGPIE (c) x-ray images of the Christmas tree effect on MAGPIE.

However, this phenomenon also deeply affects the implosion dynamics².

²It will be interesting to notice that this effect has been eradicated by the prepulse technique on the SPHINX generator [10] .

Chapter 2

A Magnetohydrodynamic Model for Z-pinch simulations

Improving the x-ray production of the Z-pinch requires improving our comprehension of their physics. Unfortunately, like in the vast majority of HEDP cases, the processes involved cannot be easily solved analytically and require multidimensional numerical modelling. In order to achieve this task, we make use of a parallel, three-dimensional resistive Eulerian magnetohydrodynamic (R-MHD) code known as GORGON [11] and developed at Imperial College.

2.1 Overview of Gorgon

GORGON has been written to solve problems related to Z-pinch and resistive MHD in general. In that sense, a lot of attention was brought during its development to keep its structure flexible, scalable and relatively user-friendly. The guideline was to build the kernel around mature methods (like finite difference) which would ensure reliable responses to varied questions.

The main purpose of this code is to explicitly solve on an Eulerian three-dimensional grid the MHD equations of continuity, single momentum, ions and

electrons energy, the Ohm's law and the heat flow[12]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (2.1)$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla (p_i + p_e) + \mathbf{j} \times \mathbf{B} \quad (2.2)$$

$$\frac{\partial \varepsilon_i}{\partial t} + \nabla \cdot (\varepsilon_i \mathbf{v}) = -p_i \nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{q}_i + \Delta_{ie} \quad (2.3)$$

$$\frac{\partial \varepsilon_e}{\partial t} + \nabla \cdot (\varepsilon_e \mathbf{v}) = -p_e \nabla \cdot \mathbf{v} - \nabla \cdot \mathbf{q}_e + \eta |\mathbf{j}|^2 - \Lambda + \Delta_{ei} \quad (2.4)$$

with ρ the density, $\mathbf{v}$ the velocity and η the resistivity. The ions and electrons internal energies, respectively ε_i and ε_e are given by:

$$\varepsilon_i = \frac{p_i}{(\gamma - 1)} \quad (2.5)$$

$$\varepsilon_e = \frac{p_e}{(\gamma - 1)} + Q(\bar{Z}) \quad (2.6)$$

where p_i and p_e are the ions and electrons pressure, $\gamma = 5/3$ the adiabatic index for monoatomic gas and $Q(\bar{Z})$ the potential ionization energy depending on the average ionization charge $\bar{Z}$. This latter is originally obtained using an approximate analytic representation of the Thomas-Fermi model[29], a good but nevertheless limited approximation as we will see later. The ions and electrons thermal fluxes are given by $\mathbf{q}_i = -\kappa_i \nabla T_i$ and $\mathbf{q}_e = -\kappa_e \nabla T_e$. $\kappa_{i/e}$ is the thermal conductivity, η the resistivity and Λ the radiative losses. Elastic collisions between ions and electrons are assumed, what gives for the energy exchange rates $\Delta_{ie} = -\Delta_{ei}$.

From the user point of view, setting up a Z-pinch simulation with GORGON is a reasonably straightforward process. The first interesting element to notice concerns the wire initialisation. The transition from solid to plasma is not modelled in the code. Therefore, the empiric solution to this issue is to set up the wires as cells containing relatively cold plasma around $T = 0.1$ eV. This seemingly

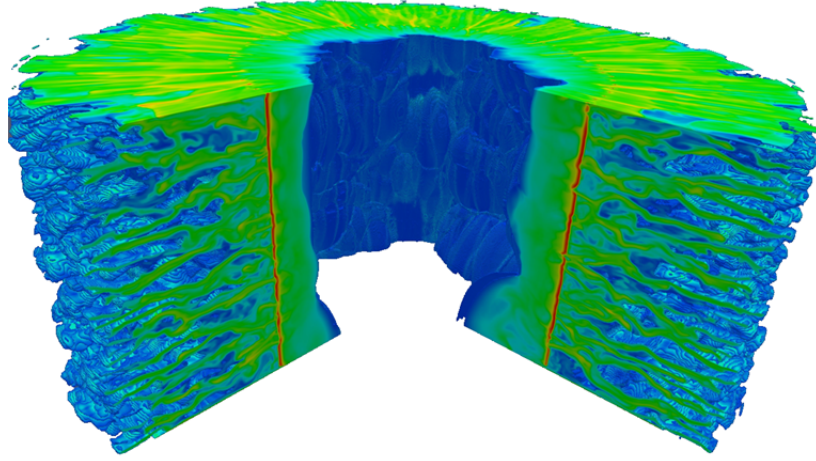


Figure 2.1: Typical Gorgon simulation of a nested W array on Z (20 μm resolution)

arbitrary temperature is a free parameter allowing the recovery of the expected wire ablation rate. In the original version of the code, the regions representing the electrodes are considered to be thermally insulated and highly conductive cells ($\eta = 10^{-6}$), although this does not realistically model the electrodes (no ablation or emission effects can occur).

2.2 Field solver

The key feature of GORGON electromagnetic field solver is the way both $\mathbf{E}$ and $\mathbf{B}$ are treated in terms of the vector potential $\mathbf{A}$ ($\mathbf{E} = -\partial\mathbf{A}/\partial t$ and $\mathbf{B} = \nabla \times \mathbf{A}$). This technique ensures the constraint $\nabla \cdot \mathbf{B} = 0$ is preserved.

In general, the major part of a simulation volume is occupied by vacuum, a state represented in the code by cells of low density ($\rho_{vacuum} < 10^{-4} \text{ kg.m}^{-3}$) and high resistivity. For those cells, only the vacuum form of Maxwell equations is preserved. Injecting the expression of the current from the Ohm's law into the full Ampere's law ($\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + (1/c^2)\partial\mathbf{E}/\partial t$) gives the equation to advance the magnetic field:

$$\frac{\partial^2 \mathbf{A}}{\partial t^2} = -c^2 \nabla \times \nabla \times \mathbf{A} - \frac{\mu_o c^2}{\eta} \frac{\partial \mathbf{A}}{\partial t} + \frac{\mu_o c^2}{\eta} \mathbf{v} \times \nabla \times \mathbf{A} \quad (2.7)$$

where μ_0 is the magnetic permeability.

This formulation facilitates the implementation of an explicit solution scheme for the magnetic solver, a method far less computationally expensive than an implicit one. Indeed, while requiring to adjust the timestep of the simulation in regard to the Alfvén speed (which can be very high in the case of Z-pinch simulations), explicit solver do not necessitate the inversion of big matrices and can easily be distributed across several machines for parallelization.

Circuit model

The current is imposed to the system by setting the boundaries conditions for the magnetic field. Three options are offered to the user to perform this last task: approximation of the current shape by a sinusoidal function $I(t) = I_{max} \sin(\pi t / 2\tau)$ (where τ is the characteristic pulse rising time of the generator studied), utilisation of a file containing the actual experimental current data or modelling of the generator current with a circuit model (injecting the electrode potential V_{load} as a feedback from the MHD computations to get the load impedance in real time (fig 2.2). In first approximation, this last option is equivalent to solving a system of differential equations of the type:

$$\begin{cases} d_t I_{gen} = (V_{gen} - R_{gen} I_{gen} - R_{loss}(I_{gen} - I_{load})) / L_{gen} \\ d_t I_{load} = (R_{loss}(I_{gen} - I_{load}) - V_{load}) / L_{feed} \end{cases} \quad (2.8)$$

with V_{gen} , I_{load} , L_{feed} , R_{loss} respectively standing for the generator voltage, the current in the load, the convolute inductance and the losses total resistance. A good modelling of this latter time-dependent parameter is crucial in order to properly evaluate the current and thus the energy deposition in the pinch.

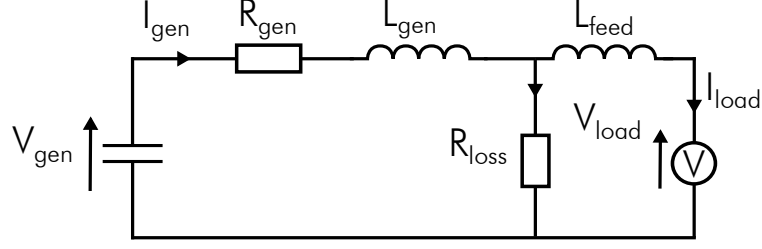


Figure 2.2: Simple schematic of GORGON circuit model

2.3 Radiative losses

An exhaustive treatment of the physics involved in Z-pinch experiments would at least require a detailed resolution of the atomic physics, radiation transfers and magnetohydrodynamics equations on the computational grid. Indeed, Z-pinch plasmas are very strong x-ray sources under constantly changing optical depth conditions which radiate their energy over a wide range of the spectrum. For the most part of the experiment and in the case of low-Z materials (e.g. Aluminium), those sources remain optically thin, and the emitted energy can leave the plasma.

Nevertheless, in some situations, spatially and frequency dependent “optical traps” can be formed that absorb this radiative energy, locally affecting the dynamic of the pinch. This may be the case for high-Z materials in the very dense regions of the imploded pinch where the density has reached such a level that the photons are trapped into the plasma. Under these circumstances, the thermalization of the radiation field pushes the formerly thin source up to its black body limit. In the likelihood that the volume of plasma considered was subjected to magnetic compression, the increased thermal pressure resulting from the stronger opacity may be consistent enough to balance the external applied forces and stop the said compression. It seems therefore crucial to account for the coupling of the radiation field with the MHD in the resolution of the Z-pinch physics.

Unfortunately, the necessity to operate in three dimensions in order to properly reproduce several plasma behaviors makes the treatment of radiation transfers a very cumbersome task. As a matter of fact, a correct approach to this problem

would require to resolve the intricate interplays of photoemission-photoabsorption between the different regions of the simulation. Without the use of approximations or computational tricks, the complexity of this task is in the order of N^2 , N being the number of plasma cells modelled. The average GORGON simulation containing billions of those cells, such a resolution performed in a reasonable time remains beyond the reach of our current supercomputing capabilities.

Another approach had therefore to be adopted. In a first and relatively crude approximation, the impossibility of including radiative interactions between cells lead to consider the transfer problem locally. In this scheme, the isotropic emission coefficient for continuum transitions (free-free and bound-free [25]):

$$J_{ff+bf} = 1.69 \times 10^{38} n_e T_e^{1/2} \sum Z^2 n_i(Z) \left(1 + \frac{E_i^\infty}{T_e} \right) \text{ W.cm}^{-3}$$

is weighted by a fit factor in order to take into consideration the bound-bound transitions. The total amount of radiative power losses from one cell is therefore evaluated using the mean Planck opacity of this cell (see 3.1.2 and 4.4) and subsequently removed from the electron energy equation (2.4). In this way, the opacity of each computational region represents the total amount of optical depth that photons emitted from this same region will encounter during their journey through the grid.

2.4 Requirements of the model

Although the previous approach has been proven to be very fast and successful in the reproduction of many Z-pinch x-ray pulses characteristics (notably the total energy and pulse width), it has several inconveniences. First of all, the approximation of bound-bound transitions by the use of fitting factors, besides being questionable, is obviously a serious barrier to any attempt to implement some

synthetic x-ray diagnostics. Secondly, this lack of spectral resolution, also encountered in the treatment of opacities, prevents the modelling of frequency dependent dynamical processes. Finally, and from the point of view of code sustainability, the resolution of atomic radiative transitions being at the base of any radiation transfer code, it will be necessary, as a preliminary step for implementing such a code, to have at our disposal a model capable of accounting for these transitions.

The inline model

The main purpose of this work was therefore to develop a fast and nonetheless reliable atomic model that can be run in parallel with the three-dimensional MHD solver of GORGON. The function of this inline code was primarily to simulate the transitions from optically thin to optically thick regime while producing time-dependent filtered synthetic bolometers and PCD signals. The computational requirements related to speed, flexibility (particularly the ability to include different materials in the simulation) and spectral resolution led us to base our implementation on a Screened-Hydrogenic Model (SHM) with nl splitting and to evaluate the line emission for each transition calculating an average opacity and source function over an approximation of the Voigt width (a full treatment with several points per line would be far too computationally expensive to be run inline). Originally only designed for Local Thermodynamic Equilibrium (LTE) conditions, the code evolved making use of a computationally inexpensive modification of the SAHA equation in order to mimic Non-LTE plasma conditions.

The offline model

The offline version of this model, built as a standalone application, was developed to be used as a post-processing tool providing detailed synthetic diagnostics data (spatially integrated spectra of Z-pinch plasma, filtered synthetic MCP images,

etc...) from Z-pinch simulation outputs. Based on the same kernel as its inline counterpart, this code has a much more elaborate treatment of the line profiles and is also parallelizable across multiple nodes using the MPI library. This was made possible by the fast and memory efficient access to the spectral information offered by a custom implementation of a self-balancing binary search tree data structure.

Chapter 3

Radiative processes in Z-pinch plasmas

The matter constituting the load of a Z-pinch undergoes several phase transitions during the experiment. The material of a cylindrical wire array, for example, will be found successively under the form of a solid (originally), a liquid/gaseous mixture (wire core through the ablation stage [32]) and a plasma (for the rest of the experiment). Although in theory every single one of these states is susceptible of releasing some photons, it is experimentally observed that the measured x-ray output is negligible before the formation of the precursor column, revealing that the principal source of emission is the plasma. In consequence, our study will only focus on the atomic and radiation physics of ionized and fully dissociated elements, disregarding any emission occurring from less excited states of matter (e.g. from molecular electronic transitions).

In the first part of this chapter, we present the general ideas relative to the emission of radiation in plasmas. Beginning with the introduction to the spectral line emission, we subsequently examine the release of radiation through continuous processes. This naturally leads us to study different kind of population equilibriums and to introduce some existing computational approach developed in order

to solve these issues, which constitutes the second part of this chapter.

3.1 Atomic line emission

Spectral line emission constitutes the main source of radiative power from Z-pinch plasma. This process corresponds to the transition of a bound electron from a given energy level (or excited state) to a lower one. When this happens, a photon with an energy $h\nu$ equal to the energy difference between the two levels is emitted. The atomic energy states being quantized, the distribution of the photons radiated by bound-bound transitions has a discrete aspect and some “lines” can be observed in the spectra.

These lines are identified by the ionization state of their emitter, the upper energy level of the transiting electron and the lower one. If an element of atomic number Z is ionized $Z - 1$ times (only one electron left), it will be said to be in a H-like state. Correspondingly, the same element ionized $Z - 2$ times will be in a He-like state, and so on. Traditionally, the electron shells are labeled K,L,M,N,O,P,Q for the principal quantum numbers $n=1,2,3,4,5,6$ and 7 , going from the innermost shell outwards. The transitions from the levels $2,3,4,\text{etc}...$ to the shell K ($n=1$) for H-like ions and He-like ions are respectively referred to as Lyman- α , Ly- β , Ly- γ , etc... and He- α , He- β , He- γ , etc... : they are called K-shell transitions¹. Equivalently, L-shell transitions are from any levels to the shell L ($n=2$), M-shell transitions to the shell M ($n=3$), and so forth. Table 3.1 and figure 3.1 summarize these considerations.

By selecting a material easily ionizable (of moderate atomic number), it is possible to design a Z-pinch load which, during the stagnation phase, will radiate away the energy stored in the plasma as high energy photons in K,L,or M-shell lines.

¹warning: for some historical reasons, H- $\alpha, \beta, \dots \neq$ Ly- $\alpha, \beta, \dots$ but corresponds to the Balmer lines (L-shell) $3, 4, \dots \rightarrow 2$

Transition	Designation
$2p \rightarrow 1s$	Ly- α
$3p \rightarrow 1s$	Ly- β
$4p \rightarrow 1s$	Ly- γ
$1s2p \rightarrow 1s^2$	He- α
$1s3p \rightarrow 1s^2$	He- β
$1s4p \rightarrow 1s^2$	He- γ

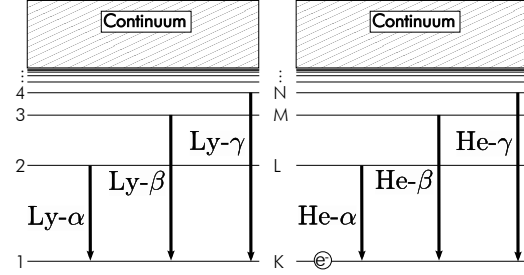


Table 3.1: Designation of the principal K-shell lines

Figure 3.1: H-like and He-like ions line transitions diagram

3.1.1 The Einstein probability coefficients

Let us now consider the radiative processes between two levels of a given ion. In the quantum mechanical picture, there are three different possible radiative transitions connecting the two levels, all governed by three different probability rates named the Einstein coefficients (fig 3.2).

First of all, there is a probability A_{21} per unit time that an electron in the higher shell 2 will undergo a radiative transition to the shell 1. Therefore, the number of such transition per unit volume per unit time is $n_2 A_{21}$, with n_2 the electron population density of level 2. Secondly, and in the presence of an incident radiation intensity I_ν , an electron from the lower level may absorb a photon of energy $h\nu_{21} = E_2 - E_1$ and thus transit to the level 2, the probability of this process per unit volume per unit time being given² by $n_1 4\pi I_\nu B_{12}$. Finally, an electron from level 2 may undergo a stimulated emission to level 1, a transition resulting from the “negative absorption” of an incident photon of energy $h\nu_{21}$ (see annexe A.2).

In order to derive the relationship between the coefficients, let us assume that our ions have been placed in a black body cavity in thermal equilibrium at temperature T . Under these conditions, the principle of detailed balancing (see 3.3.1) gives us a relationship between the rate of emission and absorption for a given

²warning: $[A_{21}] = \text{s}^{-1} \neq [B_{12}] = \text{erg}^{-1} \cdot \text{cm}^2 \cdot \text{Hz}$

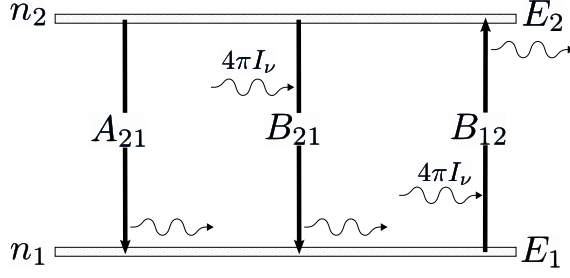


Figure 3.2: Einstein coefficients for spontaneous emission (A_{21}), stimulated emission (B_{21}) and absorption (B_{12}).

transition:

$$n_2 A_{21} + n_2 4\pi I_\nu B_{21} = n_1 4\pi I_\nu B_{12} \quad (3.1)$$

which translates the fact that in thermal equilibrium, the number of photons emitted by spontaneous or stimulated transitions is balanced by the number of photons absorbed. Reorganizing (3.1) and recalling that, here, $I_\nu = I_{\nu p}$ and the excited state populations follow the Boltzmann distribution $n_2/n_1 = (g_2/g_1) e^{-h\nu_{21}/kT}$, we obtain:

$$4\pi I_{\nu p} = \frac{A_{21}}{B_{21} ((g_1 B_{12}/g_2 B_{21}) e^{h\nu_{21}/kT} - 1)} \quad (3.2)$$

This latter equation is verified for any value of T only if:

$$\begin{cases} g_1 B_{12} &= g_2 B_{21} \\ A_{21} &= \frac{8\pi h \nu_{21}^3}{c^2} B_{21} = \frac{8\pi h \nu_{21}^3}{c^2} \frac{g_1}{g_2} B_{12} \end{cases} \quad (3.3)$$

It is important to notice that although (3.3) was derived using the assumption of thermodynamic equilibrium, the relation connecting the Einstein coefficients is totally independent of any temperature and holds independently of the presence or absence of any equilibrium.

3.1.2 Radiation transfer and spectral line emission

The evaluation of the amount of radiative energy released by a volume of plasma requires to solve the radiative transfer equation for the light propagating through this plasma. In order to derive this equation, let us consider an elementary cylinder of base area dA and height l located at a point in space and oriented in such a way that the direction of the radiation Ω coincides with the axis of the cylinder (fig 3.3). During the time dt , an amount of radiation $I_\nu dA dt$ flows into the left base of the cylinder. Concurrently, an amount $(I_\nu + dI_\nu) dA dt$ flows out from the right base. If we call s the coordinate along the propagation direction, the change in intensity of the light beam as a result to its passage through the cylinder is given by:

$$dI_\nu = \frac{\partial I_\nu}{\partial t} \frac{ds}{c} + \frac{\partial I_\nu}{\partial s} ds \quad (3.4)$$

and is the consequence of the emission and absorption of light in this same cylinder. The radiative energy emitted in the cylinder during the time dt per unit solid angle is $j_\nu(1 + c^2 I_\nu / (2h\nu^3)) dA dt ds$ while the energy absorbed during the same period is $\kappa_\nu I_\nu dA dt ds$ (see A.2). Therefore, grouping together the terms representing the absorption and stimulated emission gives us the following balance equation for the radiation in the cylinder:

$$\frac{1}{c} \frac{\partial I_\nu}{\partial t} + \frac{\partial I_\nu}{\partial s} = j_\nu - \kappa_\nu I_\nu \left(1 - \frac{c^2}{2h\nu^3} \frac{j_\nu}{\kappa_\nu}\right) \quad (3.5)$$

From the previous part, we can easily infer the relationship between the volume emission coefficient j_ν and the Einstein coefficient for spontaneous emission in the case of a transition $2 \rightarrow 1$:

$$\int_0^{+\infty} j_\nu d\nu = \frac{n_2 A_{21} h \nu_{21}}{4\pi} \quad (3.6)$$

$$\stackrel{3.3}{=} n_2 \frac{2h\nu_{21}^3}{c^2} \frac{g_1}{g_2} B_{12} h \nu_{21} \quad (3.7)$$

Similarly, we can write the relationship between the absorption coefficient κ_ν and the Einstein coefficient for absorption:

$$\int_0^{+\infty} \kappa_\nu d\nu = n_1 h \nu_{21} B_{12} \quad (3.8)$$

Substituting an expression of B_{12} from (3.8) into (3.7) and after some rearranging we obtain the definition of the source function S_ν ³:

$$S_\nu = \frac{j_\nu}{\kappa_\nu} = \frac{2h\nu_{21}^3}{c^2} \frac{n_2}{n_1} \frac{g_1}{g_2} \quad (3.9)$$

Typically, in Z-pinch plasmas, the speed of light far exceeds the speed of the fluid and the characteristic spatial scales range from micrometers up to centimetres. Consequently, the transit time of the radiation through the plasma is far smaller than the evolution time of parameters such as the density and temperature. As a result, we can assume that the source j_ν and sink κ_ν terms as well as the boundary conditions are not time dependent. From these considerations and by substituting (3.9) into (3.5), we can now write a stationary version of the radiation transfer equation:

$$\begin{aligned} \frac{\partial I_\nu}{\partial s} &= j_\nu - \kappa_\nu I_\nu \left(1 - \frac{n_2}{n_1} \frac{g_1}{g_2} \right) \\ &= \kappa'_\nu (S'_\nu - I_\nu) \end{aligned} \quad (3.10)$$

where $\kappa'_\nu = \kappa_\nu (1 - n_2 g_1 / (n_1 g_2))$ and $S'_\nu = j_\nu / \kappa'_\nu$ are respectively the absorption coefficient and source function accounting for the stimulated emission. This last expression can be integrated over the cylinder height to give, assuming the homogeneity (but not necessarily the thermal equilibrium) of the elementary plasma

³Note: Under thermodynamic equilibrium conditions, the Boltzmann distribution holds and the expression for the source function is equivalent to the Kirchhoff's law.

volume (i.e. $\kappa_\nu = \text{constant}$) :

$$I_\nu(l) = S'_\nu(1 - e^{-\kappa'_\nu l}), \quad (3.11)$$

We define the optical depth $\tau'_\nu = \kappa'_\nu l$ as a measure of the plasma transparency at a certain frequency ν . If τ'_ν is large, the plasma will be called optically thick (i.e. opaque), in the opposite case, it will be called thin (transparent).

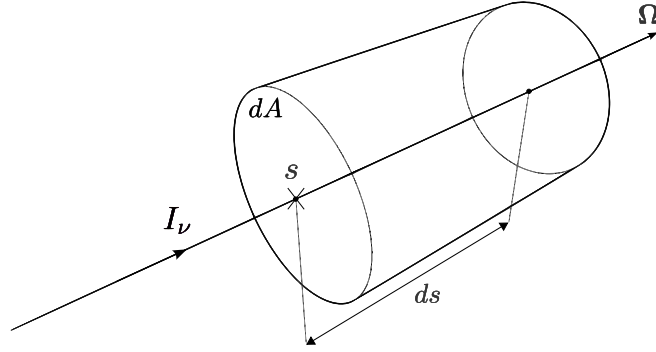


Figure 3.3: Schematic for the derivation of the radiation transfer equation

3.1.3 Spectral line shape

3.1.3.1 Classical theory

The classical model represents the bound-bound transitions as the harmonic (spontaneous emissions) and forced (induced emissions) oscillations of electrons about some equilibrium position around the nucleus. During these oscillations, the electrons are accelerated and therefore release some radiation. In the spontaneous case, solving the classical equation of motion for the damped harmonic oscillator:

$$m\ddot{r} + m(2\pi\nu_0)^2 r + m\gamma\dot{r} = 0 \quad (3.12)$$

leads, for small damping ($\nu_0 \gg \gamma$), to the solution:

$$r = a_0 e^{-\frac{\gamma}{2}t} \cos(2\pi\nu_0 t) = a(t) \cos(\omega_0 t) \quad (3.13)$$

with γ the damping constant due to the “frictional forces” (radiation losses in our case) and ν_0 the natural frequency of the oscillator. The total energy of the oscillator, $E = E_{pot} + E_{kin} = (kr^2 + m\dot{r}^2)/2$ is thus given at time t by:

$$E(t) = \frac{1}{2}m\omega_0^2 a^2(t) = E(0)e^{-\gamma t} \quad (3.14)$$

and the rate of energy loss by:

$$-\frac{\partial E}{\partial t} = \gamma E(0)e^{-\gamma t} = \gamma E(t) \quad (3.15)$$

According to classical electromagnetic, we know that this rate can be equated to the amount of energy released by an accelerated charge (see footnote 1 in 3.2.1):

$$-\frac{\partial E}{\partial t} = \frac{2e^2}{3c^3} \langle \ddot{r}^2 \rangle \quad (3.16)$$

where $\langle \ddot{r}^2 \rangle = \omega_0^4 a^2(t)/2 = \omega_0^2 E(t)/m$ (averaging over one cycle). Equating (3.15) and (3.16) allows us to evaluate the damping constant:

$$\gamma = \frac{8\pi e^2 \nu_0^2}{3mc^3} \text{ [s}^{-1}\text{]} \quad (3.17)$$

From (3.13) we see that the amplitude of the oscillation decay as $e^{-\gamma t/2}$, the corresponding energy decay following an exponential with a time constant of $1/\gamma = \tau_{class}$. As a consequence, the emission is not anymore at the natural frequency of the oscillator ν_0 but is spread over a frequency range on the order of $1/\tau_{class}$. To be more specific, we can derive the intensity of the frequency spectrum, multiplying the Fourier transform of r ($R_\nu = \hat{r}_\nu$) by its complex conjugate:

$$I_\nu = R_\nu R_\nu^* \simeq I_0 \frac{(\gamma/4\pi)^2}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2} \quad (3.18)$$

We recognize in this expression the Lorentz distribution which admits a maximum for $\nu = \nu_0$ and a Full width at half maximum (FWHM) $\delta\nu = \gamma/2\pi$.

Similarly, we can obtain a solution for the induced emission case considering the equation of motion for the forced harmonic oscillator:

$$m\ddot{r} + m(2\pi\nu_0)^2 r + m\gamma\dot{r} = eE_0 e^{i2\pi\nu t} \quad (3.19)$$

where E_0 is the external electric field of an incident monochromatic light wave of frequency ν . The solution of this equation is:

$$r = \frac{eE_0}{4\pi^2 m} \frac{1}{\nu_0^2 - \nu^2 + i\nu(\gamma/2\pi)} e^{i2\pi\nu t} \quad (3.20)$$

Multiplying (3.19) by $\dot{r}$ (obtained from the last equation) and averaging over the time provides the energy absorbed by the electron per unit time. Dividing this latter expression by the time-averaged energy flux of the light wave ($cE_0^2/8\pi$) leads to the formula for the absorption cross section:

$$\sigma_\nu = \frac{e^2\gamma}{4\pi mc} \frac{1}{(\nu - \nu_0)^2 + (\gamma/4\pi)^2} \quad (3.21)$$

An excited oscillator can also lose its energy by collisions. It can be shown that, in this situation, its motion is still described by (3.20). The main difference appears in the expression of γ which in this case contains the sum of the natural width (3.17) with a quantity $\propto 1/\tau_{coll}$, where τ_{coll} is the average time between two collisions. Similarly, the form of the cross section (3.21) remains the same if γ accounts for the collisions.

Let us now assume that an atom contains a certain number of oscillators f_k , each with a natural frequency ν_{0k} . The total absorption coefficient for a density n_i of such atom is given:

$$\kappa_\nu = n_i \sum_k f_k \sigma_{\nu k}$$

Typically, the frequency interval between the different ν_{0k} is much greater than the width of the absorption cross section and only one term subsists in the previous equation. The total energy absorbed at frequency ν_0 by oscillators placed under an incident flux of photons with a radiant energy density U_ν will therefore be expressed by

$$\int_0^{+\infty} U_\nu c \kappa_\nu d\nu = n_i U_\nu c f \int_0^{+\infty} \sigma_\nu d\nu$$

Thus, the absorption per atom is characterized by :

$$f \int_0^{+\infty} \sigma_\nu d\nu \stackrel{3.21}{=} \frac{\pi e^2}{mc} f \quad [\text{cm}^2 \cdot \text{Hz}] \quad (3.22)$$

is only dependent of the number of oscillators.

3.1.3.2 Quantum theory

Let us now make the transition from classical to quantum oscillators and consider the emission and absorption of light by an electron in the simple case of our two-level atom. In the quantum mechanical picture, the uncertainty principal states that the value of the bound state energies is uncertain by an amount $\Delta E \sim h/\Delta t$, with $\Delta t = 1/A_{21}$ the “lifetime” of the states in question, equal to the reciprocal of the probability that a spontaneous transition to a lower level occurs. This uncertainty on the energy levels results on an uncertainty on the spectral lines frequency $\Delta\nu \sim \Delta E/h \sim 1/\Delta t$ which is on the order of γ , the damping constant of the classical theory. The total width of an energy level 2 is thus given by the sum of the probabilities of transitions to lower levels:

$$\Gamma_2 = \sum_{k<2} A_{2k}$$

The principle of detailed balancing gives us a relationship between the probabilities of emission and absorption for a given transition. If we place our atom under an

incident flux of photons with a radiant energy density U_ν , the energy absorbed by electrons in the excited state 1 transiting to 2 per unit time per unit volume is:

$$\int_0^{+\infty} n_i^1 U_\nu c \sigma_{\nu,1 \rightarrow 2} d\nu = n_i^1 U_\nu c \int_0^{+\infty} \sigma_{\nu,12} d\nu = n_i^1 U_\nu c h \nu_{21} B_{12}$$

where:

$$B_{12} = \frac{1}{h \nu_{21}} \int_0^{+\infty} \sigma_{\nu,12} d\nu \quad (3.23)$$

is the Einstein coefficient for absorption (here we have assumed that the changes in U_ν are negligible across the spectral interval of the line width). Equating the area of the spectral line with the classical expression given in (3.22), we can derive the quantum-mechanical equivalent of the absorption cross section between the two levels:

$$\sigma_{\nu,12} = \frac{e^2 \Gamma_{12} f_{12}}{m c 4 \pi} \frac{1}{(\nu - \nu_{21})^2 + (\Gamma_{12}/4\pi)^2} \quad (3.24)$$

Here $\Gamma_{12} = \Gamma_1 + \Gamma_2$ has replaced γ and contains the widths of the upper and lower levels. This last formula introduces the oscillator strength f_{12} of the line, a dimensionless value equal to the number of classical oscillators equivalent to one real atom for a particular transition. By integrating (3.24) with respect to the frequency and substituting in (3.23), we find a relationship between the Einstein absorption coefficient and the oscillator strength:

$$f_{12} = \frac{m c}{\pi e^2} h \nu_{21} B_{12} \quad (3.25)$$

Knowing the relationship between the Einstein coefficients (3.3), a general expression for the emission probability in term of the oscillator strength for absorption

can be obtained:

$$A_{21} = \frac{g_1}{g_2} \frac{8\pi^2 e^2 \nu_{21}^2}{mc^3} f_{12} = \frac{g_1}{g_2} 3\gamma f_{12} = -3\gamma f_{21} \quad (3.26)$$

where f_{21} is the negative oscillator strength for emission:

$$f_{21} = -\frac{g_1}{g_2} f_{12} = -\frac{A_{21}}{3\gamma}$$

3.1.3.3 Line broadening mechanisms

The main difficulty in the calculation of the line emission and absorption is the evaluation of the line shapes. It is well-known from experimental evidence that line profiles are broadened and shifted. In Z-pinch plasmas, two main mechanisms responsible for those effects can be identified.

The first, called Doppler broadening, is a result of the so-called ‘‘Doppler effect’’. The observed frequency of a photon emitted by a source moving with the velocity $v_x \ll c$ along the line of sight (axis x) will be shifted by an amount $\Delta\nu = \pm \nu_0(v_x/c)$ from its initial frequency ν_0 (the sign depending on the direction of propagation). Under thermal conditions, the ions velocities are described by the Maxwellian distribution:

$$\begin{aligned} f(v_x) dv_x &= \sqrt{\frac{m_i}{2\pi k T_i}} e^{-m_i v_x / (2k T_i)} dv_x \\ &\Leftrightarrow \\ f(\nu) d\nu &= \sqrt{\frac{m_i c^2}{2\pi k T_i \nu_0^2}} e^{-m_i c^2 (\nu - \nu_0)^2 / (2k T_i \nu_0^2)} d\nu \end{aligned}$$

where m_i and T_i are respectively the ion mass and temperature. In the last equation we recognize the expression of a Gaussian profile

$$\Phi_{Gauss}(\nu, \sigma) d\nu = \frac{1}{\sigma \sqrt{2\pi}} e^{-(\nu - \nu_0)^2 / 2\sigma^2} d\nu \quad (3.27)$$

where $\sigma = \nu_0 \sqrt{kT_i/m_i c^2}$ is the standard deviation leading to the Doppler Full Width at Half Maximum (DFWHM) :

$$\Delta\nu_{DFWHM} = \sigma\sqrt{8\ln 2} \quad (3.28)$$

The higher the ion temperature and emission frequency, the wider the spread of the shifts and thus the width of the lines will be.

The second effect is called “pressure broadening” and is related to the previously mentioned possibility of collisions and perturbations between the emitters. The nature of the interactions and particles concerned may be diverse. For instance, the perturbations can be caused by the Van der Waals force between neutral particles, the neutral resonance between identical species or the electric field between charged particles. In this last case, the interaction between the atom and the field, the so-called the Stark effect, can be linear in E for hydrogen or quadratic for any other atom. It can be shown that, in plasmas, the related “Stark broadening” dominates the resonance and Van der Waals ones, its effect being equivalent to the addition of a quantity γ_{Stark} to the natural width of the line (i.e. the original Lorentzian profile is conserved).

The two types of broadening being independent, their combined effect can be described by taking the convolution of the Gaussian and Lorentzian distribution:

$$\Phi_{Voigt}(\nu, \sigma, \gamma) = \Phi_{Gauss} \star \Phi_{Lorentz} = \int_{-\infty}^{+\infty} \Phi_{Gauss}(\nu', \sigma) \Phi_{Lorentz}(\nu - \nu', \gamma) d\nu'$$

Here, ν and ν' are relative to the line center. The resulting Voigt profile is usually expressed in term of the reduced frequency $w = \nu/(\sigma\sqrt{2})$ and the damping constant $a = \gamma/(\sigma\sqrt{2})$, representing the relative importance of the Lorentzian and

Gaussian components:

$$\Phi_{Voigt}(w, \sigma, \gamma) = \frac{1}{\sigma\sqrt{2\pi}} \frac{a}{\pi} \int_{-\infty}^{+\infty} \frac{e^{-w'}}{(w - w') + a^2} dw' \quad (3.29)$$

No analytic solution exists for this integration, nevertheless, estimations can be computed and tabulated as it will be seen in the next chapter. It is important to notice that due to the exponential decay of the Gaussian, the wings of the lines are determined almost entirely by the Lorentzian profile. On the other hand, for a small damping constant a , the central part of the profile is given by the Gaussian component.

3.2 Continuous emission

This section details the various physical processes resulting in the production of continuous emission and absorption spectra. The approaches adopted in the derivation of the different quantities are the ones proposed by Zel'dovich[47] and Thorne et al. [43] and assume LTE conditions. We will see that while the total intensity of radiation emitted by such processes is often orders of magnitude smaller than, say, the maximum intensities of the spectral lines, continuum transitions are of primordial importance for the experimentalist.

3.2.1 Bremsstrahlung

It is well known from classical electrodynamics that charged particles undergoing an acceleration emit radiation. Let us consider in a plasma an electron of velocity v located at a distance r of a positively charged ion. This electron evolves in the external Coulomb field produced by this charge and therefore experiences an acceleration along $\mathbf{r}$ resulting in the release of some radiation and the corresponding decrease of its kinetic energy (fig 3.4).

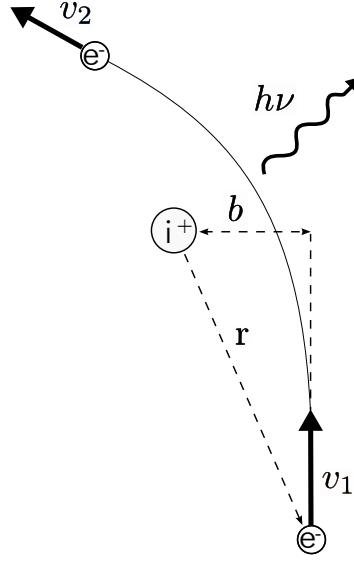


Figure 3.4: Bremsstrahlung emission

If the associated deceleration is small, i.e. if the radiative loss is negligible in comparison with the initial kinetic energy, the electron describes an hyperbolic orbit in the reference frame attached to the ion. This so-called bremsstrahlung process (from bremsen "to brake" and Strahlung "radiation", literally "braking radiation") and its inverse can be summarized by the following equation:

$$X^\alpha + e^- + \varepsilon_1 \rightleftharpoons X^\alpha + e^- + \varepsilon_2 + h\nu \quad (3.30)$$

with $\varepsilon_1 - \varepsilon_2 = h\nu$ the difference in electron kinetic energy released as radiation and α the ionization state. On each side of the equation (3.30), the electron is in a free state and its kinetic energy can take any value. Consequently, the emission and absorption spectra induced by free-free transitions will be continuous.

We now consider a beam of parallel electrons with a density n_e traveling at a velocity $v \ll c$ and incident on the ion with the impact parameter b . In the classical picture, an electron flux $n_e v$ passing through the elementary ring of area $2\pi b db$ around the ion emits a radiant energy of $\Delta E_\nu n_e v 2\pi b db d\nu$ [erg.s⁻¹], with $\Delta E_\nu = 16\pi^2 e^2 \hat{a}_\nu^2 / (3c^3)$ accounting for the total energy emitted⁴ by an electron

⁴We recall the classical result for non-relativistic velocities: $\Delta E_t = 2e^2 a_t^2 / (3c^3)$

during its journey and $\hat{a}_\nu$ being the Fourier transform⁵ of the acceleration $a(t)$. In this context, the effective radiation dq_ν , the energy emitted in the frequency interval $d\nu$ per ion per unit electron flux is obtained integrating over the impact parameter:

$$dq_\nu = d\nu \int_0^\infty \Delta E_\nu 2\pi b db \quad [\text{erg.cm}^2] \quad (3.31)$$

The exact classical calculations of the acceleration experienced by electrons along their hyperbolic trajectory around an ion of charge Z_α gives for the effective radiation:

$$dq_\nu = \frac{32\pi^2}{3\sqrt{3}} \frac{Z_\alpha^2 e^6}{m^2 c^3 v^2} g^{ff} d\nu \quad [\text{erg.cm}^2] \quad (3.32)$$

with g^{ff} a factor introduced in order to take care of the discrepancy between the classical and the quantum-mechanical calculations, otherwise known as Gaunt factor. It is interesting to notice that (3.32) only holds if $E_{kin} = \frac{1}{2}mv^2 \ll I_H Z^2$, i.e if the electron initial kinetic energy is smaller than the energy of the first Bohr orbit (see 3.2.2). In quantum-mechanical terms, the concept of impact parameter does not have a clear meaning and the latter formula is better expressed as the product of the emitted photon energy $h\nu$ times the cross section of emission $d\sigma_\nu$:

$$dq_\nu = h\nu d\sigma_\nu \quad [\text{erg.cm}^2] \quad (3.33)$$

Emission coefficient

We can now derive the expression for the bremsstrahlung emission coefficient. In a plasma consisting of ions with a density n_i^α , the energy emitted by the electrons having a velocity between v and $v+dv$ in the frequency interval $d\nu$ per unit volume per unit time is:

$$h\nu n_i^\alpha n_e v f(v) d\sigma_\nu(v) dv = n_i^\alpha n_e v f(v) dq_\nu(v) dv \quad [\text{erg.cm}^{-3}.\text{s}^{-1}] \quad (3.34)$$

⁵By definition, $\hat{a}_\nu = (2\pi)^{-1} \int_{-\infty}^{+\infty} a_t e^{-i2\pi\nu t} dt$

Under thermal conditions, the electron velocities are described by a Maxwellian distribution $f(v) dv = 4\pi(m/(2\pi kT_e)^{3/2} \exp(-mv^2/2kT) v^2 dv$. Using (3.32) and integrating (3.34) with respect to the velocities from $v_{min} = h\nu$ (minimum velocity of electrons capable of emitting a photon) to $+\infty$ we obtain the spectral emission coefficient due to bremsstrahlung:

$$J_\alpha^{ff}(\nu) d\nu = \frac{32\pi}{3\sqrt{3}} \left(\frac{2\pi}{kT_e m} \right)^{1/2} \frac{Z_\alpha^2 e^6}{mc^3} n_i^\alpha n_e e^{-h\nu/kT_e} d\nu g^{ff} \quad [\text{erg.cm}^{-3}.\text{s}^{-1}] \quad (3.35)$$

from which we can derive the integrated emission coefficient for free-free transitions, summing the contribution of each ion :

$$J^{ff} = \sum_\alpha \int_0^\infty J_\alpha^{ff}(\nu) d\nu = \frac{128\pi^3 e^6}{3\sqrt{3}hc^3(2\pi m)^{3/2}} (kT_e)^{1/2} n_e \sum_\alpha Z_\alpha^2 n_i^\alpha g^{ff} \quad [\text{erg.cm}^{-3}.\text{s}^{-1}] \quad (3.36)$$

From (3.35) we see that the exponential decay observed in bremsstrahlung spectra is due to the tail of the Maxwellian distribution function for the electron velocity.

Absorption coefficient

In Local Thermodynamic Equilibrium (see 3.3.1), the absorption coefficient κ_α^{ff} and cross section σ^{ff} for free-free transitions can be directly derived recalling the expression of the Kirchhoff's law (see A.2):

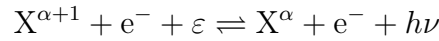
$$\kappa_\alpha^{ff}(\nu) = \frac{j_\alpha^{ff}}{I_{\nu p}} = \frac{J_\alpha^{ff}}{4\pi I_{\nu p}} = n_i^\alpha \sigma^{ff} \quad [\text{cm}^{-1}] \quad (3.37)$$

where:

$$\sigma^{ff}(\nu) = \frac{16\pi^2 Z_\alpha^2 e^6 n_e}{3\sqrt{3}hc(2\pi m)^{3/2}(kT_e)^{1/2}\nu^3} g^{ff} \quad [\text{cm}^{-2}] \quad (3.38)$$

3.2.2 Radiative recombination

The derivation of the spectral characteristics in the case of bound-free transitions is a little bit different from the previous one. Using our classical picture of an electron making a close approach to an ion, the recombination process could be described as the transfer of this same electron from an hyperbolic orbit (where its energy is $E > 0$) to an elliptic one (characterized by an energy $E < 0$) (fig 3.5a). During the transition, the energy difference between the two orbits is emitted as a photon $h\nu$. In quantum mechanics, states with negative energy are discrete, therefore, the electron completes its journey “captured” by one of the ion orbital shell (fig 3.5b). This process and its reverse (photoionization) are represented by:



with $h\nu = \varepsilon - E_k^{\alpha+1}$, $|E_k^\alpha|$ being the ionization energy of an electron in the shell k of an atom in the ionization state α . The minimum frequency of an emitted or absorbed photon is set by this energy gap. As a result, emission and absorption spectra for electron recombination exhibit a “sawtooth” appearance.

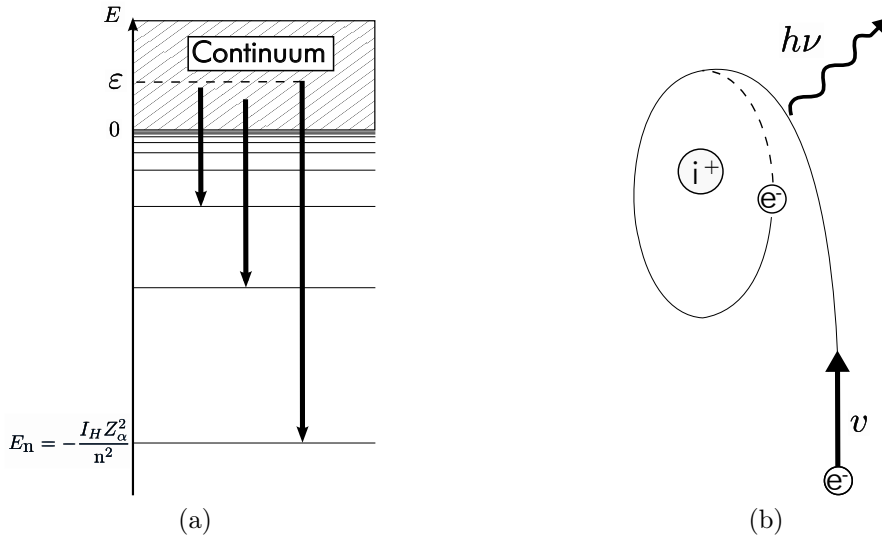


Figure 3.5: (a) Energy diagram showing the free-bound electron transitions (b) Classical transfer from an hyperbolic orbit to an elliptic one

Emission coefficient

In order to evaluate the coefficients for the bound-free transition, let us express the energy emitted in the frequency interval $d\nu$ by the radiative capture of electrons having a velocity between v and $v + dv$. As stipulated above, the final energy state of the electrons is now discrete, implying that there is a finite number of level Δk corresponding to any emission in $d\nu$. In the case of hydrogen-like ions, the energy levels of the bounded electrons are described by the principal quantum number n and given by (see 4.2) :

$$E_n = -\frac{I_H Z_\alpha^2}{n^2} \text{ with } I_H = \frac{2\pi^2 m e^4}{h^2}$$

We can therefore replace Δk by Δn and reformulate the expression (3.33) as $\Delta q_\nu = (dq_\nu/d\nu)\Delta\nu = h\nu \sigma_{cn}\Delta n$, where σ_{cn} is the average capture cross section in Δn . Knowing that $\Delta\nu/\Delta n = (1/h) \Delta h\nu/\Delta n = (1/h)|dE_n/dn|$ and using (3.32), we obtain for the electron capture cross section:

$$\sigma_{cn} = \frac{128\pi^4 e^{10} Z_\alpha^4}{3\sqrt{3} m c^3 h^4 v^2 \nu n^3} g^{bf} \quad (3.39)$$

Recalling that $mv^2/2 = h\nu + E_n$, using the variable change $v dv = h/m d\nu$, and summing for all the excited levels $n \geq n_{0,\alpha}$ (where $n_{0,\alpha}$ is the ground level in the ionization state α), we have for the electron recombination spectral coefficient :

$$\begin{aligned} J_\alpha^{bf}(\nu) d\nu &= h\nu n_i^{\alpha+1} n_e v f(v) \sigma_{cn}(v) dv \\ &= 4\pi \frac{128\pi^4 m e^{10} Z_\alpha^4}{3\sqrt{3} (2\pi m k T_e)^{3/2} c^3 h^2} n_i^{\alpha+1} n_e e^{-h\nu/kT_e} d\nu \sum_{n > n_{0,\alpha}} \frac{1}{n^3} e^{-E_n^\alpha/kT_e} g^{bf} \end{aligned} \quad (3.40)$$

Absorption coefficient

The use of the Saha ionization formula (see 4.3.1) for the expression of $n_i^{\alpha+1} n_e = 2(2\pi m k T_e/h^2)^{3/2} n_i^\alpha \tilde{Z}_{\alpha+1} e^{-|E_0^\alpha|/kT_e} / \tilde{Z}_\alpha$ allows us to write the former equation in

function of the recombined ion density. The ratio of the excited ion population density to the total population in the state α being given by the Boltzmann equation $n_i^{n,\alpha}/n_i^\alpha = g_n \exp(-(E_n^\alpha - E_0^\alpha)/kT_e)/\tilde{Z}_\alpha$ we can rewrite (3.40) for the transition in one level n as :

$$J_{n,\alpha}^{bf}(\nu) d\nu = 4\pi \frac{256\pi^4 m e^{10} Z_\alpha^4 \tilde{Z}_{\alpha+1}}{3\sqrt{3} c^3 h^5 n^3} n_i^{n,\alpha} e^{-h\nu/kT_e} d\nu g^{bf} \quad (3.41)$$

For hydrogen-like ions, the partition function $\tilde{Z}_{\alpha+1} = 1$ and $g_n = 2n^2$, integrating with respect to ν and summing for n and α , the total emission coefficient can be formulated as:

$$J^{bf} = 4\pi \frac{128\pi^4 m e^{10}}{3\sqrt{3} c^3 h^6} kT_e \sum_{n,\alpha} n_i^{n,\alpha} \frac{Z_\alpha^4}{n^5} e^{-|E_n^\alpha|/kT_e} g^{bf} \quad (3.42)$$

We can now extract the absorption coefficient $\kappa_{n,\alpha}^{bf}$ and cross section $\sigma_{n,\alpha}^{bf}$ for bound-free transitions following the method employed in the previous part:

$$\kappa_{n,\alpha}^{bf}(\nu) = \frac{j_{n,\alpha}^{ff}}{I_{\nu p}} = \frac{J_{n,\alpha}^{ff}}{4\pi I_{\nu p}} = n_i^{n,\alpha} \sigma_{n,\alpha}^{bf} \quad (3.43)$$

where the expression of the cross section:

$$\sigma_{n,\alpha}^{bf}(\nu) = \frac{64\pi^4 m e^{10} Z_\alpha^4}{3\sqrt{3} c h^6 \nu^3 n^5} g^{bf} \quad (3.44)$$

is called the Kramers' formula.

Temperature measurement

As previously mentioned, Bremsstrahlung and electron recombination processes are a very useful tool for the Z-pinch experimentalist. Indeed, in the optically thin case, we observed that the frequency dependence of the free-free (3.35) and bound-free (3.41) emission coefficients spectra are dominated by the term $e^{-h\nu/kT_e}$.

Consequently, a semi-logarithmic plot of the j_ν^{xf} 's versus the photons energy displays straight lines of negative slope $-1/kT_e$ from which the plasma electrons temperature T_e can be trivially inferred, provided that the measurements are time and spatially resolved.

3.3 A variety of Equilibria

We saw from the previous parts that the evaluation of the different radiative quantities requires the calculation of the population densities. As, from a spectroscopic point of view, we are mainly concerned with the radiative processes, we have so far neglected to account for the effect of collisions. However, it turns out that the electron collisional processes play a very important role in the population dynamic and in the establishment of various equilibriums.

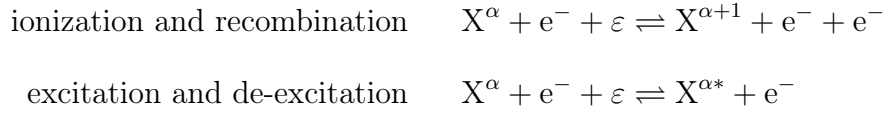
3.3.1 Local Thermodynamic Equilibrium

Previously, we have mentioned that the principle of detailed balancing could be applied under LTE conditions. Now is the time to investigate what it means.

So far, in our derivation of the radiative quantities we have encountered four temperature dependent distributions related to the radiative (Planck), kinetic (Maxwell), excitation (Boltzmann) and ionization (Saha) energies. Let us now consider an ideal case where some radiation and particles are enclosed in a certain volume and maintained at the constant temperature T . Thermodynamic arguments show that, after a certain time, the four distribution will adopted the same temperature T , a situation known as thermodynamic equilibrium. The principle of detailed balancing states that, under these conditions, every mechanism that leads to a transition in one direction must be balanced by its exact inverse. In other words, for every photon emitted there must be a photon absorbed at the same frequency, and for every collisional excitation there must be a collisional

de-excitation between the same energy levels.

Nevertheless, in real case scenario, the radiative energy distribution is often far from equilibrium as this requires the plasma to be optically thick at all frequencies. In the so-called Local Thermodynamic Equilibrium (LTE) conditions, it is therefore possible to find locally a common temperature T for the Maxwell, Boltzmann and Saha distribution. The applicability of LTE is conditioned by the predominance of electron collisional processes over radiative ones. The former processes can be represented by:



The numbers of electron collisional excitation and de-excitation between two levels 1 and 2 per unit volume per unit time are respectively given by $n_1 n_e C_{12}$ and $n_2 n_e C_{21}$. Here, the two collisional coefficients $C_{12} = \langle v \sigma_{12}(v) \rangle$ and $C_{21} = \langle v \sigma_{21}(v) \rangle$ are defined in term of the cross-sections for collisional processes $\sigma_{ij}(v)$. Using the principle of detailed balancing in LTE

$$n_1 n_e C_{12} = n_2 n_e C_{21} \quad (3.45)$$

thus

$$\frac{C_{12}}{C_{21}} = \frac{n_2}{n_1} \xRightarrow{\text{Boltzmann}} \frac{\langle v \sigma_{12}(v) \rangle}{\langle v \sigma_{21}(v) \rangle} = \frac{g_2}{g_1} e^{-(E_2 - E_1)/kT} \quad (3.46)$$

It is important to notice that, as the collisional cross-sections only depend of atomic parameters, the last relation must hold as long as the electron velocities follow a Maxwellian at the definable temperature T . Equation 3.46 is therefore independent of LTE assumption (although it was derived from it).

Recalling our two level atom model, an expression describing a general equi-

librium between upwards and downwards rates can be written as follows:

$$n_2 A_{21} + n_2 4\pi I_\nu B_{21} + n_2 n_e C_{21} = n_1 4\pi I_\nu B_{12} + n_1 n_e C_{12} \quad (3.47)$$

With the conditions that I_ν is small, equation (3.47) becomes:

$$n_2 A_{21} + n_2 n_e C_{21} = n_1 n_e C_{12} \quad (3.48)$$

Assuming that the electron density is large, we recognize the Boltzmann distribution of (3.46) as expected for LTE. This last condition is fulfilled only if :

$$n_e \gg \frac{A_{21}}{C_{21}} \quad (3.49)$$

It can be shown ([43]) that the cross-section for electron collisional excitation $\sigma_{12} \propto 1/v^2$, and from (3.3) we know that $A_{21} \propto \nu^3$, so $A_{21}/C_{21} \propto \text{constant} \times v \nu^3 = \text{constant} \times (\Delta E)^3 \sqrt{T_e}$. From Thorne, a more rigorous treatment leads to :

$$n_e \gg 1.7 \times 10^{14} (\Delta E)^3 \sqrt{T_e} \quad (3.50)$$

where T_e and ΔE are the electron temperature and the energy gap of the transition in eV. Condition (3.50) is easily satisfied for transitions between high level states (with a small energy separation) and at low temperature.

In Z-pinch plasmas, the situation is a bit more complicated as the range of temperature and density is indeed very large. Let us take for example the case of a nested copper array experiment (80/40 10.97 μm in $\emptyset$) on the Z generator and consider the final diameter at stagnation to range between 0.5mm-0.5cm (i.e. an ion density $n_i \approx 5 \times 10^{21} - 5 \times 10^{19} \text{ cm}^{-3}$). Figure 3.6 presents a comparison between the evolution of the free electron densities (calculated from the Saha

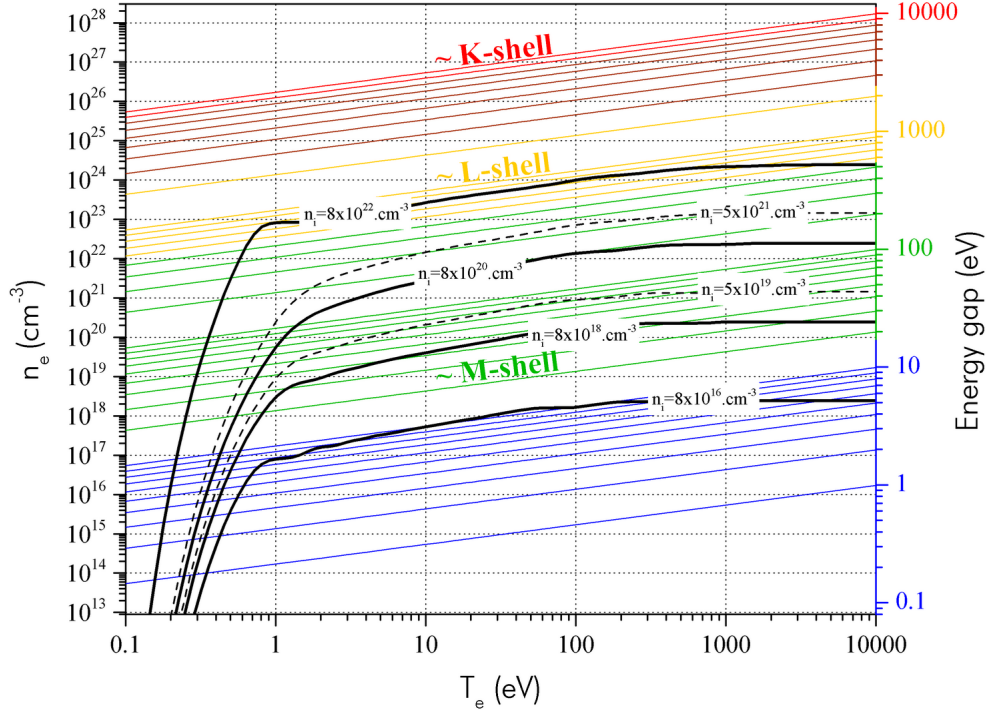


Figure 3.6: (Black lines) Saha free electron densities for Cu densities from 1 to 10^{-6} solid density versus approximated LTE thresholds (equation 3.50) for different energy gaps (colored lines)

equation) for a range of copper⁶ densities, with respect to the temperature, versus the stationary LTE thresholds (given by equation 3.50) for different energy gaps . For temperatures above 1 keV (usual at stagnation), the copper is in a H/He-like state but only levels separated by less than ~ 200 eV (in the highest density/smaller diameter at stagnation case) and ~ 40 eV (for the lowest density) can be considered in LTE. The plasma is said to be in partial LTE where only the population of the highest states can be evaluated without any knowledge of the transition rates. The situation is in fact more complicated than this simple approximation as the conditions in the pinch are transient and LTE can only be established if enough time is given for the thermal equilibration of the plasma.

⁶we choose copper as it is the load material with the highest Z for which we have reliable atomic tables

3.3.2 Coronal Equilibrium

The second most important kind of equilibrium one can encounter in plasmas is called Coronal Equilibrium. This situation arises when the electron density at a given temperature is not high enough to ensure LTE conditions and the radiation density is low as well (common in low density plasma similar to the one of the Sun's corona). Under these conditions, it is assumed that upward atomic transitions are caused by collisions between electrons and ions while downward transitions occur by spontaneous emission, and equations 3.48 becomes , for $A_{21} \gg n_e C_{21}$:

$$\begin{aligned} \frac{n_2}{n_1} &= n_e \frac{C_{12}}{A_{21}} \\ &= n_e \frac{\langle v \sigma_{12}(v) \rangle}{A_{21}} \stackrel{3.46}{\ll} \frac{g_2}{g_1} e^{-(E_2-E_1)/kT} \end{aligned}$$

The latter inequality, which requires the knowledge of the cross-section for electron collisional excitation and the radiative rate for spontaneous emission, guarantees that the population ratio in Coronal Equilibrium is lower than the Boltzmann value (i.e. the higher excited states are more difficult to reach). The same type of argument holds considering this time the collisional ionization and three body recombination transitions. Similarly, assuming that the radiative recombination rate exceeds the collisional excitation one, we can infer that the average ionization in Coronal Equilibrium will be less than its value in LTE.

3.3.3 Collisional Radiative Equilibrium

Unfortunately, our simple two level atom model with its corresponding radiative rates, already inappropriate for use in the treatment of Coronal Equilibrium, is totally incapable of accounting for all the possible transitions between the various ionization and excited states. A more complete picture could therefore be the one described in figure 3.7 and containing the radiative and collisional rates for

excitation, de-excitation, ionization and recombination transitions.

A full and detailed treatment of this problem requires solving the spatial and time dependent evolution of the many state populations. Usually, when no assumption of Local Thermodynamic Equilibrium can be made (i.e. in NLTE), the method employed in order to evaluate the distribution of excitation/ionization consists in considering the rates equations for the principal ionic states and solving the resulting system with the time history of the electron density and temperature (see for example [34]):

$$\frac{dP_n}{dt} = \sum_{k=1, k \neq n}^{\infty} P_k Q_n (C_{k \rightarrow n} + R_{k \rightarrow n}) - \sum_{k=1, k \neq n}^{\infty} P_n Q_k (C_{n \rightarrow k} + R_{n \rightarrow k}) \quad (3.51)$$

where the evolution of the population P_n of the state n is calculated using the collisional $C_{x \rightarrow y}$ and radiative $R_{x \rightarrow y}$ rates along with the occupation factor Q_x accounting for the fraction of the shell x which is on average empty⁷.

Nevertheless, when the temperature is low and the level of ionization moderate (transitions to M-shell, L-shell or above), this Detailed Configuration Accounting (DCA) approach, while capable of spectroscopic accuracy, is rarely used. Indeed, in practice, this would require following the evolution of millions of individual ionic species with very large statistical weights, a task far too computationally expensive. Several methods have been developed to overcome this limitation. One of the older one, the “average-atom” model (developed in 1947 by Mayer originally for LTE), replaces the requirement of following each ionic species with the requirement of following the principal quantum shell occupancies. These occupancies, although obtained by averaging the populations over the different ionic configurations, can be used to statistically retrieve the details of the individual ionic states. The obvious advantage of this method lies in the drastic reduction of the number of differential equations required to solve the various populations.

⁷ $Q_x = (1 - P_x/D_x)$ where D_x is the electronic degeneracy of the shell x .

However, the amount of information lost in the averaging processes often forbids its application to synthetic spectroscopy.

The next level of refinement in the evaluation of the populations came with the introduction of the Superconfiguration collisional radiative models (see [3] and [4]). These models account for the overwhelming statistical weights of excited levels by grouping those same states into sets of “effective levels”, or Superconfigurations (SC). The approach taken assumes partial LTE: within each set, the configurations are assumed to be in LTE and the populations given by the Boltzmann distribution evaluated at an effective temperature; between the SCs, populating and depopulating “channels” are calculated solving the rate equations. Comparisons between advanced SC and detailed-level accounting models have shown good agreement for average ion charges, SC populations and effective temperatures [24].

Finally, some hybrid models combining a small subset of very detailed levels with a complete set of configuration and Superconfiguration-averaged levels have been proposed [23].

The approaches presented here have been proven to be very effective in the calculation of the different NLTE populations of various ions under a wide range of conditions. Nonetheless, to our knowledge, none has demonstrated the ability to run in parallel with a three-dimensional resistive Eulerian MHD code, solving the populations and radiation of billions of cells in a realistic time.

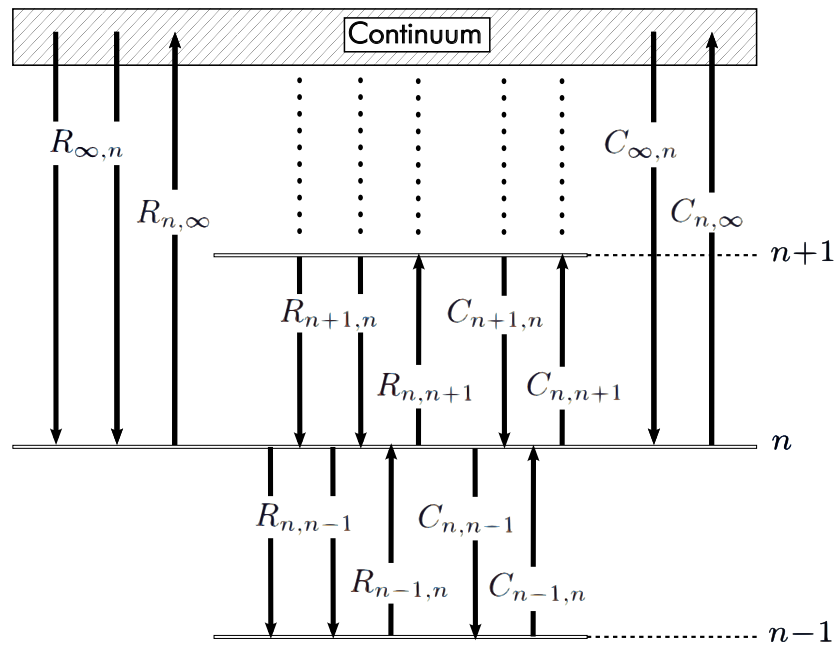


Figure 3.7: A more complete picture of the collisional and radiative transitions

Chapter 4

A new atomic model for Gorgon

In this Chapter, the main components of the new atomic model developed for the three-dimensional resistive Eulerian MHD code Gorgon are introduced. The first section presents the general ideas and constraints relative to the implementation of a radiation solver running in parallel with a magnetohydrodynamic one. Section 4.2 and 4.3 respectively describe the approaches taken in the code for the energetic and populations calculations. Finally, in section 4.4, the issue of the opacities is addressed. Although many aspects of the description focus on the structure of the inline version of the code, most of the concepts and characteristics presented here are also relevant to the offline implementation described in Chapter 5.

4.1 Overview

The development of the atomic model introduced in this part started from the need for a general and flexible tool that could improve the radiation treatment in Z-pinch simulations and be used as a post processing engine with synthetic spectra capabilities subsequently.

Predicting the energetic and spectral characteristics of Z-pinch sources is a delicate task. Indeed, we saw in the previous chapters that Z-pinch plasma con-

ditions were spread across a wide range of parameter space and could locally undergo transitions from optically thin to optically thick regimes, this latter point necessitating a close coupling of the radiation and magnetohydrodynamic solvers. In the case of Gorgon, the computational size and resolution requirements of a typical Z-pinch simulation places a special emphasis on the optimization of any additional Physics solver integrated into the main program. Unfortunately, it was found that the original method selected to solve this issue, while very fast, was also questionable and inaccurate. On the other hand, it appeared that alternative solutions providing a good level of spectroscopic accuracy (DCA) were far too computationally expensive to be implemented in parallel.

We therefore investigated the possibility of a third approach that would combine some of the advantages of the detailed configuration accounting methods while maintaining the overall runtime reasonable. The new scheme presented is based on a Screened-Hydrogenic model with l-splitting and a computationally inexpensive modification of the Saha solver. Although far from being capable of reproducing every single spectral detail present in the results of Z-pinch experiments, this model has demonstrated a good ability to mimic the radiative output of Z-pinch plasmas in a variety of NLTE conditions.

4.1.1 Implementation

Figure 4.1 illustrates the flow chart of the new model structure and its interface with Gorgon. The code has been built as a discrete module that could take the place of the former radiation solver scheme without requiring a total re-design of the program architecture. The limitations on the radiative transfer capabilities being what they are, the treatment has been kept local (see 4.4) and the effect of the radiation escaping each cell of the Eulerian grid is still represented by a loss term in the electron energy equation.

At each timestep, Gorgon provides the model with the total material density and the electron and ion temperatures in the cells. These information are then combined with the Atomic Physics data calculated in the pre-processing phase (ionization energy, excitation, partition functions, etc... see section 4.2) and supplied to a population solver (section 4.3). Once the occupancies of the different ion energy states as well as the average ionization level and free electron density have been determined, the radiation solver takes over and evaluates, with the cells dimension, the total losses from the different radiative processes (section 4.4).

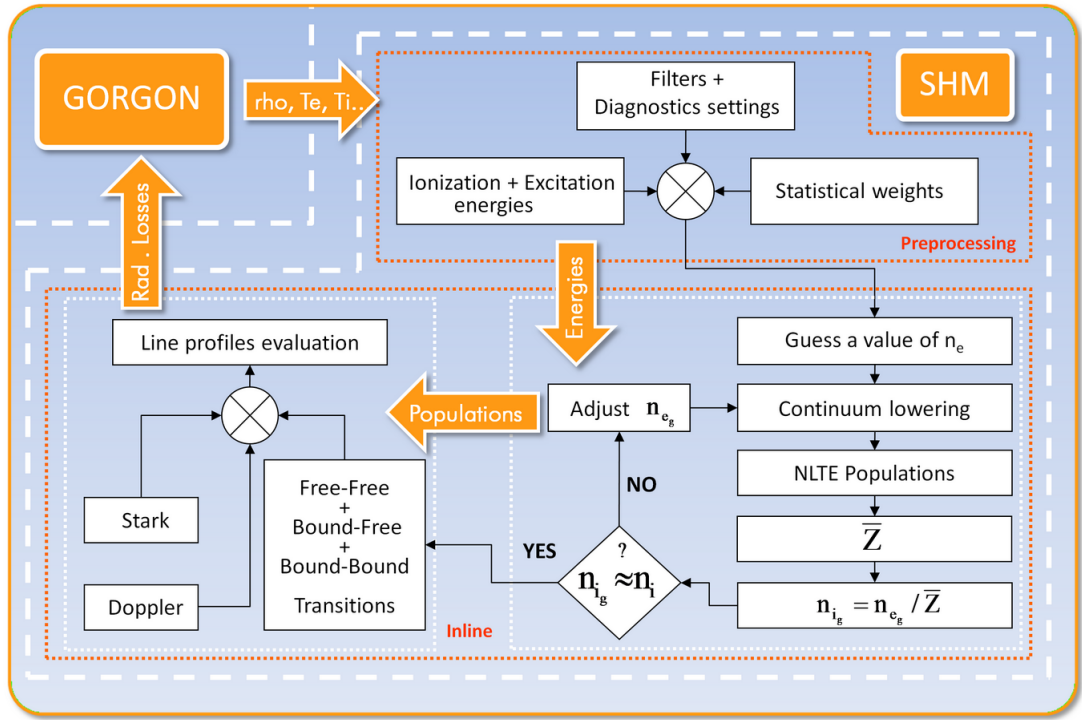


Figure 4.1: Flowchart of the new model

4.1.2 Optimization

Every single step described above is constrained by some computational expense considerations. Several strong approximations and optimization techniques have been used in this code (specifically for the calculation of the opacities Sec 4.4), but one in particular deserved to be noticed, the memoization of the exponential

function.

Memoization is an optimization technique aimed to speed-up computation by caching in memory the results of a previously processed function. It is the usual trade of memory for speed: when a call to a memoized function is made using a set of input parameters that has already been processed during the run time of the program, CPU cycles are saved by directly accessing the cache instead of executing the function code another time. However, memoization, unlike other look-up table methods, populates the cache results during the execution (i.e “on the fly”) and is therefore more flexible.

The exponential function is omnipresent in the resolution of Atomic Physics problems. For instance, it appears in the formulation of every energy distribution (Planck, Maxwell, Boltzmann, Fermi-Dirac, Saha), in the terms of the partition function and in the solution of the radiation transfer equation. Unfortunately, exponentiation routines of typical math libraries, involving numerous calls to slow machine level instructions, represent a performance bottleneck. An alternative consists in using the Taylor Series expansion:

$$\forall x \in \mathbb{R} : \exp(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!} \quad (4.1)$$

which is rapidly convergent for $|x| < 1$ but requires otherwise a number of iterations increasing with $|x|$ in order to maintain the same decimal precision. Thus, in the context of our calculations, (4.1) could have been used to evaluate $e^{-h\nu/kT}$ in the Rayleigh-Jeans region of the spectra (where $h\nu \ll kT$) while optimized methods would have been employed elsewhere. Nevertheless, the frequency of the calls, the similarity in the input parameters and the low cost of accessing the memory ultimately led to opt for the memoization of this function.

4.2 Atomic Physics

A detailed description of the structure of an atomic system must take into account the kinetic and potential energies of the electrons in the Coulomb field of the nucleus, the electrostatic interactions between those electrons, the many relativistic and radiative processes as well as any potential external effect that could affect these parameters. The complexity of the task is tremendous and any treatment of a more than trivial configuration requires a high level of approximation.

The stationary states of an N-electron atom are described by the time-independent Schrödinger equation:

$$\hat{H}\Psi(\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_N) = E\Psi(\mathbf{q}_1, \mathbf{q}_2, \dots, \mathbf{q}_N) \quad (4.2)$$

where Ψ is the wave function, eigenfunction of the Hamiltonian corresponding to the eigenvalue E , and $\mathbf{q}_i$ a variable regrouping the spatial $\mathbf{r}_i$ and spin coordinates.

The non-relativistic Hamiltonian of the system $\hat{H}$ is given by:

$$\hat{H} = \sum_{i=1}^N \left(\frac{-\hbar^2}{2m} \Delta_i - \frac{Ze^2}{r_i} \right) + \sum_{i,j=1, i \neq j}^N \frac{e^2}{r_{ij}} \quad (4.3)$$

where $r_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$ and the Laplacian Δ_i is defined, in Cartesian coordinates, as:

$$\Delta_i = \nabla_i^2 = \frac{\partial^2}{\partial x_i^2} + \frac{\partial^2}{\partial y_i^2} + \frac{\partial^2}{\partial z_i^2} \quad (4.4)$$

The first energy term in the r.h.s of (4.3) corresponds to the electrons-nucleus interaction and the second one represents the effect of electrostatic repulsion between the electrons.

Exact analytical solutions of the Schrödinger equation are only known in the case of Hydrogen-like atoms. In this particular context and expressing Δ_i in

spherical polar co-ordinates, the eigenfunctions

$$\Psi(\mathbf{q}) = R_{nl}(Z, r)Y_{lm_l}(\theta, \varphi)\chi_{m_s} \quad (4.5)$$

can be formulated as the product of functions with separated variables. This last point allows to split (4.2) into two equations, one involving the radial part r and the other one the angular coordinates θ and φ . The properties of the well-known spherical harmonics $Y_{lm_l}(\theta, \varphi)$ and spin function χ_{m_s} being independent of the shape of the central field, it can be shown that the radial part of (4.5) verifies the following equation:

$$\frac{-\hbar^2}{2m} \left(\frac{d^2}{dr^2} - \left(E + \frac{Ze^2}{r} \right) - \frac{l(l+1)}{r^2} \right) rR_{nl}(Z, r) = 0 \quad (4.6)$$

For $E > 0$, this equation admits a solution for any value of E (continuous) and l (discrete). Otherwise, solutions only exist for the following values of E :

$$E = -\frac{I_H Z^2}{n^2} \quad \text{with} \quad I_H = \frac{2\pi^2 m e^4}{h^2} = \frac{m e^4}{2\hbar^2} \quad (4.7)$$

with the ancillary condition that $n \geq l + 1$. We call n , l , m_l and m_s respectively the Principal, Orbital, Magnetic and Spin quantum number. The first three ones are integers satisfying

- $n \in [1; \infty]$
- $l \in [0; n - 1]$
- $m_l \in [-l; l]$

The spin quantum number can take two possible values, $1/2$ and $-1/2$.

For an Hydrogen atom, the energies of states having the same n but different l are the same: those are called degenerate, and the number of states with the same energy is called the degeneracy of the level ($2n^2$ for the hydrogen atom). In a more general context (i.e. for atoms with many electrons), the energy is also

dependent on l . This dependency can be inferred considering the terms in the radial part of the Schrödinger equation (4.6). The first and second term represent the total and potential energy of the system. Therefore, in order to conserve the dimensional homogeneity of the equation, the third term must as well be identify to an energy (more specifically to the orbital kinetic one), which requires that

$$\frac{\hbar^2 l(l+1)}{2mr^2} = \frac{1}{2}mv^2 \implies \hbar^2 l(l+1) = (mrv)^2 = L^2 = \text{angular momentum squared}$$

This explains why l , quantizing the orbital kinetic energy and the magnitude of the angular momentum of each orbital

$$|\mathbf{L}| = L = \hbar\sqrt{l(l+1)}$$

is called the orbital quantum number. The projection of the angular momentum vector $\mathbf{L}$ onto a fixed direction in space (conventionally the z-axis) is quantized by $L_z = m_l \hbar$ to values one unit of angular momentum apart.

Electrons are fermions, and the Pauli exclusion principle forbids two of them to occupy the same state, i.e, to have the same set of quantum numbers. This limit the number of available places in the different shells. For each of the n possible values of l , there are $2l + 1$ values of m_l , and for each of them, two possible values for m_s . These states can be mapped out (fig 4.2), energy vertically, angular momentum horizontally. For historical reasons, electrons having $l = 0, 1, 2, 3, 4, 5$ are known as s, p, d, f, g, h electrons respectively. The electron configuration describes the value of n and l taken by the electrons of an atomic system, the number of electron in each sub-shell (set of electrons with the same nl values) being shown as a superscript. For example $1s^2 2s^2 2p^2$ represents the electronic configuration of atomic Carbon in its ground state.

n				
6	$\uparrow\downarrow$			
5	$\uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$	
4	$\uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$
3	$\uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$	
2	$\uparrow\downarrow$	$\uparrow\downarrow \uparrow\downarrow \uparrow\downarrow$		
1	$\uparrow\downarrow$			
m_l	0	+1 0 -1	+2 +1 0 -1 -2	+3 +2 +1 0 -1 -2 -3
l	0	1	2	3
	s	p	d	f

Figure 4.2: Ground state of Tungsten: $[\text{Xe}]4f^{14}5d^46s^2$

4.2.1 The Screened Hydrogenic Model

So far, we have only treated the case of a one electron system. Leaving the spin aside for the moment, let us reconsider (4.2) for a N-electron atom:

$$\hat{H}\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = E\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) \quad (4.8)$$

Solving this system necessitates solving in a 3N-Dimensional space a large set of partial derivative equations for which the presence of the electron interaction term in 4.3 prevents any variable separation. Indeed, even if, for high Z materials, every single e^2/r_{ij} term is negligible compared to Ze^2/r_i , there is no guarantee that their cumulative effect will not result in the inter-electron energies being comparable to the electron-nucleus ones¹.

The general method to solve the last equation was developed by Hartree, Slater and Fock (the full details of the derivation can be found in the literature). The idea is to assume that each electron is independent and subject to a central potential V that combines the effect of the nucleus and the other (N-1) electrons. Considering

¹this is actually the case for low ionized material

that the potential V is function of r only leads to what is called the central field model. V tends to $-Ze/r$ close to the origin and asymptotically to $-(Z-N+1)/r$, the main difficulty resides in evaluating its intermediate values for a complex atom. Indeed, in this case, for each radial position, V is also function of the charge distributions and therefore only represents one electron configuration.

In the 1940's Slater and Mayer developed the formalism of a practical and relatively easy to use atomic model [27] adding to the central field and independent electron considerations the hypothesis that each electron evolves in a different Coulomb potential, function of the effective charge Z_k . This approach has the main advantage of facilitating the calculations of the atomic configuration energies and establishes the basis of the Screened-Hydrogenic Models (SHM). Under these conditions, the electronic wave functions are the classical Hydrogenic ones

$$\Psi_k(\mathbf{q}) = R_{nl}(Z_k, r)Y_{lm_l}(\theta, \varphi)\chi_{m_s} \quad (4.9)$$

and the total energy of the system is in consequence given by:

$$E_T = -I_H \sum_{k=1}^{k_{max}} P_k \frac{Z_k^2}{n_k^2} \quad (4.10)$$

where P_k is the population of the electron group k (shell or sub-shell) for which the same effective charge is assumed and k_{max} the last index of such a group. The common action of all the electrons on a given one is equivalent to the partial screening of the nuclear charge this electron would “see” in the absence of the others (fig 4.3):

$$Z_k = Z - \sum_{k'=1}^{k_{max}} \sigma_{kk'} P_{k'} + \alpha_k \quad (4.11)$$

with α_k a model-dependent constant. From the last equation, we observe that the effective charge Z_k is simply defined by the populations of the shell k and a set of tabulated screening constants $\sigma_{kk'}$, independent of the atomic system considered

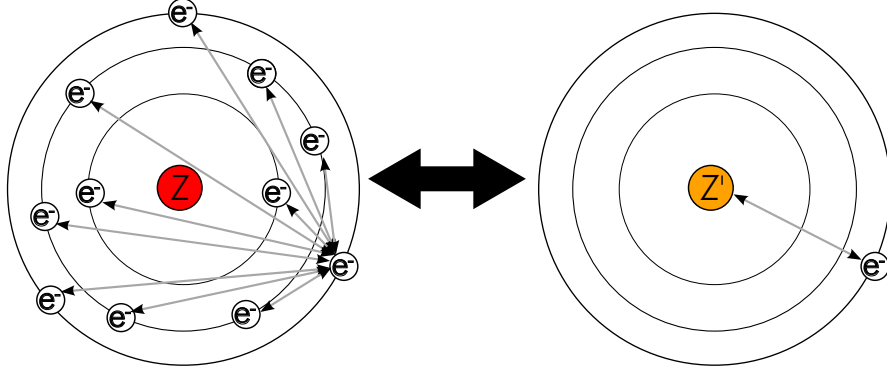


Figure 4.3: The nucleus charge is screened by the other electrons, $Z' < Z$

but different for each version of the model.

As a matter of fact, since the first publication of the Screened-Hydrogenic method, many flavors of the approach have been developed by several authors ([38],[29],[31]). Each one has its own particularities, set of screening constants and assumption on the degeneracy. In this work, we have adopted the method developed by Faussurier et al. which accounts for the l -dependence of the electronic energy levels and screening coefficients ([17] and [18]). In this formalism, the effective charges are:

$$Z_k = Z - \sum_{k'=1}^{k_{max}} \sigma_{kk'} (P_{k'} - \delta_{kk'}) \quad (4.12)$$

where $\delta_{kk'}$ is the Kronecker symbol preventing the self-screening of an electron and $\sigma_{kk'}$ the screening constants given in B.

4.2.2 Ionization and excitation energy

Let us now assume an ion in its ground state electronic configuration described by $\{(n_1 l_1)^{P_1}, (n_2 l_2)^{P_2}, \dots, (n_{k_{max}} l_{k_{max}})^{P_{k_{max}}}\}$.

In our model, each monoelectronic energy ε_k is obtained deriving the total energy E_T with respect to the population of the subshell k ($k = (nl)$):

$$\varepsilon_k = \frac{\partial E_T}{\partial P_k}$$

Therefore, in order to evaluate the ionization energy of an electron in this subshell, one will have to successively calculate the total energy of the ground state configuration, remove one electron from k , and finally subtract the previous energy from the one of the new configuration $\{(n_1 l_1)^{P_1}, \dots, (n_k l_k)^{P_k-1}, \dots, (n_{k_{max}} l_{k_{max}})^{P_{k_{max}}}\}$:

$$\begin{aligned} \text{for the ionization state } \alpha \quad E^\alpha &= -I_H \left(\sum_{i=1, i \neq k}^{k_{max}} P_i \frac{Z_i^2}{n_i^2} + P_k \frac{Z_k^2}{n_k^2} \right) \\ \text{for the ionization state } \alpha + 1 \quad E^{\alpha+1} &= -I_H \left(\sum_{i=1, i \neq k}^{k_{max}} P_i \frac{Z_i^2}{n_i^2} + (P_k - 1) \frac{Z_k^2}{n_k^2} \right) \\ \implies E_{ionization}(k, \alpha) &= E^{\alpha+1} - E^\alpha \end{aligned}$$

with Z'_k the effective charge of the subshell k after the configuration change. Similarly, the ionization energy for a subshell $j > k_{max}$ (excited state) can be evaluated by promoting an electron from a internal shell of the ground state (in practice, we use k_{max}) to j , resulting in the excited configuration

$$\{(n_1 l_1)^{P_1}, (n_2 l_2)^{P_2}, \dots, (n_{k_{max}} l_{k_{max}})^{P_{k_{max}}-1}, P_j\}$$

The new energy is then calculated and subtract from $E^{\alpha+1}$ to get the ionization energy in the subshell j :

$$\begin{aligned} E_j^\alpha &= -I_H \left(\sum_{i=1}^{k_{max}-1} P_i \frac{Z_i^2}{n_i^2} + (P_{k_{max}} - 1) \frac{Z_{k_{max}}^2}{n_{k_{max}}^2} + \frac{Z_j^2}{n_j^2} \right) \\ \implies E_{ionization}(j, \alpha) &= E^{\alpha+1} - E_j^\alpha \end{aligned}$$

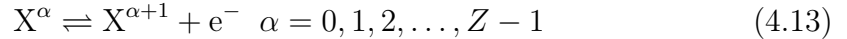
As it will be seen in Chapter 5, the model predictions are in good agreement with experimental measurements of ionization energies. Nevertheless, in order to improve the predictability and flexibility of the code, a scheme to combine the energies calculated by the SHM with the atomic tables from NIST has been implemented.

4.3 Population calculations

Considering the unfriendly combinatorics of any DCA method, the questions of which and how many energy levels and transitions to include in an atomic model are primordial. Use too few, and the population solvers do not converge to the correct solution while the spectra miss some important features. Use too many, and the problem is intractable. In our approach, the choice of not averaging the populations and the computational constraints led to the somewhat arbitrary decision of including in priority states and transitions that were experimentally observed, completing the sets with code generated configurations up to the limit of affordability.

4.3.1 Saha solver

As discussed in Chapter 3, in LTE, the evaluation of the different populations in a gas does not require the knowledge of the transition rates and is uniquely determined by the density and temperature. From thermodynamic considerations, we then recall that the ionization equilibrium symbolized by the reaction



is associated with a minimum of the free energy (i.e. a minimum of the energy available to perform some work). This latter is given by:

$$F = -kT \ln \mathcal{Z}_T \quad (4.14)$$

with $\mathcal{Z}_T$ the total partition function of the system. For an ideal gas consisting of free electrons and ions in different charge states

$$\mathcal{Z}_T = \frac{\mathcal{Z}_e^{N_e}}{N_e!} \cdot \prod_{\alpha=0}^Z \frac{\mathcal{Z}_\alpha^{N_\alpha}}{N_\alpha!} \quad (4.15)$$

with $\mathcal{Z}_x$ and N_x respectively the partition function and number density of the particle x . Substituting (4.15) in (4.14) we obtain:

$$F = -kT \left(\sum_{\alpha=0}^Z N_\alpha \left(\ln \frac{\mathcal{Z}_\alpha}{N_\alpha} + 1 \right) + N_e \left(\ln \frac{\mathcal{Z}_e}{N_e} + 1 \right) \right) \quad (4.16)$$

By setting equal to zero the variation δF with respect to the change in the number of α -ions arising from the ionization reaction (4.13)

$$\delta F = -kT \left(\delta N_\alpha \ln \frac{\mathcal{Z}_\alpha}{N_\alpha} + \delta N_{\alpha+1} \ln \frac{\mathcal{Z}_{\alpha+1}}{N_{\alpha+1}} + \delta N_e \ln \frac{\mathcal{Z}_e}{N_e} \right) = 0 \quad (4.17)$$

and noticing that $-\delta N_\alpha = \delta N_{\alpha+1} = \delta N_e$ we have

$$\frac{N_{\alpha+1} N_e}{N_\alpha} = \frac{\mathcal{Z}_{\alpha+1} \mathcal{Z}_e}{\mathcal{Z}_\alpha} \quad (4.18)$$

Each partition function $\mathcal{Z}_x$ can be written as the product of the contributions from the translational and electronic partition functions

$$\begin{aligned} \mathcal{Z}_x &= \mathcal{Z}_{translational} \cdot \mathcal{Z}_{electronic} \\ &= \left(\frac{2\pi m_x kT}{h^2} \right)^{3/2} V \cdot \sum_{s=0}^{smax} g_s e^{-E_s^x/(kT)} \end{aligned}$$

where m_x is the mass of the particle, V the volume, and E_s and g_s respectively the energy and statistical weight of the electronic configuration s . The statistical weight of a given configuration is the product of the statistical weights of its

subshells:

$$\begin{aligned}
g_s &= \prod_{k=1}^{kmax(s)} C_{max(P_k)}^{P_k} \\
&= \prod_{k=1}^{kmax(s)} \frac{max(P_k)!}{(max(P_k) - P_k)! P_k!} = \prod_{k=1}^{kmax(s)} \frac{(2(2l_k + 1))!}{(2(2l_k + 1) - P_k)! P_k!}
\end{aligned}$$

The masses of the $(\alpha + 1)$ st and α th ion being quasi-identical, the contribution of their translational partition functions disappear from (4.18). We can factor out the part of the electronic partition functions corresponding to the ground state energy

$$\begin{aligned}
\mathcal{Z}_{electronic} &= e^{-E_0^x/(kT)} \sum_{s=0}^{smax} g_s e^{-(E_s^x - E_0^x)/(kT)} \\
&= e^{-E_0^x/(kT)} \tilde{Z}_x
\end{aligned}$$

with $\tilde{Z}_x$ the modified electronic partition function. The free electron partition function is simply the product of the statistical weight of the electron (equal to 2) with its translational partition function. Taking all these considerations into account and dividing by V , we finally obtain for (4.18) :

$$\frac{n_i^{\alpha+1} n_e}{n_i^\alpha} = 2 \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} \frac{\tilde{Z}_{\alpha+1}}{\tilde{Z}_\alpha} e^{-(E_0^{\alpha+1} - E_0^\alpha)/(kT)} \quad (4.19)$$

This relation is known as the Saha equation. It can be noticed that the energy difference between the ground states $E_0^{\alpha+1} - E_0^\alpha$ corresponds to the ionization energy in stage α .

The determination of the populations necessitates solving the system of α -equations described in (4.19). In the first place, the scheme consists in guessing a value for the electron density. This guess can be educated by calling in advance the very fast Thomas-Fermi solver originally present in Gorgon. Then, defining

the functions

$$S_{\alpha+1,\alpha} = \frac{n_i^{\alpha+1}}{n_i^\alpha}$$

we have

$$n_i^\alpha = (S_{\alpha,\alpha-1} \times S_{\alpha-1,\alpha-2} \times \dots \times S_{1,0}) n_0 = f_\alpha n_i^0 \quad (4.20)$$

and for the total ion density

$$n_i = \sum_{\alpha=0}^Z n_i^\alpha = \left(1 + \sum_{\alpha=1}^Z f_\alpha \right) n_i^0 \quad (4.21)$$

Dividing (4.20) by (4.21) we obtain the fractional populations from which we can derive the average charge state $\bar{Z}$:

$$\bar{Z} = \sum_{\alpha=0}^Z \alpha \frac{n_i^\alpha}{n_i} = \frac{\sum_{\alpha=0}^Z \alpha f_\alpha}{\left(1 + \sum_{\alpha=1}^Z f_\alpha \right)} \quad (4.22)$$

n_e can therefore be adjusted to reflect the discrepancy between the temporary ion density $n_i = n_e / \bar{Z}$ and its known value (provided by Gorgon). The whole process is then repeated until convergence.

4.3.2 Continuum lowering

So far, in our derivation of the Saha equation, we have considered the case of perfect gases with no Coulomb interactions. Nevertheless, in a plasma, the potential distribution near and in a given ion is influenced by the distribution of its own bound electrons but also by the presence of neighboring free electrons, ions and neutral atoms. The effects of these perturbations are of two kinds: a time-averaged effect, altering the energy levels available to the ion, and a time-dependent one, which broaden these levels (see 3.1.3.3). The former one is usually

called “pressure ionization” or “continuum lowering” as it results in the lowering of the ionization potential energies while simultaneously limiting the number of terms in the ion electronic partition function (removing the highest excited states close to the continuum).

Let us now consider, around each ion of a plasma, a spherically symmetric non-uniformly charged cloud of free electrons and ions. In the low density limit, the scale over which the electrons screen out the electric field is much greater than the distance between the ions. The characteristic radius of the sphere is therefore given by the Debye length λ_D and the Coulomb corrections to the thermodynamic function can be calculated using the Debye-Hückel model. If the volume of the sphere is V , according to the general equation of electrostatics, the Coulomb energy of the gas inside the sphere is given by:

$$E_{coul} = \frac{1}{2} \sum_{\alpha} n_i^{\alpha} \frac{eZ_{\alpha}}{d} (-eZ_{\alpha}) \cdot V$$

Recalling the expression of the Debye length $\lambda_D = (4\pi e^2 \sum_{\alpha} n_i^{\alpha} Z_{\alpha}^2 / kT)^{1/2}$ and the thermodynamic relation $F = -T \int (E/T^2) dT$, we can derive the corresponding free energy:

$$F_{coul} = -\frac{2}{3} V e^3 \left(\frac{\pi}{kT} \right)^{1/2} \left(\sum_{\alpha} n_i^{\alpha} Z_{\alpha}^2 \right)^{3/2}$$

In a way similar to what was done in the previous part, the variation δF_{coul} with respect to the change in the number of α -ions arising from the ionization reaction can be taken

$$\delta F_{coul} = -e^3 \left(\frac{\pi}{kTV} \right)^{1/2} (\delta N_{\alpha} Z_{\alpha}^2 + \delta N_{\alpha+1} Z_{\alpha+1}^2 + \delta N_e Z_e^2) \left(\sum_{\alpha} n_i^{\alpha} Z_{\alpha}^2 \right)^{1/2}$$

and finally with $-\delta N_{\alpha} = \delta N_{\alpha+1} = \delta N_e$ and $Z_{\alpha+1} = Z_{\alpha} + 1$, $Z_e = -1$:

$$\delta F_{coul} = \frac{(Z_{\alpha} + 1) e^2}{\lambda_D} \delta N_{\alpha}$$

Adding this last quantity to the expression of δF in (4.17), one obtains the ionization equilibrium equation accounting for Coulomb interactions

$$\frac{n_i^{\alpha+1} n_e}{n_i^\alpha} = 2 \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} \frac{\tilde{Z}_{\alpha+1}}{\tilde{Z}_\alpha} e^{-(E_0^{\alpha+1} - E_0^\alpha)/(kT)} e^{(Z_\alpha+1)e^2/(\lambda_D kT)}$$

We see that the decrease in the ionization energy of an α -ion is equal to the Coulomb interaction energy of an electron located at a distance λ_D of an $\alpha+1$ -ion

$$\Delta I_{low} = \frac{(Z_\alpha + 1) e^2}{\lambda_D}$$

In the high density limit, the Debye radius is smaller than the mean inter-ion separation $R_0 = (3/4\pi n_i)^{1/3}$. Following a similar route, we can derive the decrease in the ionization energy in this case

$$\Delta I_{high} = \frac{(Z_\alpha + 1) e^2}{R_0}$$

In the code, both effects are combined in the continuous function

$$\Delta I_{\alpha+1} = (Z_\alpha + 1) e^2 \times \min(\lambda_D^{-1}, R_0^{-1})$$

4.3.3 An NLTE approximation

As it was previously discussed in Chapter 3, Z-pinch plasmas are, in the best case scenario, in partial-LTE. Therefore, it is not surprising that the first attempts to apply to a wire array simulation the new atomic model in LTE did not lead the results expected (see 6.1.2). A computationally inexpensive solution that would reproduce the principal characteristic of NLTE was required.

Since the beginning of the 1980's, Busquet et al. ([6, 7, 9, 8]) have developed a numerically simple method to transform an existing LTE code into a non-LTE one with radiation-dependent ionization. This approach, in its simplest form, can be

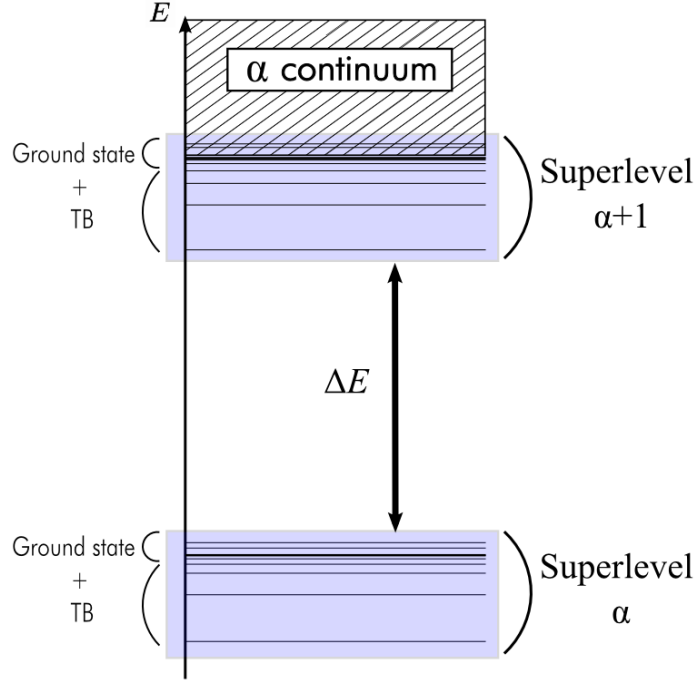


Figure 4.4: Schematic description of the Superlevels.

compared to a 0-order superconfiguration model. For a given ionization stage α , the energy gap between the excited states decreases with the excitation energies of these states. The ratio of the collisional de-excitation rates to the radiative ones scaling as ΔE^{-3} (see 3.3.1), it follows that, above a certain excitation energy, the interactions between those states are collisionally dominated. In this partial LTE, the populations in the group of excited states obey to Boltzmann/Saha statistics and form what is called a thermal band (TB). In this thermal band, one can also include some nearby levels such as the ground state of the next ionization stage $\alpha + 1$ (free level) to form a “superlevel” (fig4.4). The lower limit of the TB depends on the temperature and density and includes every single ion state in LTE. In the absence of such assumption, the global rates between two superlevels must be calculated using a classical Collisional Radiative approach.

Let us for the moment consider only two single levels of respective population densities n_1, n_2 , statistical weights g_1, g_2 and energy separation ΔE . In equilib-

rium, the populations and rates W between those levels balance:

$$\begin{aligned}\frac{n_2}{n_1} &= \frac{W_{(\text{Collisional} + \text{Radiative}) 1 \rightarrow 2}}{W_{(\text{Collisional} + \text{Radiative}) 2 \rightarrow 1}} \\ &= \frac{n_e C_{12} + 4\pi I_\nu B_{12}}{n_e C_{21} + A_{21} + 4\pi I_\nu B_{21}}\end{aligned}$$

The different rates can be obtained using the expression of the Einstein coefficients and following the estimation of the collisional excitation cross section given by Van Regemorter[44] and Mewe [28]. In the special case of a Maxwellian electron distribution with a Planckian radiation field at temperature T_r we have for the photoexcitation, photodecay (spontaneous+stimulated emission), collisional excitation and collisional de-excitation respectively:

$$\begin{aligned}4\pi I_\nu B_{12} &= \frac{g_2}{g_1} \frac{A_{21}}{e^{\Delta E/T_r} - 1} \\ A_{21} + 4\pi I_\nu B_{21} &= A_{21} \left(1 + \frac{1}{e^{\Delta E/T_r} - 1} \right) \stackrel{(3.26)}{=} \frac{g_1}{g_2} \frac{8\pi^2 e^2 \Delta E^2}{mc^3 h^2} f_{12} \left(1 + \frac{1}{e^{\Delta E/T_r} - 1} \right) \\ n_e C_{12} &= n_e \frac{4\pi^2 e^4}{\sqrt{3}} \sqrt{\frac{2}{\pi m_e}} e^{-\beta} \Delta E^{-1} T_e^{-1/2} f_{12} \bar{g} \\ n_e C_{21} &\stackrel{(3.46)}{=} \frac{g_1}{g_2} n_e C_{12} e^\beta\end{aligned}$$

where $\beta = \Delta E/T_e$ and $\bar{g}$ is the gaunt factor for the transition $1 \rightarrow 2$. Neglecting the effects of the radiation field (photoexcitation-stimulated emission) and factoring out the collisional rates leads to :

$$\begin{aligned}\frac{n_2}{n_1} &= \frac{g_2}{g_1} \frac{e^{-\Delta E/T_e}}{1 + \frac{2\sqrt{3}}{c^3 h^2 e^2 \bar{g}} \sqrt{\frac{\pi}{2m}} \frac{\Delta E^3 T_e^{1/2}}{n_e}} \quad [\text{cgs, E and T in erg}] \\ &= \frac{g_2}{g_1} \frac{e^{-\Delta E/T_e}}{1 + \frac{2.74 \times 10^{12}}{\bar{g}} \left(\frac{\Delta E^3 T_e^{1/2}}{n_e} \right)} \quad [\text{E and T in eV}]\end{aligned} \tag{4.23}$$

The last formula is equivalent to the Boltzmann distribution for high electron density, low electron temperature and small energy gap. We can extend this ex-

pression in order to evaluate the ion stage populations at equilibrium, summing up the transition rates between the superlevels and averaging the transition energies:

$$\begin{aligned} \frac{n_i^{\alpha+1}}{n_i^\alpha} &= \frac{\sum W_{\alpha \rightarrow \alpha+1}}{\sum W_{\alpha+1 \rightarrow \alpha}} \\ &\simeq \frac{g^{\alpha+1}}{g^\alpha} \frac{e^{-\langle \Delta E \rangle / T_e}}{1 + \frac{2\sqrt{3}}{c^3 h^2 e^2} \sqrt{\frac{\pi}{2m}} \frac{T_e^{1/2}}{n_e} \frac{\langle \Delta E^2 f \rangle}{\langle \Delta E^{-1} f \bar{g} \rangle}} \end{aligned} \quad (4.24)$$

where the weighted average is defined as:

$$\langle x \rangle = \frac{\sum_{i \in \{\alpha\}} x_i g_i e^{-(E_i^\alpha - E_0^\alpha) / T_{eff}}}{\sum_{i \in \{\alpha\}} g_i e^{-(E_i^\alpha - E_0^\alpha) / T_{eff}}}$$

$g^{\alpha+1}$ (containing the free electrons) and g^α , statistical weights of the superlevels, are now respectively defined as $2 \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} \tilde{Z}_{\alpha+1} / n_e$ and $\tilde{Z}_{\alpha+1}$. In the model, the value taken for the average gaunt factor is around 0.2². It was found that taking the approximation $\langle \Delta E_{ionization}^3 \rangle / \bar{g} \simeq \langle \Delta E^2 f \rangle / \langle \Delta E^{-1} f \bar{g} \rangle$ does not significantly change the results. With these considerations, the system of equations in (4.24) can be redefined as:

$$\frac{n_i^{\alpha+1} n_e}{n_i^\alpha} \simeq 2 \left(\frac{2\pi m_e kT}{h^2} \right)^{3/2} \frac{\tilde{Z}_{\alpha+1}}{\tilde{Z}_\alpha} e^{-\langle \Delta E \rangle / T_e} \times \frac{1}{1 + 1.34 \times 10^{13} \langle \Delta E^3 \rangle T_e^{1/2} / n_e} \quad (4.25)$$

A formulation equivalent to the Saha equation with the term $(1 + 1.34 \times 10^{13} \langle \Delta E^3 \rangle T_e^{1/2} / n_e)^{-1}$ accounting for the departure from LTE. Similarly, the source function is no longer equal to its value in LTE: recalling the expression of the source function accounting

²A better estimate is given by Mewe: $\bar{g} = 0.15 + 0.28 \times \ln[1 + (0.562 + 1.4\beta) / (\beta + 1.4\beta^2)]$

for the stimulated emission, it reads

$$S'_\nu = \frac{j_\nu}{\kappa_\nu \left(1 - \frac{n_2 g_1}{n_1 g_2}\right)}$$

$$\stackrel{(3.9), (4.23)}{\simeq} \frac{2h\nu_{21}^3}{c^2} \left[e^{\Delta E/T_e} (1 + 1.34 \times 10^{13} \Delta E^3 T_e^{1/2} / n_e) - 1 \right]^{-1}$$

4.4 Opacities

As it was previously mentioned, even if the radiation from each cell of the Eulerian grid is considered to be isotropic, the number of those cells prevents any non-local treatment (e.g. ray-tracing) of the radiation transfer equation. Moreover, the number of bound-bound transitions calculated in each volume element by the new model only exacerbates these limitations.

For each one of these transitions, a detailed description of the emission necessitates a multi-point evaluation of the opacity across the line profile (see next chapter). In the context of an inline implementation, an approximation method was developed. Let us consider the total power emitted by a line transition centered at the frequency ν_0 , from (3.11) :

$$P_T = \int_0^{+\infty} S'_\nu (1 - e^{-\tau'_\nu}) d\nu \quad (4.26)$$

We recall the expression of the optical depth $\tau'_\nu = \kappa'_\nu dl = j_\nu dl / S'_\nu$, where dl is the mean optical path of the photons in a cell. The frequency dependent emission coefficient can be expressed as the product of the total emission of the line $j_{bb} = n_2 A_{21} h \nu_{21} / 4\pi$ with its frequency dependent profile $\Phi_{V oigt}$. If we assume that the variation of the source function across the line is negligible then $S'_\nu \simeq S'(\nu_0) = S'_0$, and for (4.26) we obtain:

$$P_T \simeq S'_0 \int_0^{+\infty} (1 - e^{-j_{bb} \Phi_{V oigt} dl / S'_0}) d\nu$$

We recognize in the integral the so-called equivalent width of the line.

In the case of a weak line, the optical depth $\tau'_v = \frac{j_{bb}\Phi_{Voigt}dl}{S'_0} \ll 1$ and a Taylor expansion of the exponential gives

$$P_{weak} \simeq j_{bb}dl \int_0^{+\infty} \Phi_{Voigt} d\nu = j_{bb}dl$$

the Voigt profile being normalized to unity. For strong lines, around the central frequency, an interval $[\nu_0 - \Delta; \nu_0 + \Delta]$ exists in which the optical depth is greater than unity

$$P_{strong} \simeq S'_0 \left(\int_0^{\nu_0 - \Delta} (1 - e^{-\tau'_\nu}) d\nu + \int_{\nu_0 - \Delta}^{\nu_0 + \Delta} (1 - e^{-\tau'_\nu}) d\nu + \int_{\nu_0 + \Delta}^{+\infty} (1 - e^{-\tau'_\nu}) d\nu \right)$$

The central term in the previous expression can be approximated by 2Δ , as $e^{-\tau'_\nu} \ll 1$ on the major part of the interval. By taking the Taylor expansion of the two other terms (for which $\tau'_v \leq 1$), we finally get

$$P_{strong} \simeq 2 \left(\Delta + \frac{j_{bb}dl}{S'_0} \int_{\nu_0 + \Delta}^{+\infty} \Phi_{Voigt} d\nu \right) \quad (4.27)$$

The evaluation of this expression necessitates the determination of the value of Δ , which in turn requires solving for Δ the equation $\tau'_\nu = 1$, or

$$\Phi_{Voigt}(\Delta, \sigma, \gamma) = \frac{S'_0}{j_{bb}dl} \quad (4.28)$$

Unfortunately, as discussed before, no analytic solution exists for this equation. Zaghloul[46] proposes a reformulation of the Voigt profile to a simple proper integral, enabling the use of algorithms available in the literature and included in many software packages to integrate the function with relative simplicity and

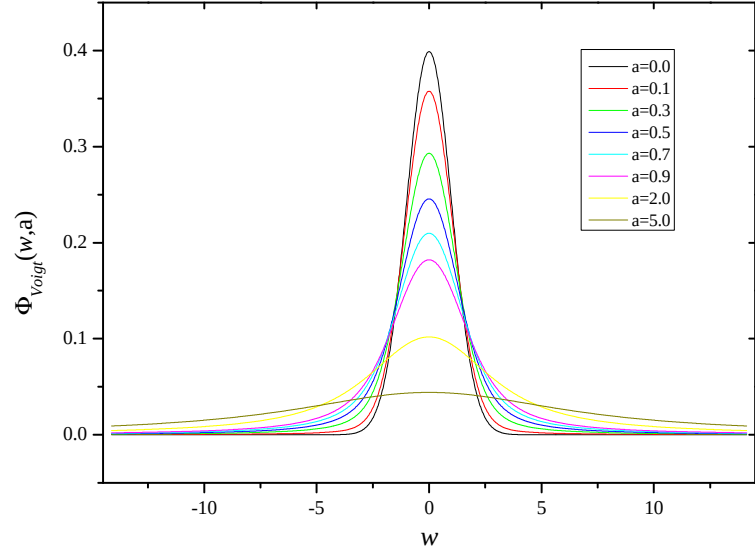
good accuracy (fig 4.5). Expressed in term of the reduced frequency w :

$$\begin{aligned} \Phi_{Voigt}(w, \sigma, \gamma) = & \frac{1}{\sigma\sqrt{2\pi}} \left(e^{a^2} \operatorname{erfc}(a) e^{-w^2} \cos(2aw) + \right. \\ & \left. \frac{2}{\sqrt{\pi}} \int_0^w e^{-(w^2-w'^2)} \sin(2a(w-w')) dw' \right) \end{aligned} \quad (4.29)$$

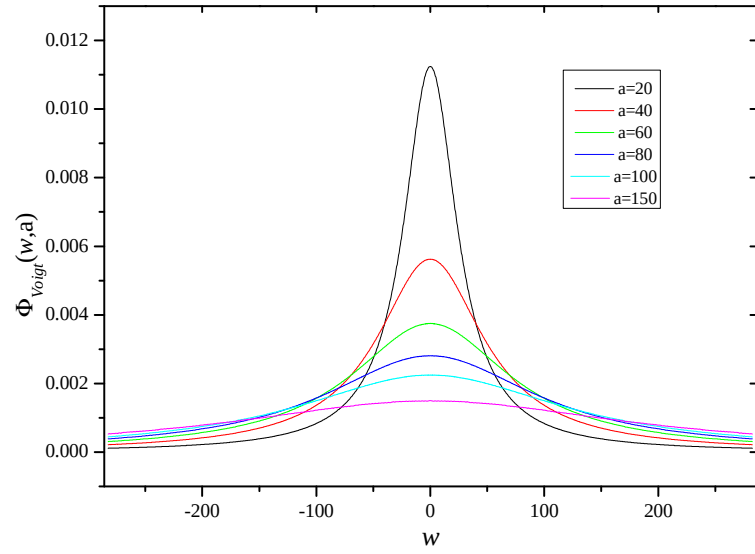
with the complementary error function defined as $\operatorname{erfc}(x) = \frac{2}{\sqrt{\pi}} \int_0^{+\infty} e^{-t^2} dt$. When the parameter a is greater than 26, an overflow occurs on 64 bits processors. A solution consists in taking the asymptotic expansion for the scaled complementary error function

$$\operatorname{erfcx}(x) = e^{x^2} \operatorname{erfc}(x) \underset{x \rightarrow \infty}{\simeq} \frac{1}{\sqrt{\pi}} \frac{1}{x} \sum_{n=0}^{+\infty} \frac{(-1)^n (2n)!}{n! (2x)^{2n}}$$

Tabulating the inverse Voigt function $\Psi : (\Phi_{Voigt}, \sigma, \gamma) \longrightarrow \Delta$ and the inverse of its integral $\Upsilon : \left(\int_{\Delta}^{+\infty} \Phi_{Voigt} d\nu, \sigma, \gamma \right) \longrightarrow \Delta$ using the standard deviation σ from the ion temperature and a simple estimate for Stark broadening[15] allows a fast inline resolution of (4.28) and (4.27).



(a)



(b)

Figure 4.5: Voigt profiles calculated using equation (4.29) for (a) small to moderate and (b) moderate to high values of the damping parameter a , respectively.

Chapter 5

Standalone implementation and comparisons

This Chapter describes in details the offline version of the new atomic model. In the first sections, the different capabilities of the standalone implementation and the specific methods developed for the production of synthetic spectra are introduced. In the last part, we compare the results obtained by a commercial Atomic Physics software package (PrismSpect) with the prediction of the model.

5.1 Version requirements

Originally, the standalone code was started as a development framework for the atomic model. The initial idea was to use it as a test area for functions and subroutines that will later be included in the inline version. In addition to this project, we were also simultaneously developing various diagnostics (synthetic XUV imaging, shadowgraphy and proton probing) to analyse the outputs of Z-pinch simulations. It soon became clear that the capabilities of the atomic code could provide some valuable additional features to this set of synthetic diagnostics.

The main interest of such an implementation was to allow the generation of

detailed synthetic spectra from the data of the simulations. Although a full 3D ray-tracing approach remained unrealistic given our current computational capabilities, in principle, it seemed reasonable to think that we could use the core of the inline version of the atomic model to simulate the behavior of diagnostics only requiring a one-dimensional spectral integration, and that without too much difficulty. Once the question of generating and propagating a spectrum through a line of cells in the computational grid would have been solved, the generalisation to the case of the entire volume and the production of synthetic filtered Microchannel Plates (MCP) images (for example) would have been trivial.

Unfortunately, we had once again to face the reality of computational speed limitations. The instinctive answer to this issue was to parallelize the code using the Message Passing Interface (MPI) library provided by the Argonne National Laboratory[1]. To understand why this measure was not sufficient, it is necessary to examine the intricate relationship between speed and data storage for this very particular situation.

Let us examine the scheme for the integration of spectral energy flux information through the grid and consider the transport of radiation along the line of sight from cells located on the outermost boundary of the simulation volume to the plane of detection. In the case of an orthographic projection (the only one considered here), the propagation path of the light beam is parallel to one axis of the grid coordinate system (fig 5.1).

Cycling through each elementary volume towards the detector, the atomic model uses the local ion and electron densities, temperatures and momentums to calculate the local frequency-dependent emissivities and opacities. For each cell, these emission and absorption spectra are combined in the radiation transfer equation to update the incident flux:

$$F_{i-\frac{1}{2}}(\nu) = F_{i+\frac{1}{2}}(\nu)e^{-\kappa'_i(\nu)dl} + 4\pi dl^2 \times S'_i(\nu) \left(1 - e^{-\kappa'_i(\nu)dl}\right) \quad (5.1)$$

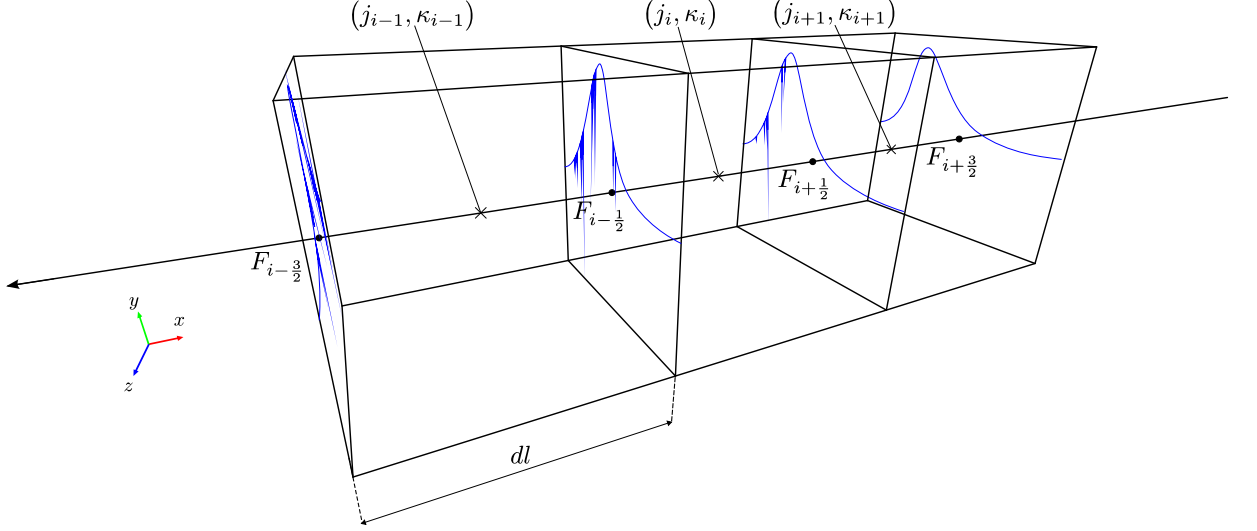


Figure 5.1: Schematic for the spectral transport through the grid.

where $F_{i-\frac{1}{2}}$ is the flux incident on the back face of the cell of index i and side-length dl (the radiation sources are assumed to be isotropic). In contrast with the inline treatment of bound-bound transitions, the offline approach does not require additional approximation of the line opacities and each profile can be sampled at several points. Hundreds of transitions being usually considered in each cell, millions of points can be inserted into the propagating spectra during its journey through the simulation volume. The position of these points in the frequency-amplitude plane being determined by the local parameters of density, temperature and momentum, the likelihood of redundant insertion is small and the amount of spectral data grows very quickly.

5.1.1 Dynamic array

The question of data storage is therefore crucial. The most common way to record the properties of an object set involves the use of a data structure called an array. A typical array is defined as a contiguous zone of the computer memory that stores a collection of indexed elements. When a value needs to be saved or retrieved from a location, the address of the corresponding memory zone is calculated and directly

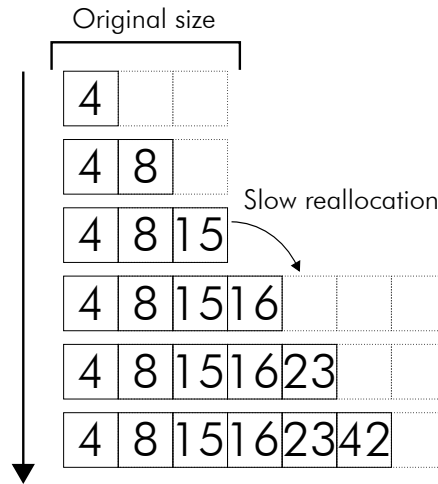


Figure 5.2: Insertion process in a dynamic array.

accessed in $\Theta(1)$ time. If the number of objects to insert is not known before runtime, as it is the case for spectral transport, a growable or dynamic array is needed. Such a structure is created by estimating at the very beginning the maximum amount of memory to be required and by allocating an array of such fixed-size. Elements can then be added or removed at the end of this reserved space in constant time (fig 5.2).

As simple as this approach is, it has several disadvantages. Firstly, if the initial estimate of the maximum size n is smaller than the number of elements to be finally inserted, a reallocation of the array (taking $\Theta(n)$ time) has to be performed when full capacity is reached. Secondly, any insertion or deletion at an arbitrary position in the array takes a linear time as it requires to move the following elements. Finally, if no simple formula links the index of the record with its value, searching for an arbitrary element may necessitate looping through every single object in the array.

5.1.2 Linked list

An alternative method consists in using a so-called linked list. Linked lists are constituted by a collection of objects or nodes, each one composed of two distinct

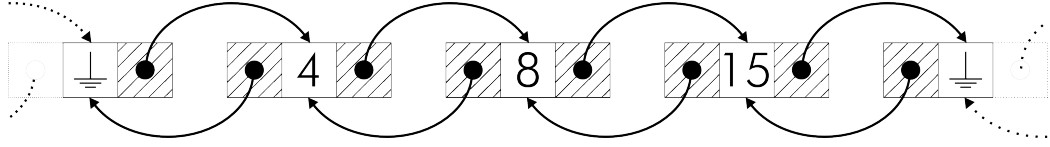


Figure 5.3: A doubly linked list.

fields: a data field, containing the information to be recorded, and a pointer field, containing the memory address of the next (and previous for doubly linked list) node (fig 5.3).

The main advantage of linked lists over dynamic arrays lies in the efficiency of insertion and deletion operations. As the data items need not be stored contiguously in the computer memory, these operations only necessitate updating the pointer field of the neighboring nodes of the location considered (in $\Theta(1)$ time). There are no constraints other than the physical memory size that limit the maximum number of records in a linked list and elements can always be inserted at the beginning/end in a constant time as no reallocation is ever required. Nevertheless, due to the sequential access to the memory, search and indexing time depend linearly on the number of nodes contained in the list ($\Theta(n)$ complexity).

5.2 A self-balancing binary search tree

The method finally adopted to solve the issue of spectral data storage was derived from a self-balancing binary search tree implementation. In computer science, a tree is a data structure using an organization of nodes mimicking an arborescent hierarchy. Each node in such a set is a parent object that may have several children located directly below it in the structure. The node possessing the highest position in the hierarchy constitutes the entry point to the tree and is called the root (tree grow downwards). A node with no children or whose children are the sentinel node (see below) is called a leaf. The length of the path between the root and a given node is the depth of this node (the root node of a tree has a depth of 0).

The collection of all nodes with the same depth is a level of the tree. The height of the tree is the distance between the root and the deepest node.

Binary trees are a special case of tree topology in which each node has a maximum of two children, one “left” and one “right”. Along with the local node data, the memory addresses of those children are stored in the pointer field of the node object. The number of nodes n in a binary tree in which the leaves are at the same level and every node other than the leaves has two children is equal to $2^{h+1} - 1$, where h is the height of the tree. A binary tree is said to be balanced if none of its leaves is much farther away from the root than the others. For such a tree, the average depth (i.e. the average number of step between the root and one leaf) can be evaluated by $\log_2 n$.

A Binary Search Tree (BST) is a binary tree with special features (fig 5.4). The data zone of a BST node contains a field for a so-called key value. This key belongs to an ordered set (real number, string of characters) with a comparison operator. The main properties of a BST are the following:

- Every node key in the tree is greater than every key contained in the left subtree of that node.
- Every node key in the tree is less than every key contained in the right subtree of that node.
- Both subtrees are also BSTs.

Let us suppose that we want to insert a given element in the BST. If the tree is null, we simply have to insert the new object at the root. Otherwise, we compare the root key to the key of the item to insert. If they are equal, we replace¹ the root data by the item data and the insertion is successful. If the key of the item is less than the root key, we point to the left subtree. If the key is greater, we point to the right subtree. The entire process is then repeated recursively for the target subtree until a leaf is reached and a new node (with the new item properties)

¹or perform any other kind of operation

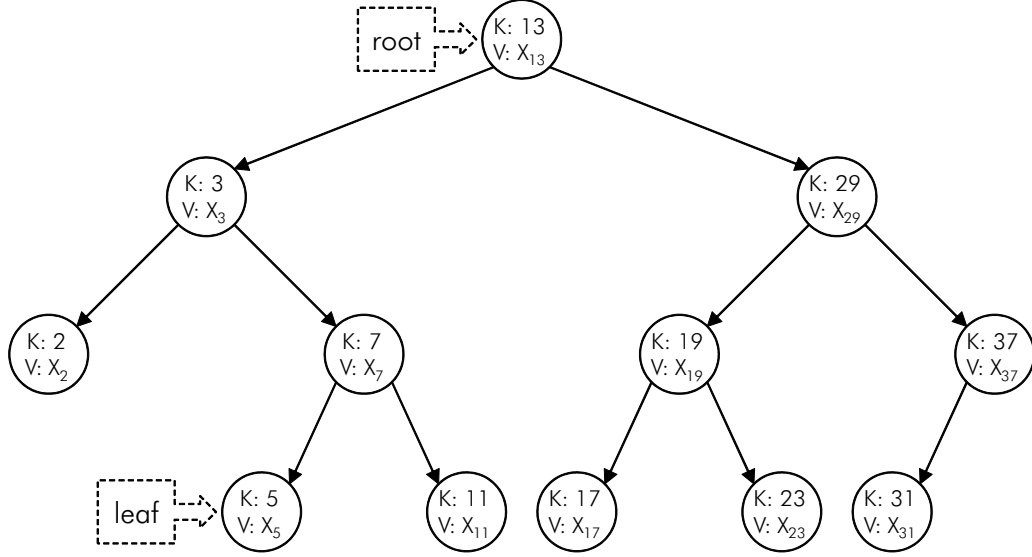


Figure 5.4: Binary Search Tree containing 12 nodes of values V and keys K .

allocated as its left or right child. The search procedure is similar to the insertion one, the recursion stopping when a matching key is found.

Search and insert procedures are very efficient on balanced tree. Let us consider the worst case scenario for a search operation performed on an hypothetical perfectly balanced tree of size $n = 4 \times 10^{19}$ (approximately the number of nitrogen particles in 1 cm^3 of air at 1 atm and 0°C): on average, it would only take $\log_2(4 \times 10^{19}) \approx 65$ steps to reach any node of that tree. Unfortunately, in general, there is no guarantee that the construction process will lead to such a balance. For instance, if the previous items were inserted in key-sorted order, the tree would degenerate into one single right branch (i.e. a linked list) of size n , with its corresponding linear time operations. The difference in performance between the two cases is tremendous and highlights the importance of keeping the tree balanced.

5.2.1 Spectral treap

The treap data structure was first introduced by Aragon and Seidel[2, 37] in 1989. Although similar in many respects to the usual species of binary search trees, treaps have the particular ability to maintain their arborescence balanced. Com-

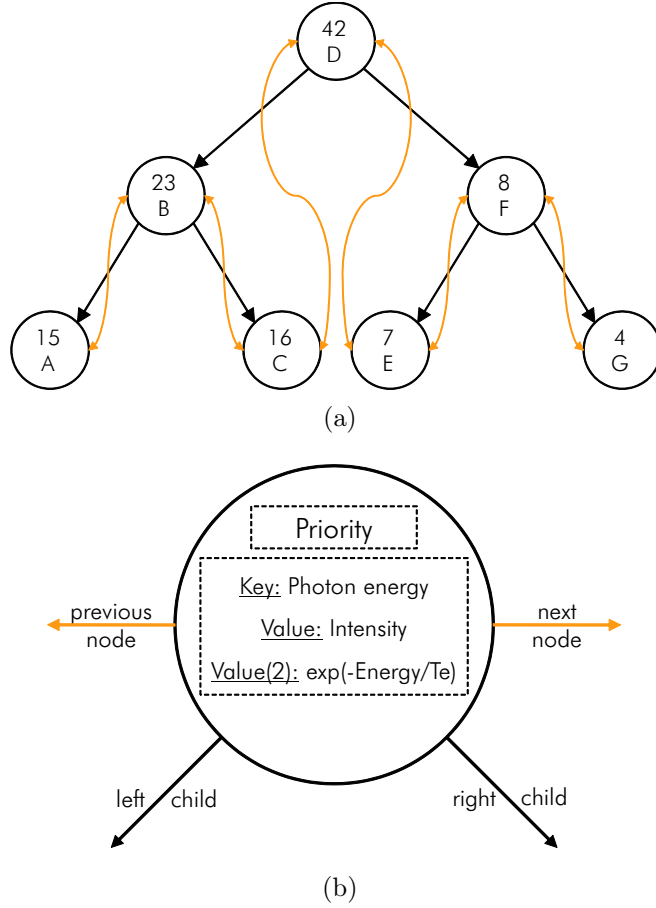


Figure 5.5: (a) A treap with alphabetic keys and numeric priorities. (b) Internal node structure. In yellow: doubly linked list for fast local operations.

pared to regular tree nodes, treap node objects have an extra field containing a randomly generated value called priority. This value, allocated at the node creation, determines its place in the hierarchy: any operation (insertion/deletion) performed on the treap, while keeping the inorder traversal order (key order) intact, must ensure that the parents have higher priorities than their children. The final structure obtained by following this rule is equivalent to a binary tree constructed by inserting the items in decreasing order of priority (i.e. priority decreasing with node depth). If the initial distribution of node priorities is random, the height of this tree is logarithmic with high probability, and so is the height of the equivalent treap (fig5.5a).

The averaged $\Theta(\log n)$ time complexity for search, insertion and deletion op-

erations makes treap ideal candidates for spectral data storage. In our approach, each spectral point is represented by a node whose key and value are respectively equal to the photons frequency and intensity. For the memoization reasons invoked in the previous chapter, this node also contains the local value of $e^{-h\nu/kT}$ in a separate field. Operations performed on line profiles often required working on a set of points with good frequency locality. A broadening process, for example, will modify the amplitude of the spectral points on the left and right of the line center. If we start by pointing to the node at this central frequency, devising a method to provide fast access to the nearby nodes is desirable. The ordinary treap structure allows such access if the child object contains a pointer to its parent. Nevertheless, traversing the treap in key order starting from one arbitrary node usually requires executing a series of conditional branch instructions. A more practical solution consists in maintaining a doubly linked list on top of the treap by adding two extra pointers to the node object (fig 5.5b).

We use a sentinel node to mark the boundaries of the treap. Besides being the left and right child of every leaf, this dummy node is also the beginning and the end of the linked list.

Tree rotation

Tree rotation is an essential process that allows changing the hierarchy position of a node without modifying the keys order.

Let us consider a very simple treap containing five nodes whose keys are alphabetically sorted. Suppose that the treap is as depicted in figure 5.6a and that the priority of the node B is higher than the one of D.

In order to preserve the hierarchy rule, a clockwise rotation around B has to be performed. This is done in two parts: first the left child pointer of B's parent (D) is reassigned to B's right child (C) (fig 5.6b) , then B's right child pointer is reassigned to D (fig 5.6c). The new structure obtained has B for root node and

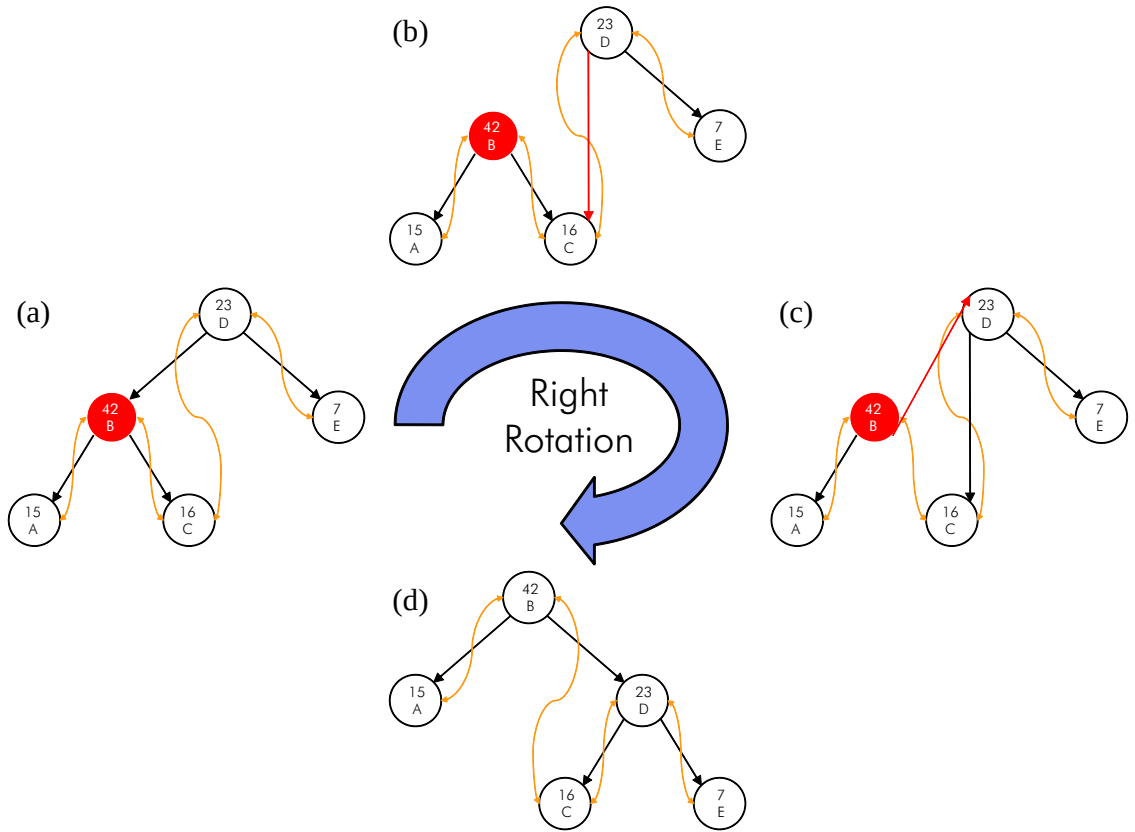


Figure 5.6: Right rotation of the treap around the node B.

complies with the priority and key orders (our doubly linked list has not been corrupted) (fig 5.6d).

Search and Insertion

Search operations in treaps are essentially similar to those in binary trees. To insert a new node of key x , generate a random priority for this node, binary search this key in the arborescence and allocate the new object at the leaf location pointed by the search result. Then, swap the position of the new node with its successive parent's until their respective priorities conform the hierarchy rule.

Deletion

To delete a node of key x , binary search this key in the tree. If the corresponding node is a leaf, simply delete it. Otherwise, as long as the node is not a leaf, swap

its position with the one of its child having the highest priority².

5.2.2 Polyline reduction

Saving spectra in treaps presents several advantages in terms of computational performance. However, the huge number of points generated during the integration processes can consequently reduce the execution efficiency. In order to lower this number, a method to filter out the non-essential nodes has been implemented. Based on the Polyline Reduction algorithm [16], it provides a flexible control over the treaps' sizes while preserving the essential spectral details.

Any given spectrum can be regarded as a sequence of n vertices X_i forming a polyline $P = \{X_i\}_{i=0}^n$. For each one of these vertices, the algorithm measures the dimensionless weight

$$w_i = \frac{\text{Distance}^2(X_i, \text{Segment}(X_{i-1}, X_{i+1}))}{\text{Length}^2(\text{Segment}(X_{i-1}, X_{i+1}))} \quad (5.2)$$

using the neighbouring points X_{i-1} and X_{i+1} (fig 5.7). This weight represents the “bumpiness” of the spectrum at the position i : the higher the irregularity, the bigger the weight. Inversely, if the three vertices are aligned, the weight is null. In that case, the two segments $X_{i-1}X_i$ and X_iX_{i+1} can be replaced by a single one, $X_{i-1}X_{i+1}$. The goal of the reduction method is therefore to remove the lightest points from the polyline, one at a time.

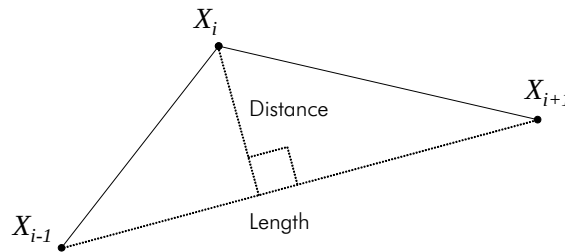


Figure 5.7: Polyline segments.

²by convention, the sentinel has a priority of -1.

In first approach, a recursive algorithm can be used to perform this task. Given a polyline of size n , cycle through the vertices calculating the individual weights. Search for the lightest node and remove it. Update the weights of the remaining $n - 1$ points. Repeat the process for the new polyline. This algorithm has $\Theta(n^2)$ complexity ($n + n - 1 + \dots + 3 = n(n + 1)/2 - 3$) and involves several redundant computations. For instance, the weights updating procedure only requires modifying the properties of the two vertices on the left and right of the lightest node.

A better approach consists in building a min-heap data structure with the vertices. A min-heap is a special case of binary tree which satisfies the heap property: if B is a child of A, then $\text{key}(A) < \text{key}(B)$. Heaps can be implemented as complete binary trees³ and therefore efficiently stored in dynamic arrays supporting $\Theta(1)$ lookup. Under these conditions, and by using the weights as keys, the position of the lightest node can be maintained at the root in $\Theta(\log n)$ operations and its removal achieved in $\Theta(1)$ time. A detailed description of the heap mechanisms can be found in the literature. Here we shall only describe the essential features of the reduction method.

The initial construction of the heap requires an $\Theta(n \log n)$ comparison sort of the n vertices weights. After the minimum value is removed from the root, the tree is reorganized in $\Theta(\log n)$ time. The extraction of the root node results in the modification of the weights of the two neighbouring vertices in the heap. The original heap structure preventing the deletion/insertion of nodes at random places, these vertices have to be propagated downwards or upwards depending on their new hierarchy position. This operation is also performed in $\Theta(\log n)$ time. The complication is caused by the fact that we have to obtain the location of the two nodes in the heap, and this without having to search through the tree (what

³binary trees in which every level, except possibly the last, is completely filled, and all nodes are as far left as possible.

would take $\Theta(n)$ time). This difficulty is overcome by storing the array index of the heap node in the vertex data structure (fig 5.8).

```

!----- Heap node type -----
Type heap_node
  sequence
  integer          :: index ! heap_index
  Type(treap_node),pointer :: p_node ! pointer to the contained treap node
  Type(heap_node),pointer :: prev   ! previous node
  Type(heap_node),pointer :: next   ! next node
  real(kind=8)          :: w ! weights
End Type heap_node
!-----

```

Figure 5.8: Fortran listing of a heap node.

Simple example

To illustrate the functioning of the algorithm, let us consider a very simple polyline containing 13 vertices $X_k = (\pi k/12, \sin(2\pi k/12))$, for $k \in [0; 12]$ (fig 5.9a). Originally, the heap is built with the weights provided by (5.2), the heap indices being the same as the vertices ones⁴ (fig 5.9b).

This structure is a min-heap if and only if each node H_k has a smaller weight than its children H_{2k+1} and H_{2k+2} , which is not the case here. The tree must be sorted: cycling through the heap array, starting from the bottom parent (H_5 in our case), swap the element with its lightest child as long as necessary (sift-down function). The weights of H_5 and H_4 are smaller than the weights of their children, so no sifting is required. However, H_3 is heavier than H_7 and H_8 . As $\text{weight}(H_7) < \text{weight}(H_8)$, H_3 is swapped with H_7 . Similarly, H_2 is swapped with H_6 and H_0 with H_2 (now containing V_6), H_5 and H_{11} . Figure 5.10b shows the state of the heap after ordering.

The first item to be removed is V_6 . Before this operation, the neighbouring

⁴to prevent the removal of the extremities, V_0 and V_{12} are defined as really heavy.

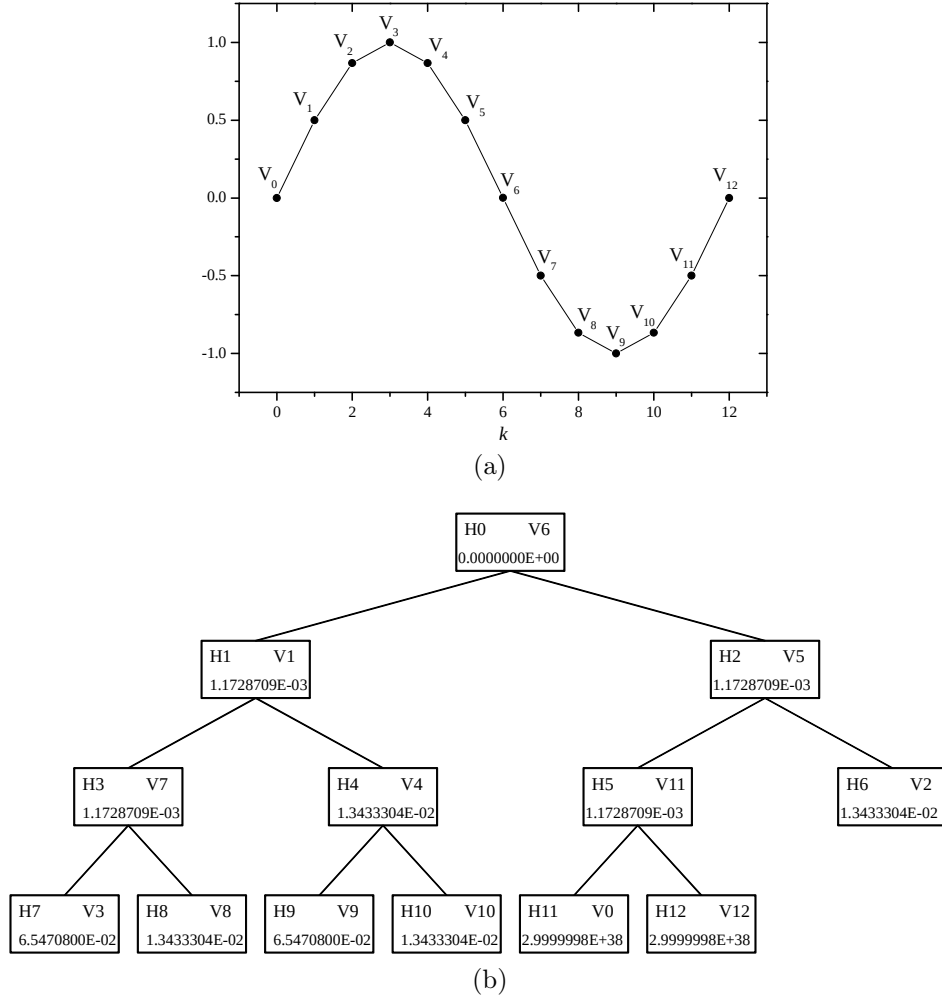
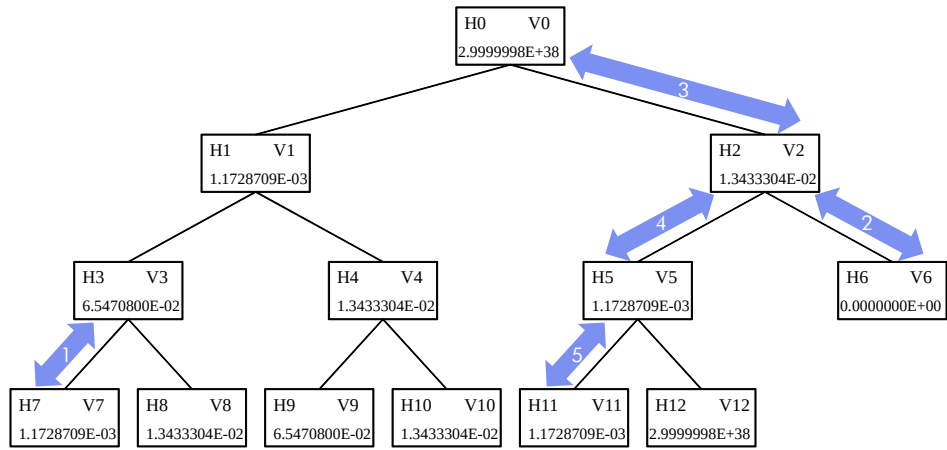


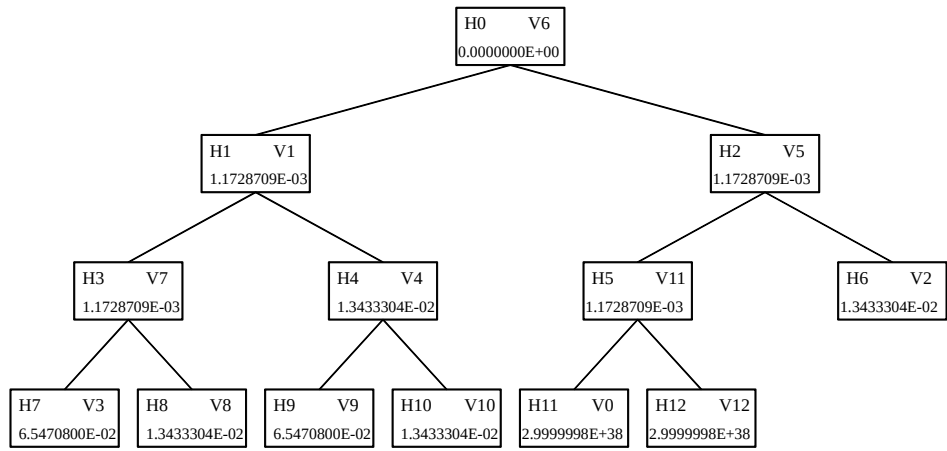
Figure 5.9: (a) Original polyline. (b) Original structure of the heap.

points (V_5 and V_7) are marked for tracking. Following the removal, and in order to keep the tree complete, the last element in H_{12} is placed at the root location and subsequently sifted down. Figure 5.11b shows the state of the resulting heap.

Now the weights of V_5 and V_7 have to be recalculated. The new weight of V_5 (defined by V_4 and V_7) is 7.9823763E-04, a value smaller than the weight of the root, so H_2 and H_0 are swapped. The new value of V_7 is also 7.9823763E-04, which is the same as the root's. Figure 5.12b shows the new state of the heap, now containing 12 vertices. Repeating this process 8 more times leads to the simplified graph in figure 5.13.

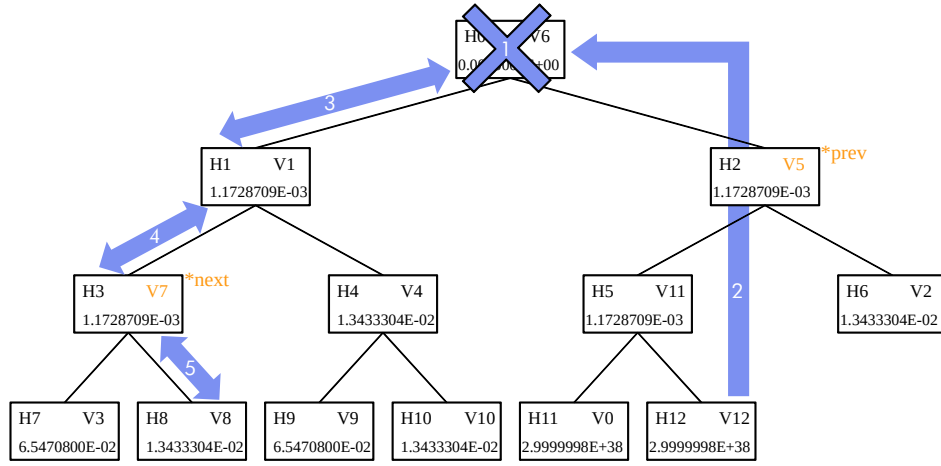


(a)

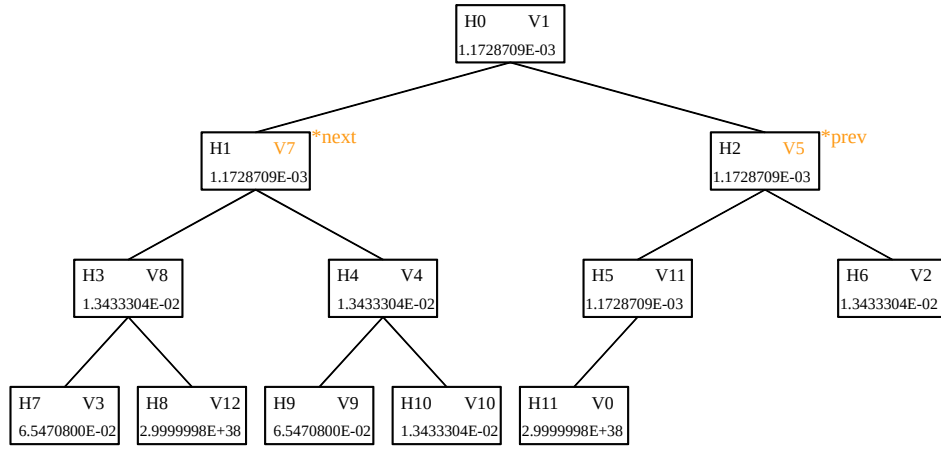


(b)

Figure 5.10: (a) Heap sorting steps (in blue). (b) Sorted heap.

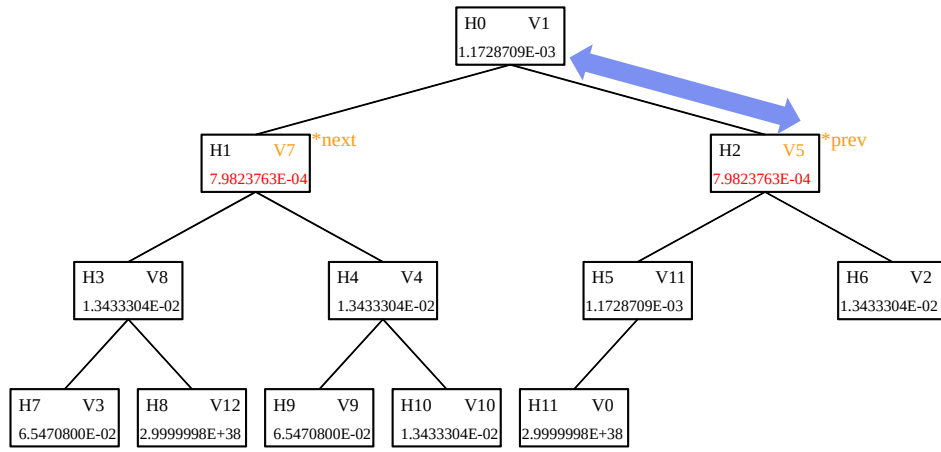


(a)

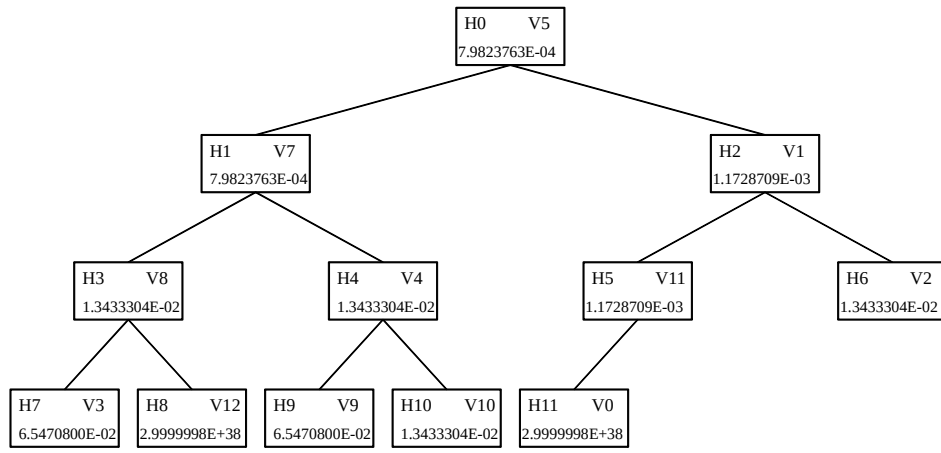


(b)

Figure 5.11: (a) First removal operations (in blue). (b) Resulting heap.



(a)



(b)

Figure 5.12: (a) First removal operations (in blue). (b) Resulting heap.

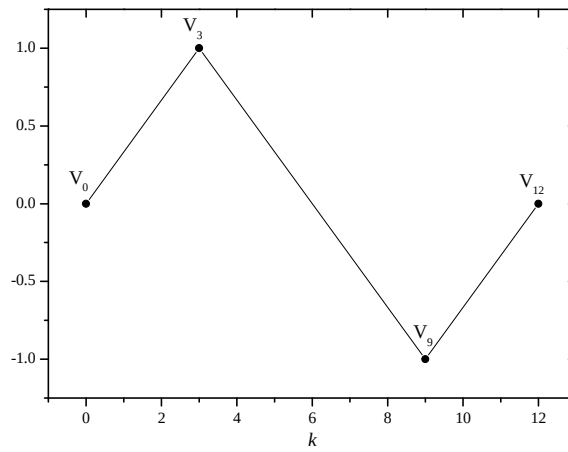


Figure 5.13: Final state of the polyline after the removal of 9 points.

5.3 Code benchmark

In this Section, the new atomic model is benchmarked using the DCA data tables from the National Institute of Standards and Technology (NIST) and Prism Computational Sciences. The spectra, integrated x-ray yields, ion population distributions and average ionizations are compared to the results obtained with PrismSPECT 4.1.0.

5.3.1 Ionization energies

As it was previously mentioned, the energy levels of the new model are a combination of the values provided by the NIST database along with some calculated by the SHM. These latter data are only generated and used when the configuration energies are unknown, which can be the case for computer-generated states not observed experimentally or ionization energies not present in the database.

In order to evaluate the accuracy of these calculations, the ionization energies of aluminium, argon, iron and copper were generated by the code and compared to the values published on the NIST website and incorporated in PrismSPECT package (Table 5.1, 5.2, 5.4 and 5.3).

As expected in the context of a screened-hydrogenic approach, for each element, the quality of the agreement increases with the level of ionization. The biggest discrepancies appear for neutral and weakly ionized atoms for which the interactions between electrons are strong. With the increase of the ionization level, these interactions are weakened and the states energies become hydrogenic: for ionization degrees above 35% the difference between the models drops below 5%.

To further improve the reliability of the results obtained for moderate and high-Z elements, the fine structure corrections proposed by Bethe and Salpeter[5] for the binding energies of electron in hydrogen-like atoms have been implemented.

Ion	SHM (eV)	NIST (eV)	PrismSpect (eV)	$\frac{(SHM-NIST)}{NIST}(\%)$	$\frac{(SHM-PrismSpect)}{PrismSpect}(\%)$
Al	9.18555	5.98576	5.99	53.46	53.35
Al ¹⁺	22.26172	18.82857	18.83	18.23	18.22
Al ²⁺	32.31934	28.44764	28.45	13.61	13.60
Al ³⁺	116.30908	119.992	119.99	3.07	3.07
Al ⁴⁺	154.18896	153.8252	153.71	0.24	0.31
Al ⁵⁺	194.56494	190.477	190.47	2.15	2.15
Al ⁶⁺	237.43556	241.76	241.43	1.79	1.65
Al ⁷⁺	282.80322	284.66	284.59	0.65	0.63
Al ⁸⁺	330.66507	330.127	330.21	0.16	0.14
Al ⁹⁺	396.86377	398.75	398.57	0.47	0.43
Al ¹⁰⁺	444.79395	441.999	442.07	0.63	0.62
Al ¹¹⁺	2087.33838	2017	2085.98	3.49	0.07
Al ¹²⁺	2304.5354	2304.1401	2304.08	0.02	0.02

Table 5.1: Ionization energies of aluminium, Al through Al¹²⁺.

5.3.2 Population and Ionization

The evolution of the ion population with respect to the density and temperature has been investigated.

The first calculations were performed in LTE for aluminium plasma of ion density $n_i = 6 \times 10^{19} - 10^{16} \text{cm}^{-3}$ ($10^{-3} - 10^{-6}$ solid density) and temperature $T_e = T_i \in [0; 2000 \text{eV}]$. The pseudo-NLTE modification presented in the previous chapter and the continuum-lowering subroutines were disabled in the SHM. PrismSpect was configured to run zero-width “Emission Visible/UV/EUV Spectroscopy” DCA simulations (using the ATBASE tables) at similar densities and temperatures. The results presented in figures 5.14a,b,c and d show a good agreement between the models for ion densities below 10^{19}cm^{-3} . The same agreement can be observed in the average ionization curves (black lines) of figure 5.15. Nevertheless, some differences appear at higher densities where the Prism curves are ahead of the SHM ones. These discrepancies may be related to dense plasma effects not

Ion	SHM (eV)	NIST (eV)	PrismSpect (eV)	$\frac{(SHM-NIST)}{NIST}(\%)$	$\frac{(SHM-PrismSpect)}{PrismSpect}(\%)$
Ar	22.68067	15.75961	15.76	43.92	43.91
Ar ⁺	35.54199	27.62995	27.63	28.64	28.64
Ar ²⁺	49.29688	40.735	40.74	21.02	21.00
Ar ³⁺	63.94824	59.58	59.81	7.33	6.92
Ar ⁴⁺	79.49805	74.84	75.0201	6.22	5.97
Ar ⁵⁺	95.93945	91.29	91.01	5.09	5.42
Ar ⁶⁺	127.55956	124.41	124.32	2.53	2.61
Ar ⁷⁺	147.19337	143.458	143.46	2.60	2.60
Ar ⁸⁺	419.85641	422.6	422.44	0.65	0.61
Ar ⁹⁺	481.59567	479.8	478.68	0.37	0.61
Ar ¹⁰⁺	545.84088	540.4	538.95	1.01	1.28
Ar ¹¹⁺	612.57623	619	618.24	1.04	0.92
Ar ¹²⁺	681.81348	685.47	686.09	0.53	0.62
Ar ¹³⁺	753.55273	755.13	755.73	0.21	0.29
Ar ¹⁴⁺	856.15228	855.47	854.75	0.08	0.16
Ar ¹⁵⁺	925.51764	918.33	918	0.78	0.82
Ar ¹⁶⁺	4124.89648	4120.6654	4120.78	0.10	0.10
Ar ¹⁷⁺	4427.2583	4426.2226	4426.11	0.02	0.03

Table 5.2: Ionization energies of argon, Ar through Ar¹⁷⁺.

Ion	SHM (eV)	NIST (eV)	PrismSpect (eV)	$\frac{(SHM-NIST)}{NIST}(\%)$	$\frac{(SHM-PrismSpect)}{PrismSpect}(\%)$
Fe	14.90625	7.9024	7.87	88.63	89.41
Fe ⁺	16.21094	16.1877	16.18	0.14	0.19
Fe ²⁺	38.10937	30.6514	30.65	24.33	24.34
Fe ³⁺	61.32813	54.801	54.8	11.91	11.91
Fe ⁴⁺	85.84374	75.0104	75	14.44	14.46
Fe ⁵⁺	111.65626	99.0634	99	12.71	12.78
Fe ⁶⁺	138.77736	124.9761	125	11.04	11.02
Fe ⁷⁺	167.20705	151.0599	151.06	10.69	10.69
Fe ⁸⁺	244.15625	233.5862	235.04	4.53	3.88
Fe ⁹⁺	272.38281	262.1026	262.1	3.92	3.92
Fe ¹⁰⁺	301.50391	290.247	290.4	3.88	3.82
Fe ¹¹⁺	331.52731	330.7898	330.8	0.22	0.22
Fe ¹²⁺	362.45316	361.042	361	0.39	0.40
Fe ¹³⁺	394.2793	392.162	392.2	0.54	0.53
Fe ¹⁴⁺	461.67386	457.0057	457	1.02	1.02
Fe ¹⁵⁺	497.01367	489.2763	489.5	1.58	1.53
Fe ¹⁶⁺	1262.28699	1262.1591	1266.1	0.01	0.30
Fe ¹⁷⁺	1362.37305	1361.9663	1356.57	0.03	0.43
Fe ¹⁸⁺	1464.96667	1469.2127	1458.14	0.29	0.47
Fe ¹⁹⁺	1570.07239	1575.5911	1573.45	0.35	0.21
Fe ²⁰⁺	1677.67383	1688.6647	1689.92	0.65	0.72
Fe ²¹⁺	1787.7832	1799.0106	1799.52	0.62	0.65
Fe ²²⁺	1967.94727	1958.5783	1953.15	0.48	0.76
Fe ²³⁺	2072.41797	2045.7391	2047.38	1.30	1.22
Fe ²⁴⁺	8840.26465	8828.0463	8836.41	0.14	0.04
Fe ²⁵⁺	9280.21875	9277.6874	9280.1	0.03	<0.01

Table 5.3: Ionization energies of iron, Fe through Fe²⁵⁺.

Ion	SHM (eV)	NIST (eV)	PrismSpect (eV)	$\frac{(SHM-NIST)}{NIST}(\%)$	$\frac{(SHM-PrismSpect)}{PrismSpect}(\%)$
Cu	12.62109	7.72638	7.73	63.35	63.27
Cu ⁺	11.39453	20.29239	20.29	43.85	43.84
Cu ²⁺	36.28906	36.8407	36.83	1.50	1.47
Cu ³⁺	62.49218	57.38	55.2001	8.91	13.21
Cu ⁴⁺	90.0078	79.85	79.9	12.72	12.65
Cu ⁵⁺	118.8125	103	103	15.35	15.35
Cu ⁶⁺	148.92578	138.9	139	7.22	7.14
Cu ⁷⁺	180.35156	?	166	NA	8.65
Cu ⁸⁺	213.08203	?	199	NA	7.08
Cu ⁹⁺	247.11717	231.9	232.5	6.56	6.29
Cu ¹⁰⁺	282.44531	265.3	266.2	6.46	6.10
Cu ¹¹⁺	378.26172	368.85	368.8	2.55	2.57
Cu ¹²⁺	412.293	400.96	401	2.83	2.82
Cu ¹³⁺	447.23044	434.94	435	2.83	2.81
Cu ¹⁴⁺	483.07413	483.91	484	0.17	0.19
Cu ¹⁵⁺	519.81635	519.99	520	0.03	0.04
Cu ¹⁶⁺	557.46088	557.06	557	0.07	0.08
Cu ¹⁷⁺	641.74603	632.94	633	1.39	1.38
Cu ¹⁸⁺	683.13281	670.5883	671	1.87	1.81
Cu ¹⁹⁺	1692.21875	1689.9	1698	0.14	0.34
Cu ²⁰⁺	1806.75793	1804	1798.65	0.15	0.45
Cu ²¹⁺	1923.80859	1915.6	1916.79	0.43	0.37
Cu ²²⁺	2043.36731	2060.6	2043.34	0.84	<0.01
Cu ²³⁺	2165.42383	2182	2183.74	0.76	0.84
Cu ²⁴⁺	2290.00195	2308.6	2308.97	0.81	0.82
Cu ²⁵⁺	2509.35938	2477.95	2482.4	1.27	1.09
Cu ²⁶⁺	2627.32397	2587.6	2588.94	1.54	1.48
Cu ²⁷⁺	11078.40527	11062.373	11073.4	0.14	0.05
Cu ²⁸⁺	11570.49805	11567.612	11570.4	0.02	<0.01

Table 5.4: Ionization energies of copper, Cu through Cu²⁸⁺.

accounted for in the new model.

Performing the same calculation in NLTE leads to a considerable change in the ion distribution profiles. The inclusion of spontaneous emission in the population rate equation significantly counterbalance the ionization processes. Consequently, for the same temperature, the average ionization state is smaller and the yield is reduced (see next section). The NLTE approximation developed for the SHM produces results following Prism full NLTE predictions for the highest densities (fig 5.15a,b and c). However, at lower density (i.e. far from LTE), several divergences are observed (fig 5.15d).

5.3.3 Spectra

The frequency integrated emission for free-free, bound-free and bound-bound transitions in LTE are in good correlation with PrismSpec (fig 5.16).

In order to further elaborate on this point, synthetic Al spectra were produced and compared to results from planar simulations of Prism. Figure 5.18 presents a comparison of the recombination and total emission spectra emitted by a volume element of side length $dx = 100$ microns. The agreement, while not being perfect (some transitions are missing in the SHM and the broadening terms are very simple) is reasonably good.

In NLTE, the situation is a bit more complicated as some differences in the ionization states lead to dissimilarities in the continuum level (e.g. the absence of one recombination edge [fig 5.19a around 2100 eV] which has a substantial impact on the shape of the total emission [fig 5.19d]). Additionally, the approximations taken seem to underestimate the emission from low density plasmas at low temperature (fig 5.17c, and d). The combined effect of these variations produces some important discrepancies between the spectra of the two models (fig 5.19).

On average, the model is more than 1000 times faster than PrismSpec.

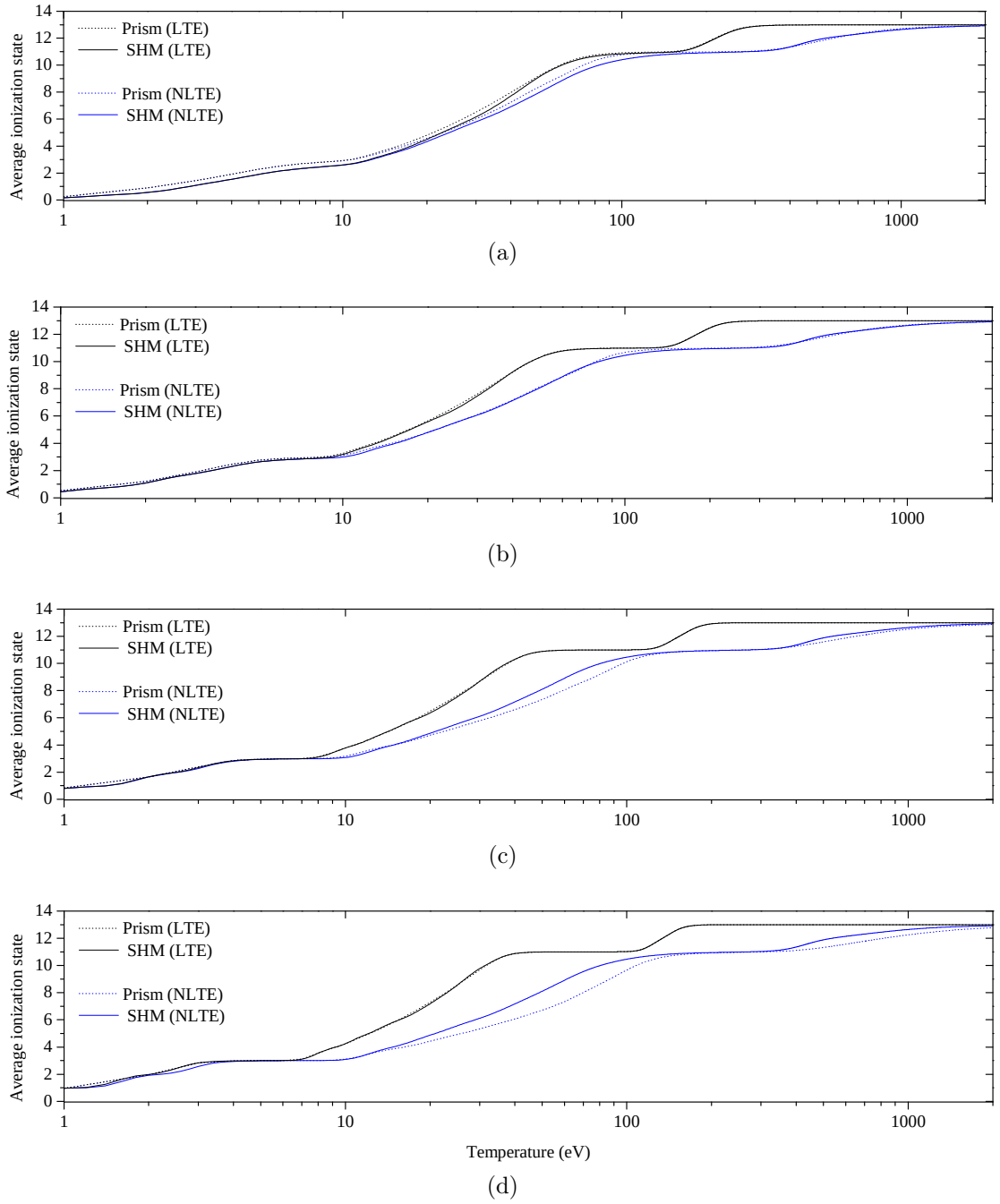


Figure 5.15: Average ionization state for aluminium in LTE/NLTE, SHM vs. PrismSPECT. $n_i \simeq 6 \times 10^{19} \text{ cm}^{-3}$ (a), $6 \times 10^{18} \text{ cm}^{-3}$ (b), $6 \times 10^{17} \text{ cm}^{-3}$ (c), $6 \times 10^{16} \text{ cm}^{-3}$ (d).

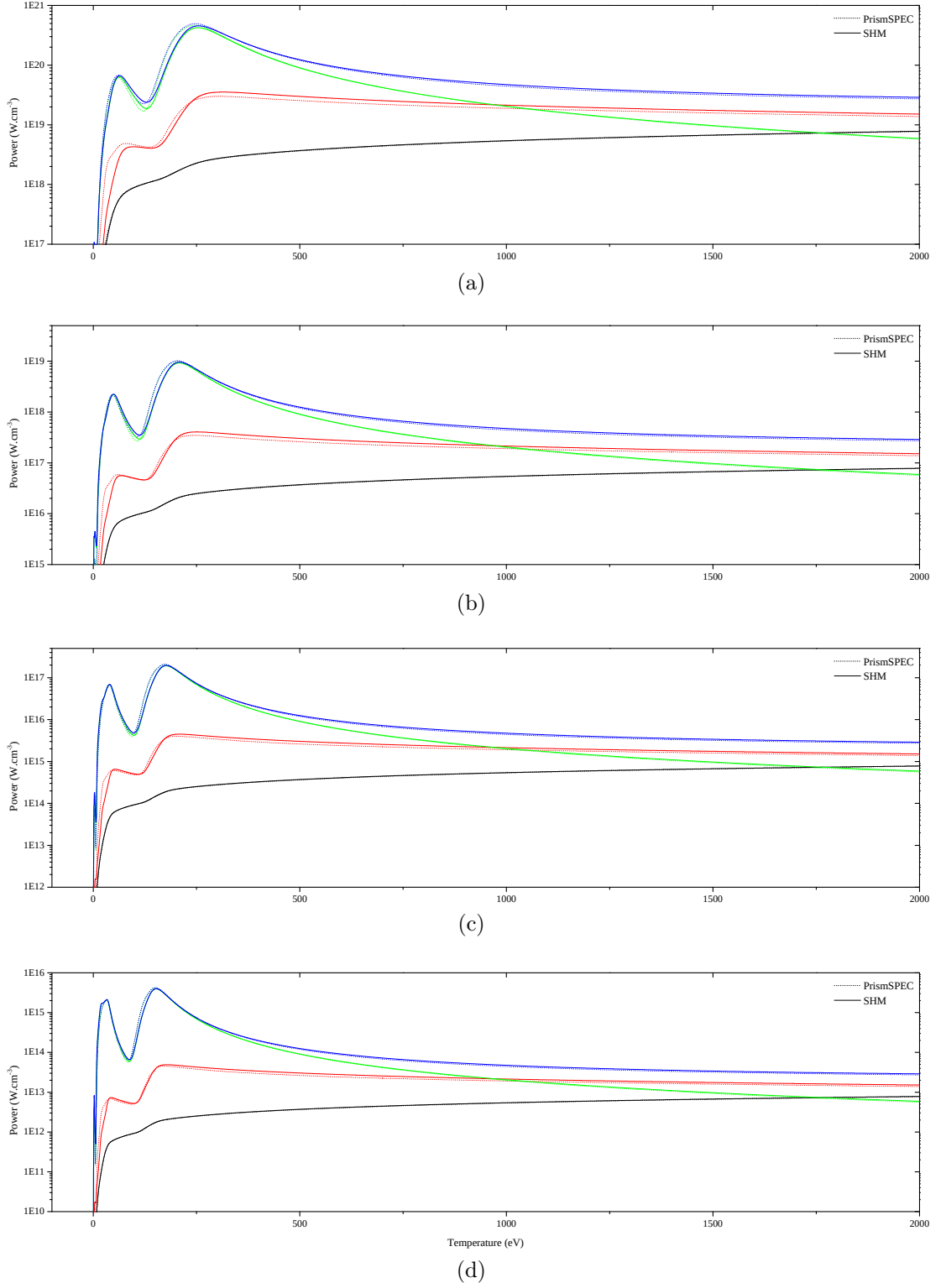


Figure 5.16: Frequency integrated free-free (black), bound-free (red), bound-bound (green) and total (blue) LTE emission. SHM vs. PrismSPECT. $n_i \simeq 6 \times 10^{19} \text{ cm}^{-3}$ (a), $6 \times 10^{18} \text{ cm}^{-3}$ (b), $6 \times 10^{17} \text{ cm}^{-3}$ (c), $6 \times 10^{16} \text{ cm}^{-3}$ (d).

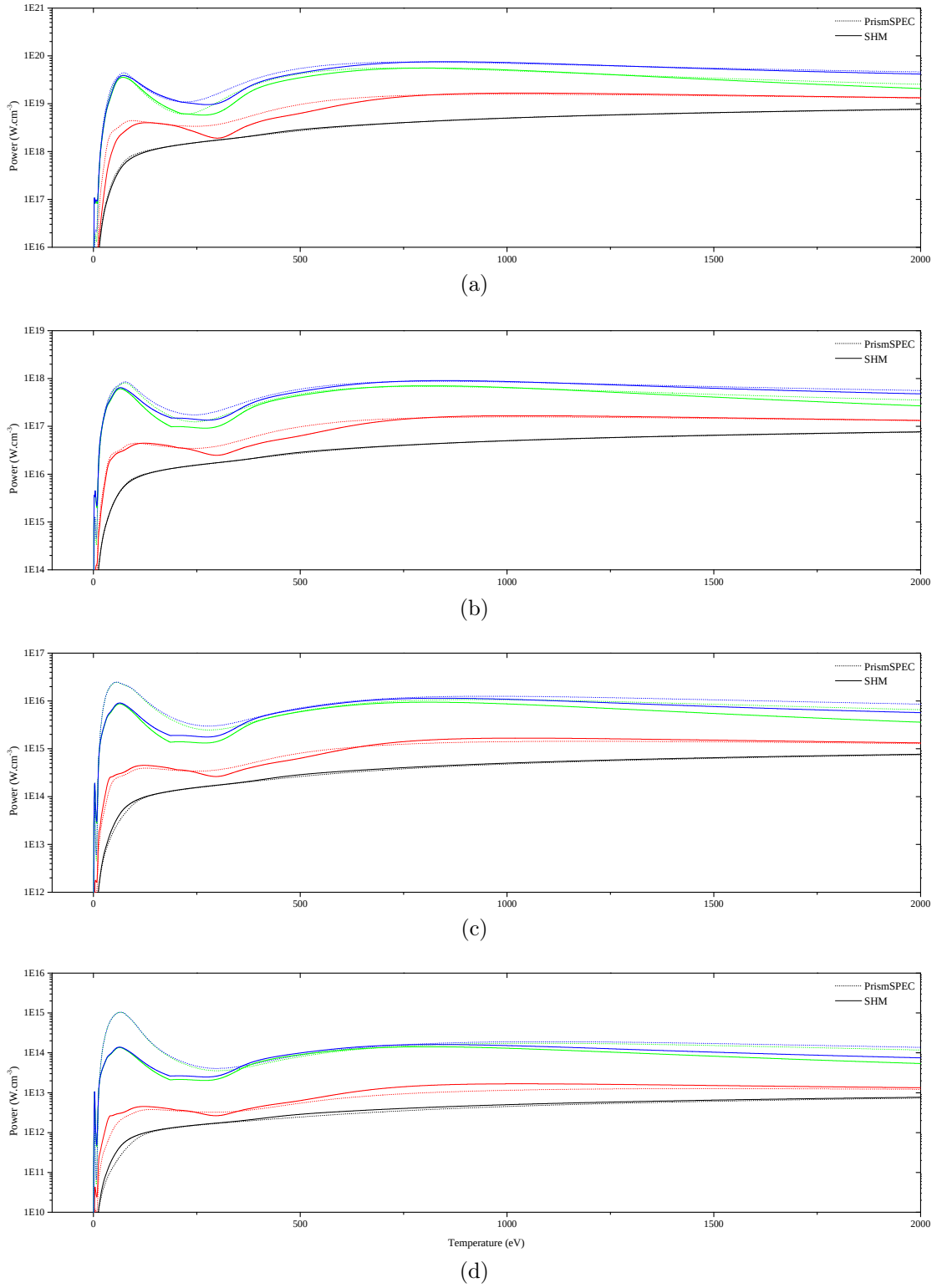
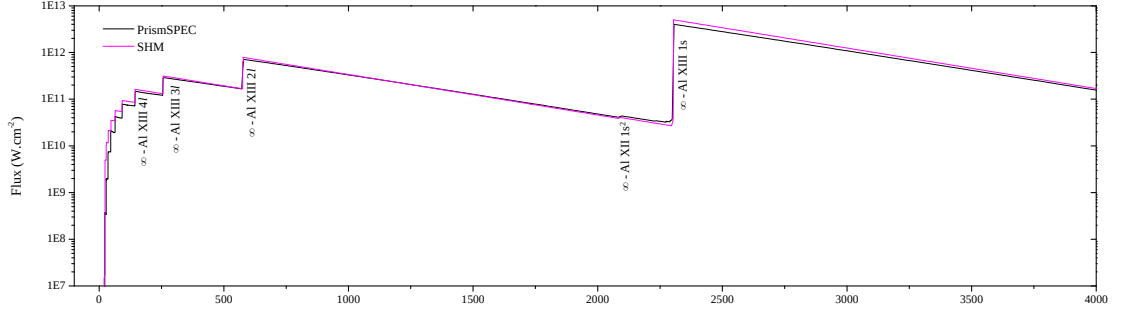
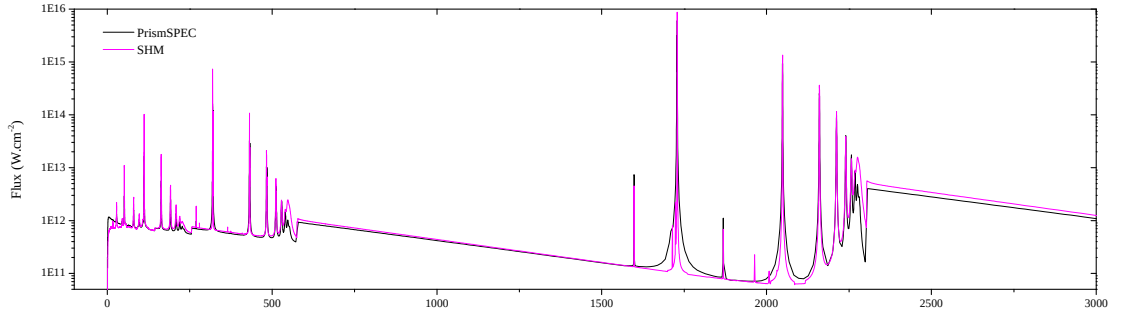


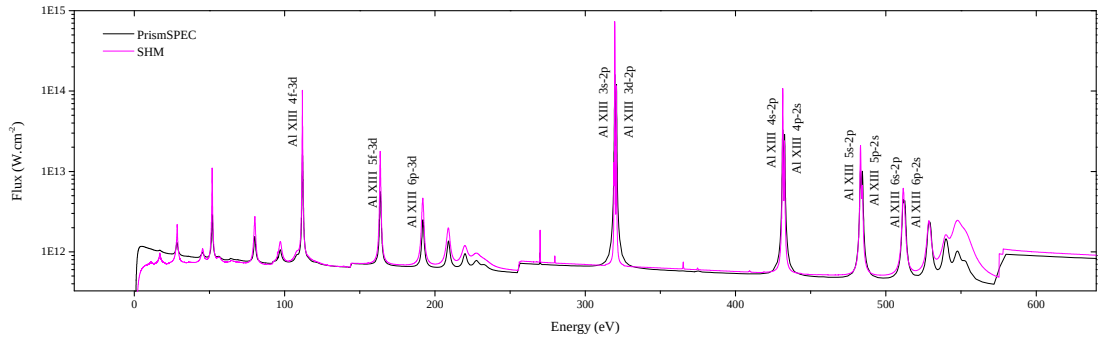
Figure 5.17: Frequency integrated free-free (black), bound-free (red), bound-bound (green) and total (blue) NLTE emission. SHM vs. PrismSPECT. $n_i \simeq 6 \times 10^{19} \text{ cm}^{-3}$ (a), $6 \times 10^{18} \text{ cm}^{-3}$ (b), $6 \times 10^{17} \text{ cm}^{-3}$ (c), $6 \times 10^{16} \text{ cm}^{-3}$ (d).



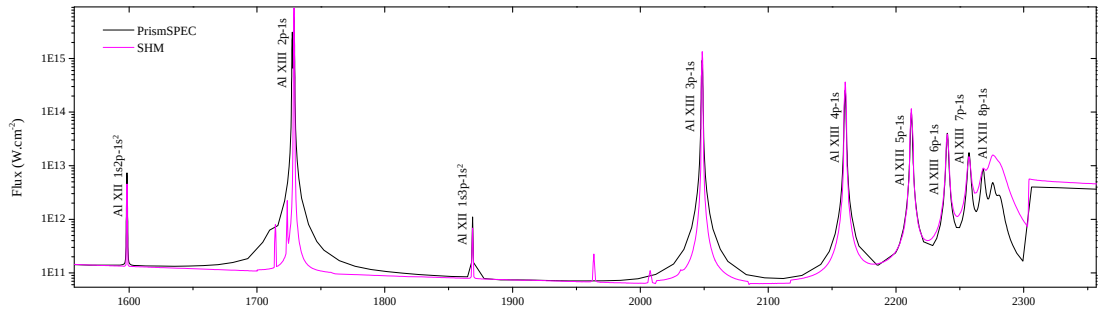
(a)



(b)



(c)



(d)

Figure 5.18: Single cell LTE Al spectra, $n_i \simeq 6 \times 10^{19} \text{ cm}^{-3}$, $T_e = T_i = 500 \text{ eV}$, $dx = dy = dz = 10^{-4} \text{ m}$. SHM vs. PrismSPECT. (a) bound-free emission, (b) total emission [0, 3000 eV], (c) total emission [0, 640 eV], (d) total emission [1550, 2350 eV].

Chapter 6

Simulation results and discussion

This chapter describes the results of Z-pinch simulations performed with the new radiative solver. In the first two sections, we discuss the modelling of cylindrical wire array experiments carried out on two different classes of Z-pinch drivers with two different types of loads. In the following section, the post-processing implementation of the model is used to generate Micro-Channel Plate (MCP) X-UV images.

6.1 Aluminium array on SPHINX

SPHINX is a Z-pinch driver developed at the Centre d'Etude de Gramat (C.E.A, France) and based on the 1 microsecond LTD technology. Operating with 16 branches of 10 LTD stages each, the machine can drive large diameter single and nested wire array loads (140 mm Ø) in 700-900 ns with peak currents of ≈ 6 MA.

6.1.1 Simulation setup

The experiment modelled in this section was performed on a single 5 cm height array composed of 150 aluminium wires of 10.4 μm diameter each (SPHINX shot 736). The total yield was measured with a set of x-ray diodes filtered by 0.5

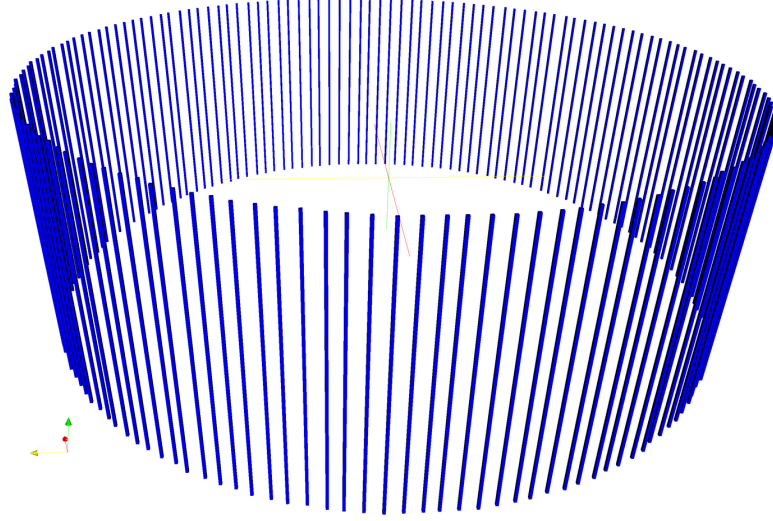


Figure 6.1: Initial state of the 150 Al wires.

μm of polyethylene and normalized using a nickel bolometer. The K-shell yield was recorded by diamond photoconductive detectors (PCD) filtered by $8\ \mu\text{m}$ of polyimide and normalized by a gold bolometer.

Due to the dimensions of the experiment ($20 \times 20 \times 5\ \text{cm}$, accounting for some mandatory vacuum space), the spatial resolution has to be limited to $5 \times 10^{-4}\text{m}$ in order to maintain the number of cells at a reasonable level. By distributing the resulting 16×10^6 volume elements across the 256 CPUs of a cluster, the 7275 time steps of the simulation can be resolved in approximately 10 hours.

As it was previously mentioned in chapter 2, phase transitions are not modelled in GORGON and the wires are initialized as low temperature high density plasma cells (fig 6.1). Their initial temperature is a free parameter allowing the recovery of the expected wire ablation rate: in our case, $T_e(0) = T_i(0) = 0.03\text{eV}$. To mimic the imperfections inherent to wire manufacturing processes, a small random perturbation is applied to this basic temperature.

The electromagnetic solver is fed with the synthetic current stemming from a simulation of the SPHINX electrical circuit (fig 6.2). This method provides the required close coupling between the synthetic pinch and its driver, a point

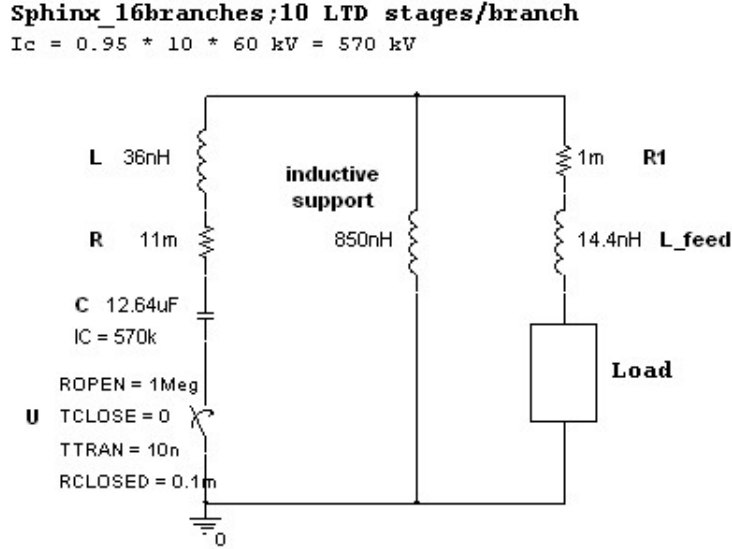


Figure 6.2: Electrical scheme of SPHINX (courtesy of H. Calamy).

of considerable importance during the implosion phase as the sudden increase of the load inductance launches a strong counter electromotive force that can dramatically reduce the current. Reciprocally, the response of the circuit to the load evolution (conditioned by its design and the potential losses) has a strong influence on the plasma conditions. Therefore, the quality of Z-pinch radiation and dynamics modelling is critically dependent on the quality of circuit modelling, and vice versa.

The radiative solver synthetic diagnostics model is setup using the experimental diagnostic responses and filters. In order to accelerate the resolution process, transitions involving configurations with subshells above $7i$ are ignored: a total of 1434 bound-bound transitions and 392 bound-free ones are accounted for.

6.1.2 Simulation results

Two types of simulations were performed, both started with the same initial conditions but carried out with or without the NLTE approximations presented in the previous chapters. Figure 6.3 shows a comparison of the density contours for the two cases in the early stages of the ablation phase (360 ns). The NLTE solver, by

accounting for spontaneous radiative transitions, reduces the excited and ionized state populations of low density plasma regions (comprising every cell of the simulation volume at that time). As a consequence, the radiative losses are limited and the resulting increased electron temperature (fig 6.3c) leads to a faster rate of expansion. The density profiles presented in figure 6.3b illustrate this fact showing the advanced position of the precursor front and the reduced wire core density in the NLTE case.

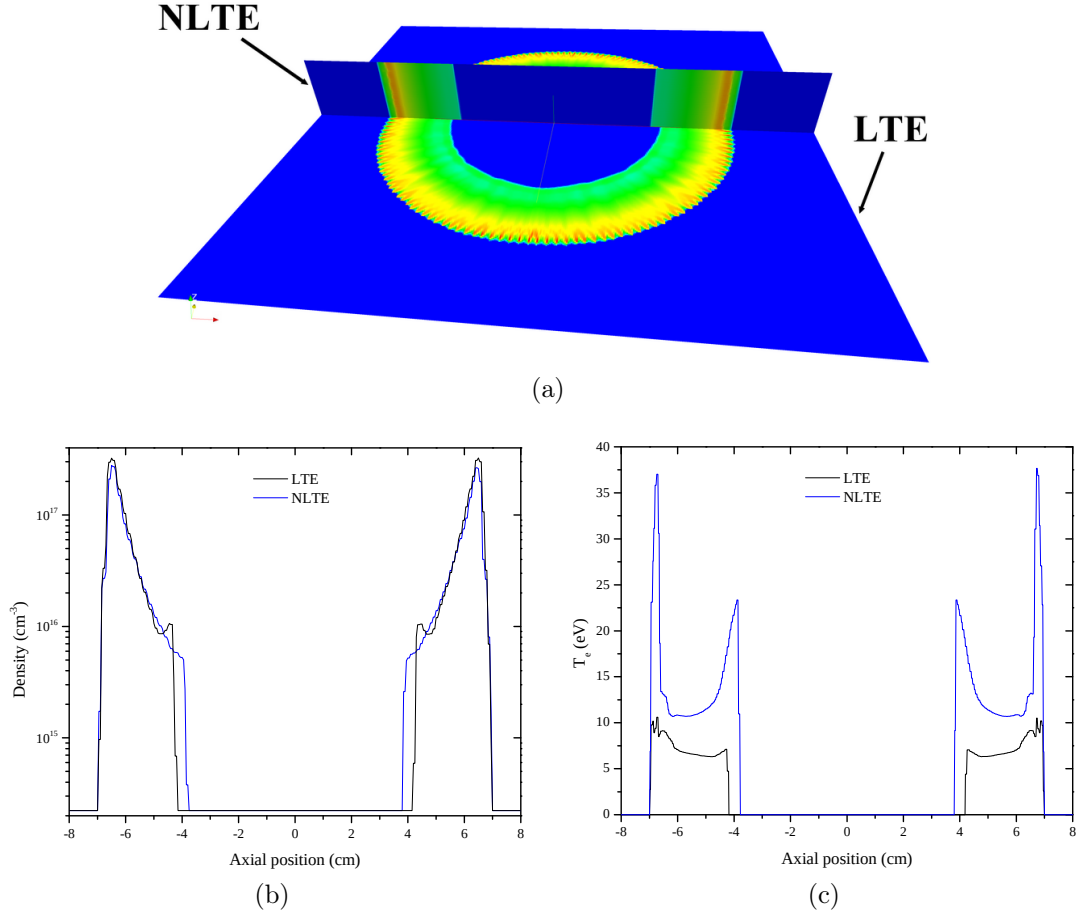


Figure 6.3: LTE vs NLTE at 360 ns (a) Density plots. (b) Ion density profiles along the x-axis. (c) Electron temperature profiles along the x-axis.

The highly unusual large diameter of SPHINX loads prevents the formation of precursor columns as the implosion phase starts before the ablation front has reached the axis. In LTE, the ablation velocity is such that at 600 ns (~ 40 ns before stagnation) the imploding wires have caught up with the precursor front

(fig 6.4a).

Conversely, at that time, the ablation front still leads the imploding shell in NLTE (fig 6.4b). For this last case, the late rendezvous has a substantial effect on the amount of trailing mass as the Rayleigh–Taylor instabilities grow over a longer distance. The density slices (figure 6.5) taken at the time of the x-ray peak

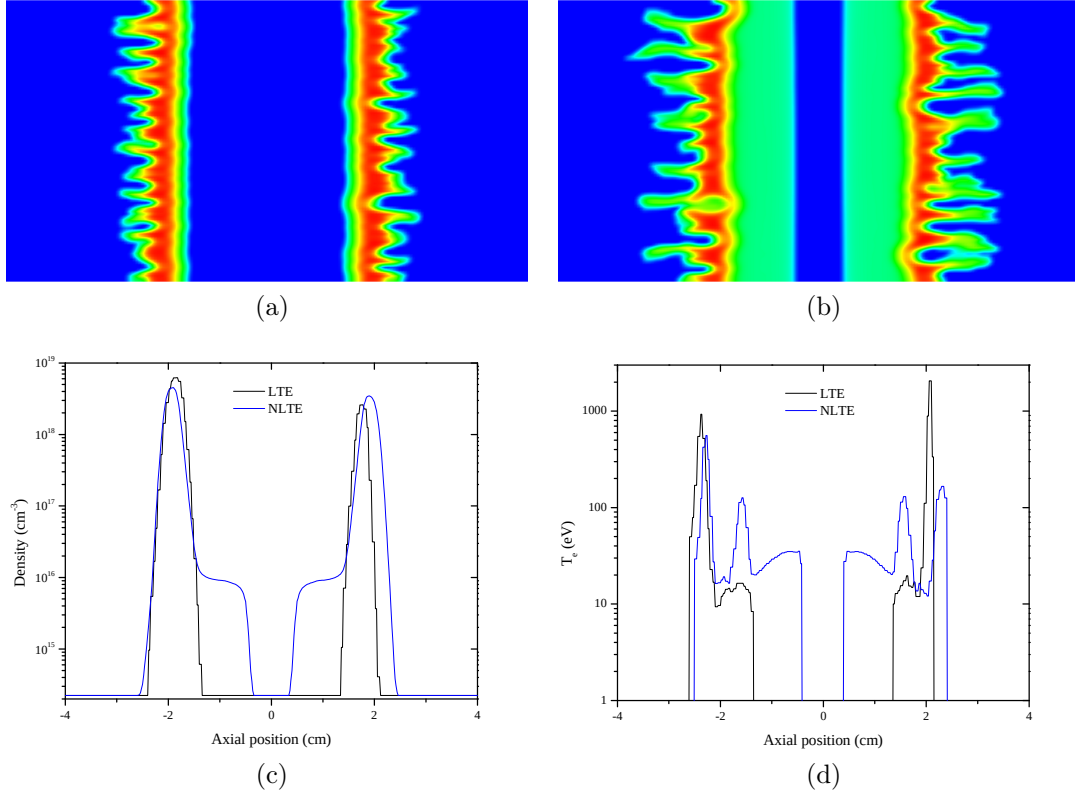


Figure 6.4: LTE vs NLTE at 600 ns (a) XZ density slice (LTE). (b) XZ density slice (NLTE). (c) Ion density profiles along the x-axis. (d) Electron temperature profiles along the x-axis.

(640 ns for LTE, 644 ns in NLTE) also highlight this point.

The maximum powers at stagnation and the energies radiated are radically different for the two models (fig 6.6b).

In LTE, the synthetic bolometers record a total of ~ 456 kJ (~ 15 TW at maximum) with ~ 94 kJ (~ 4.7 TW) in the K-shell region. This represents nearly twice the total experimental yield (230 kJ, 6.38 TW) and four times the expected K-shell (26.5 kJ, 1.03 TW) (fig 6.6a).



Figure 6.5: XZ density slices at stagnation. (a) LTE: 640 ns. (b) NLTE: 644 ns.

On the other hand, the NLTE simulation predicts a total yield of ~ 219 kJ (~ 6.10 TW at maximum) with ~ 33 kJ (~ 1.7 TW) in the K-shell region. This corresponds to a difference of less than 5% in the total energy and ~ 20 % in the K-shell. The discrepancies observed in this case are probably related to the combined effect of the wire initialization process with the poor spatial resolution and the circuit model imperfections. A comparison of the experimental and synthetic K-shell FWHM (22 ns and 12 ns respectively) would suggest that the structure of the simulated implosion is too symmetrical. By increasing the resolution of the simulation grid and adjusting the level of perturbation initially applied to the wires, the proper pulse widths and powers might be recovered. However, these modifications may not be sufficient to solve the issue of the early implosion times (observed with both models) for which no cause has been identified yet.

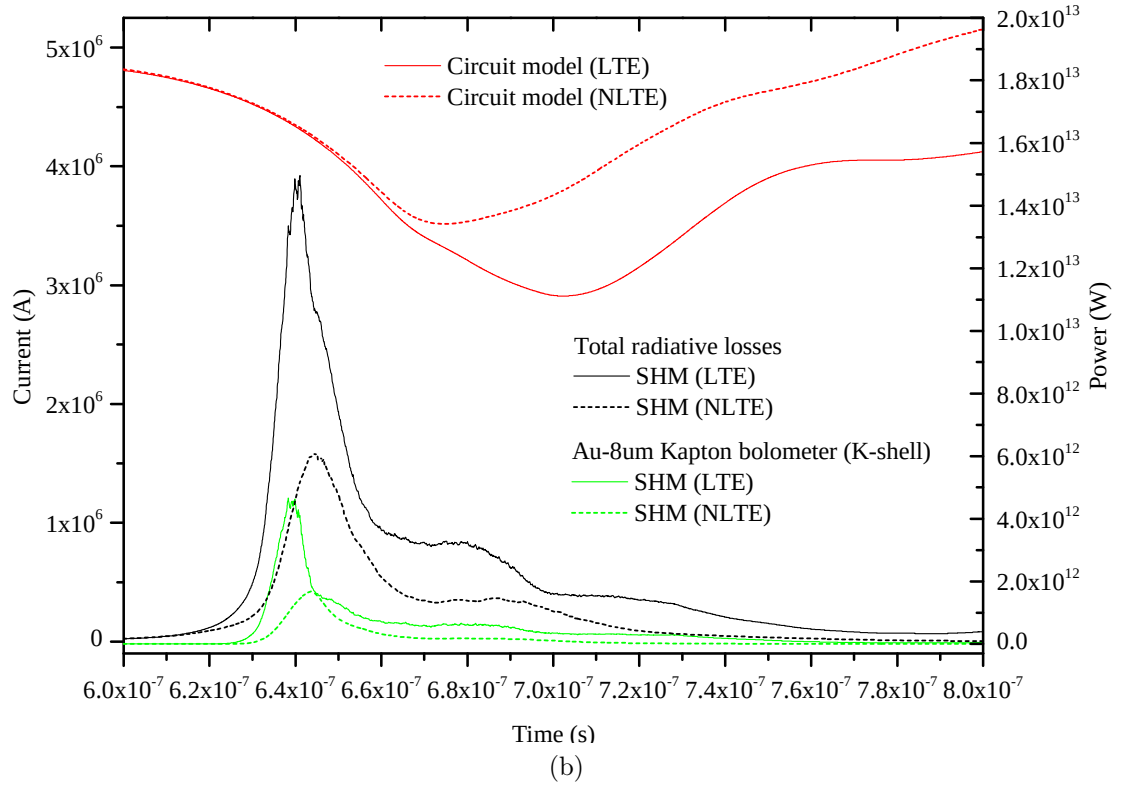
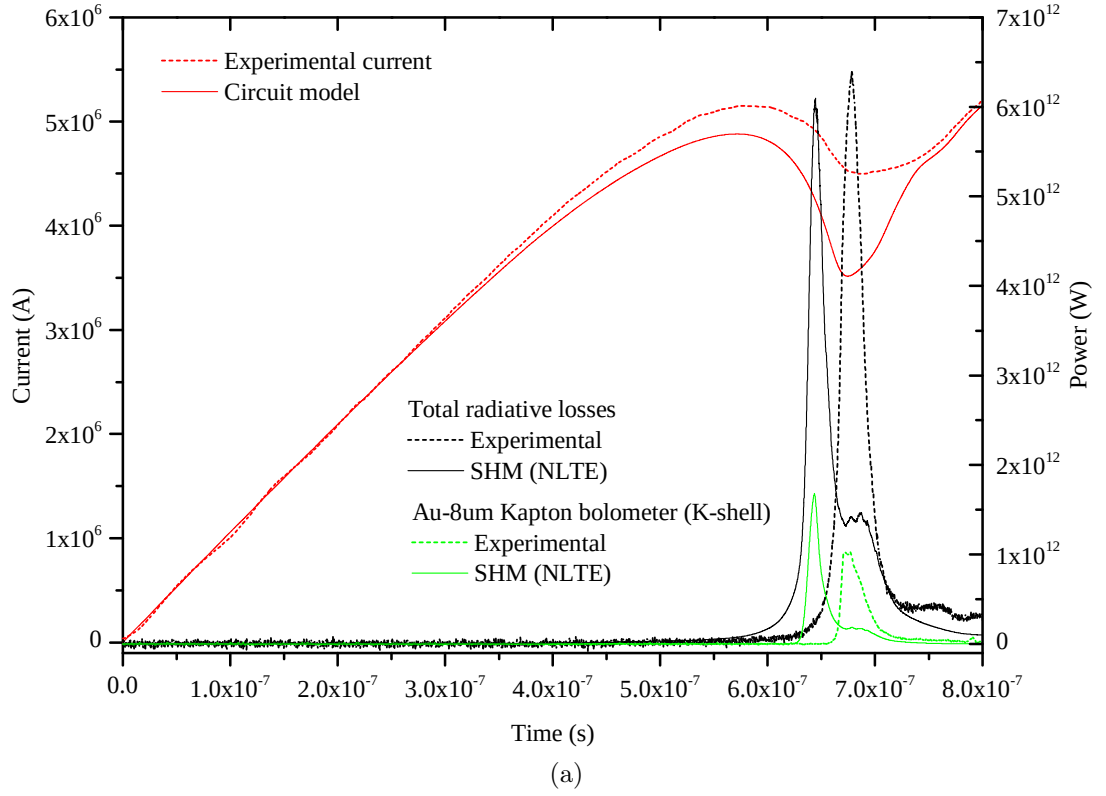


Figure 6.6: SPHINX: current and yields. (a) Experimental vs SHM (NLTE). (b) SHM (NLTE) vs SHM (LTE).

6.2 Stainless steel array on ZR

ZR is a Marx bank based pulsed power accelerator developed at Sandia National Laboratories (Albuquerque, N.M). Generating currents of ~ 20 MA in $\sim 100 - 600$ ns, the machine has demonstrated its ability to drive wire array loads producing more than 1.9 MJ of x-ray output with peak emissions > 200 TW.

6.2.1 Simulation setup

The experiment modelled in this section is the shot z1995 performed with a 70 on 35 mm, 2 cm tall nested stainless steel wire array of 1.35 mg. The total yield was measured using unfiltered diodes (with pinhole arrays to reduce the signal) normalized by bare nickel bolometers. The primary K-shell diagnostics were 0.5 mm diamond PCDs filtered by 254 μm of polyimide and normalized using gold bolometers. The L-shell yield was recorded with PCDs filtered by 8 μm of beryllium and 1 μm of Parylene-N.

The spatial resolution of the simulation was set to 250 μm and the resulting 10 368 000 volume elements distributed across 256 CPUs of Imperial College CX1 cluster. The difficulty with modelling stainless steel wire arrays emission arises from the high number of configurations and transitions to consider to properly describe the behaviour of the atomic system. In order to be as accurate as possible, excited configurations with subshells up to $10l$ (the highest subshell allowed by the SHM) were allowed. By taking into account a total of 7766 bound-bound transitions and 1485 bound-free ones in each cell, the 8649 timesteps of the simulation were resolved in less than 26 hours.

The initial temperature of the 162 wires was set to $T_e(0) = T_i(0) = 0.125$ eV and a random perturbation was applied to the mass density. For reasons similar to those previously invoked, the electromagnetic solver was fed with the current generated by a simple simulation of the ZR circuit.

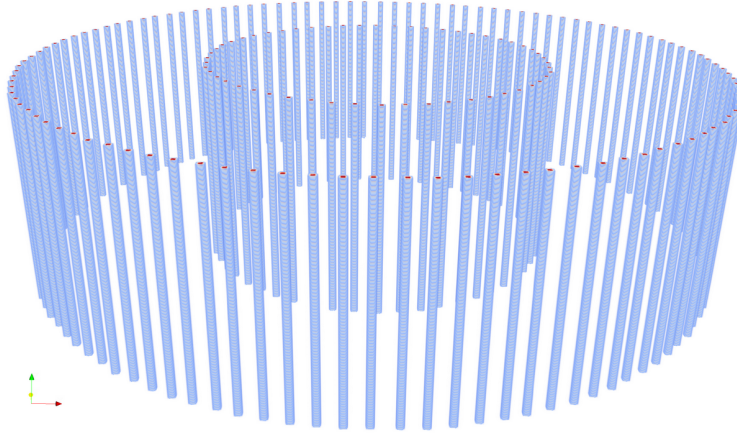


Figure 6.7: Initial state of the 162 (108/54) 8.28 μm $\varnothing$ stainless steel wires.

6.2.2 Simulation results

Figure 6.9a shows a comparison between the experimental yields and the synthetic ones in NLTE. While it is obvious that the agreement is not as good as in the previous simulation, some encouraging points deserve to be noticed.

First and foremost, the total K-shell yield (defined here as the total energy above 5 keV) is in the order of 77 kJ, diverging by less than 10 % from the experimental value (85 kJ). The biggest issue concerns the L-shell and above emissions which appear to be considerably undervalued (639 kJ of synthetic x-rays when 940 kJ are expected). One could assume, in the first place, that the main explanation for the pulse width discrepancies resides in the numerical grid imprint that degrades the symmetry of the implosion. This numerical effect, related to the slightly different velocities present in cells aligned with the simulation grid axes, imprints a square pattern on the cylindrical implosion (observable in the XY plane of figure 6.8). However, if the same simulation (with the same numerical noise) is performed in LTE, the synthetic x-ray yields are this time dramatically overestimated (343 kJ in the K-shell, 2 MJ in total) (fig 6.9b), highlighting the strong model dependence of the results.

The fact that the inline NLTE implementation underestimates the emission from low energy transitions may provide some hint about the principal source

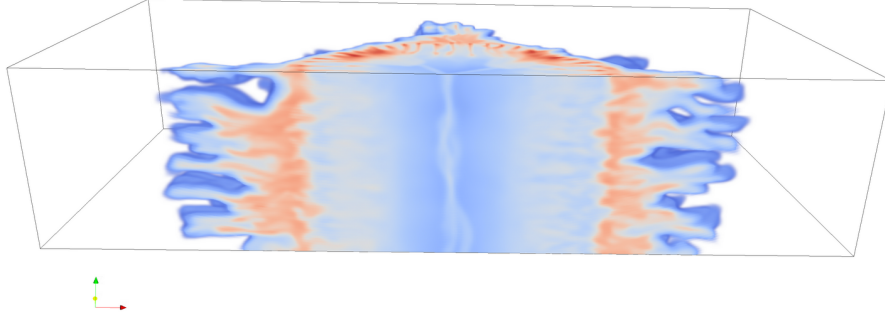


Figure 6.8: Outer array passing through the inner one ~ 20 ns before stagnation.

of discrepancies. When deriving the expression of the excited and ionized states populations (4.23 and 4.25) in chapter 4, we have deliberately assumed that the effects of the radiation field (photoexcitation-stimulated emission) were negligible. This assumption, although compatible with the moderate Z / low radiative energy density plasmas of SPHINX, may not be appropriate in the case of ZR . By accounting for those missing processes, the agreement between the experimental and simulated powers might be improved.

Indeed, the amount of radiation produced in the high frequency region of the spectrum (e.g. in the K-shell) is strongly related to the history of the emission in the highest shells. At the beginning of the simulation, the initially small deposition of energy in the cold plasma slowly increases the ionization degree and the excited level populations of the lower charge states. The high statistical weights of these configurations leads to strong radiative cooling and the subsequent reduction of the plasma temperature. However, as more energy is deposited, the low frequency region of the spectrum rapidly becomes optically thick, trapping some of the radiation in the plasma. As a consequence, the temperature increases and the ionization level rises. Therefore, not taking into account the radiation field can considerably affect the radiative cooling processes and thus the temperature and K-shell yield by artificially limiting the emission in the L-shell and above region.

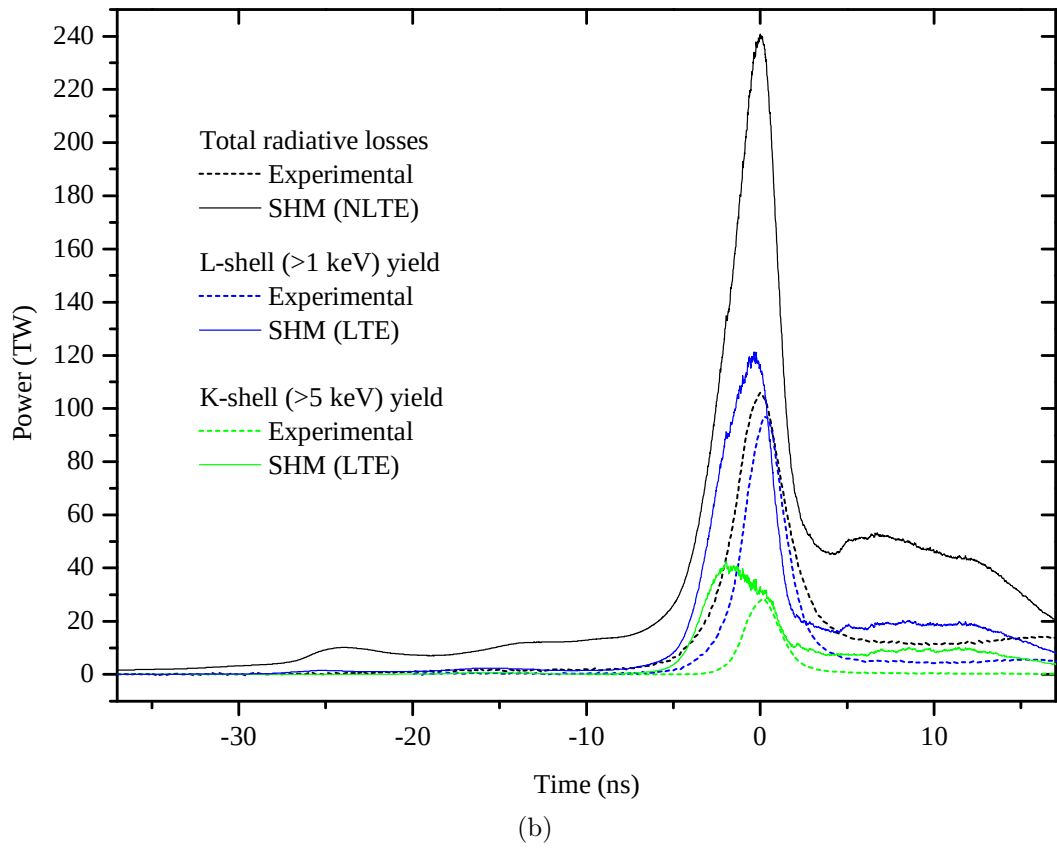
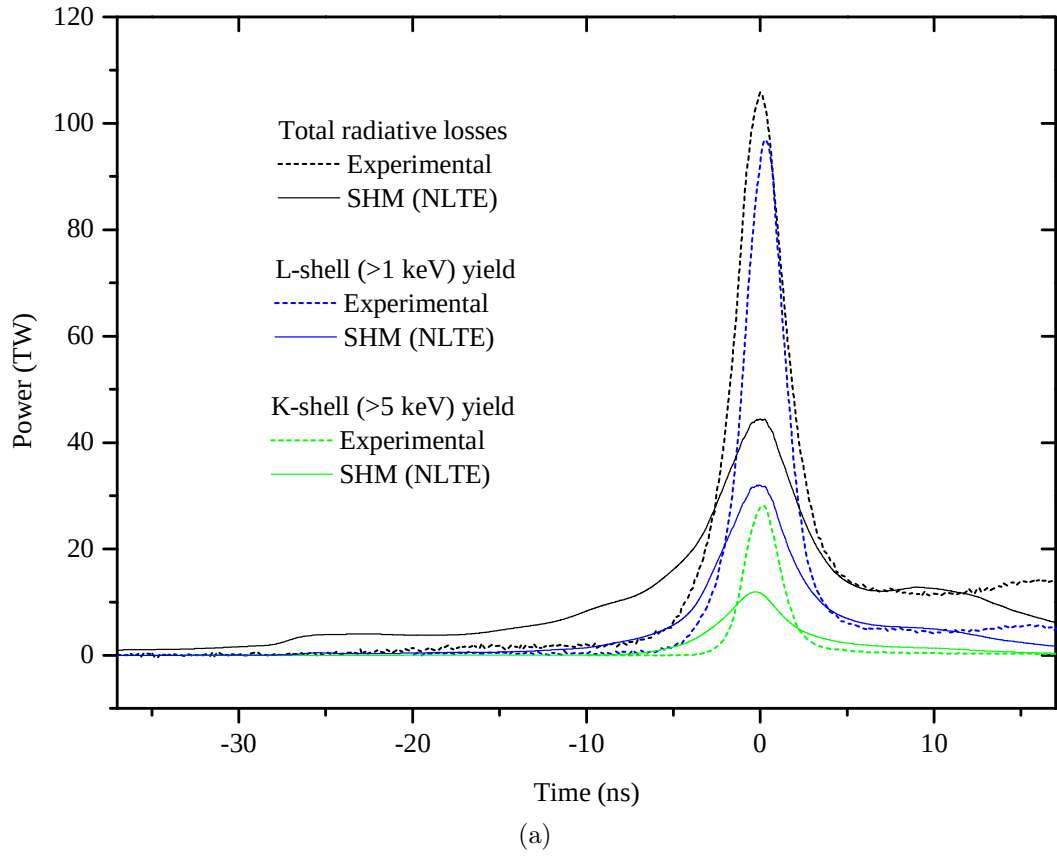


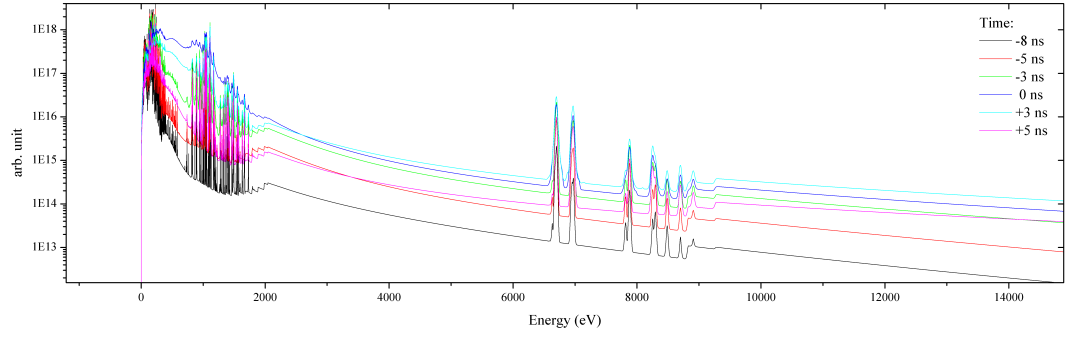
Figure 6.9: ZR yields. (a) experimental vs SHM (NLTE). (b) experimental vs SHM (LTE).

6.3 Synthetic spectra and MCP images

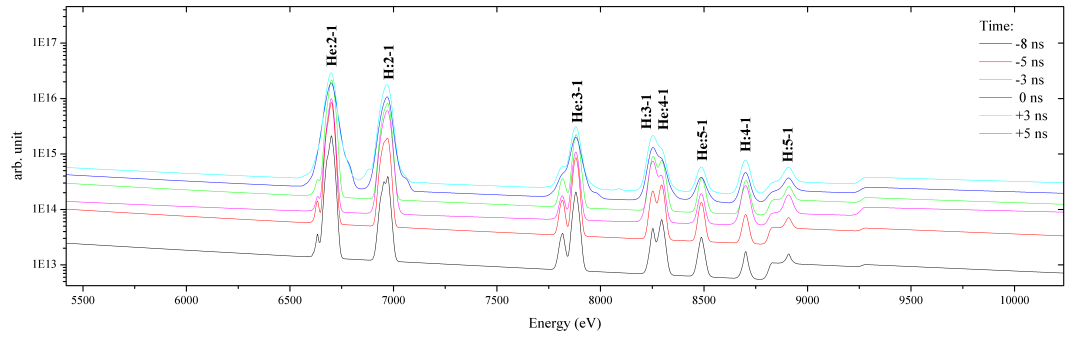
Using the scheme for the integration of spectral information presented in section 5.1, we have developed a post-processing tool generating filtered synthetic MCP images and time-dependent spatially integrated spectra.

Figures 6.10a,b, and c show the details of synthetic spectra obtained from the outputs of nested stainless steel wire array simulations on ZR and for different times before and after the X-ray peak (fig 6.10e). The high spectral resolution (0.15 eV) allows an accurate representation of the line shapes in different energy bands. By fitting the continuum above 10 keV, the evolution of the electron temperature in the pinch can be inferred. The values obtained, around 3 keV (fig 6.10d), are in good agreement with the experimental measurements[20].

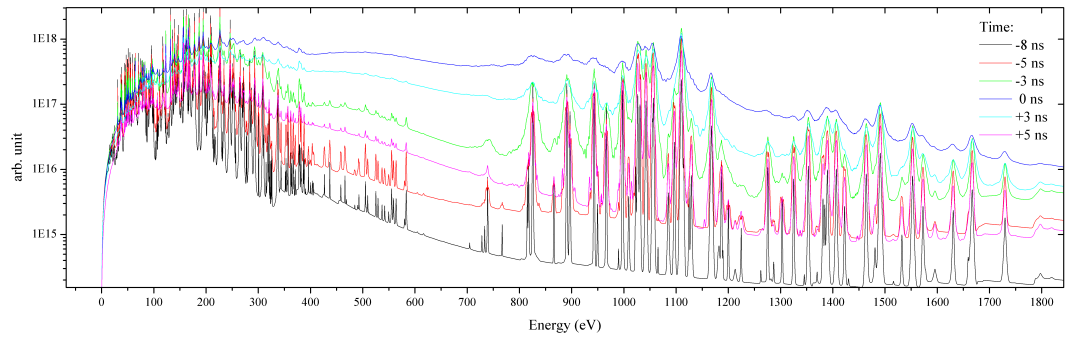
Figures 6.11 and 6.12 , show, respectively, unfiltered and filtered synthetic MCP images obtained for the same times using 254 μm of polyimide.



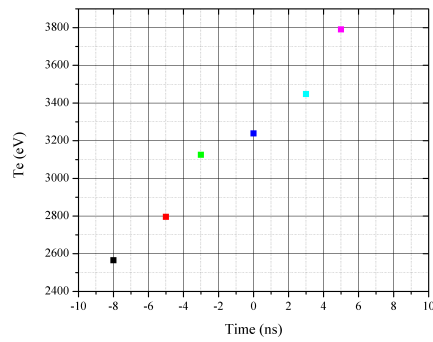
(a) Spatially integrated time-dependent synthetic iron spectra (0.15 eV resolution).



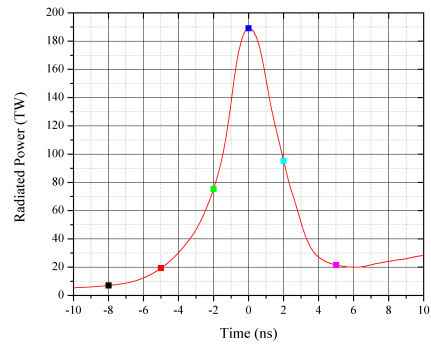
(b) Spatially integrated time-dependent synthetic iron spectra (K-shell).



(c) Spatially integrated time-dependent synthetic iron spectra (L-shell and above).



(d) Synthetic T_e from continuum fitting (>10keV).



(e) Synthetic x-ray pulse shape (LTE).

Figure 6.10

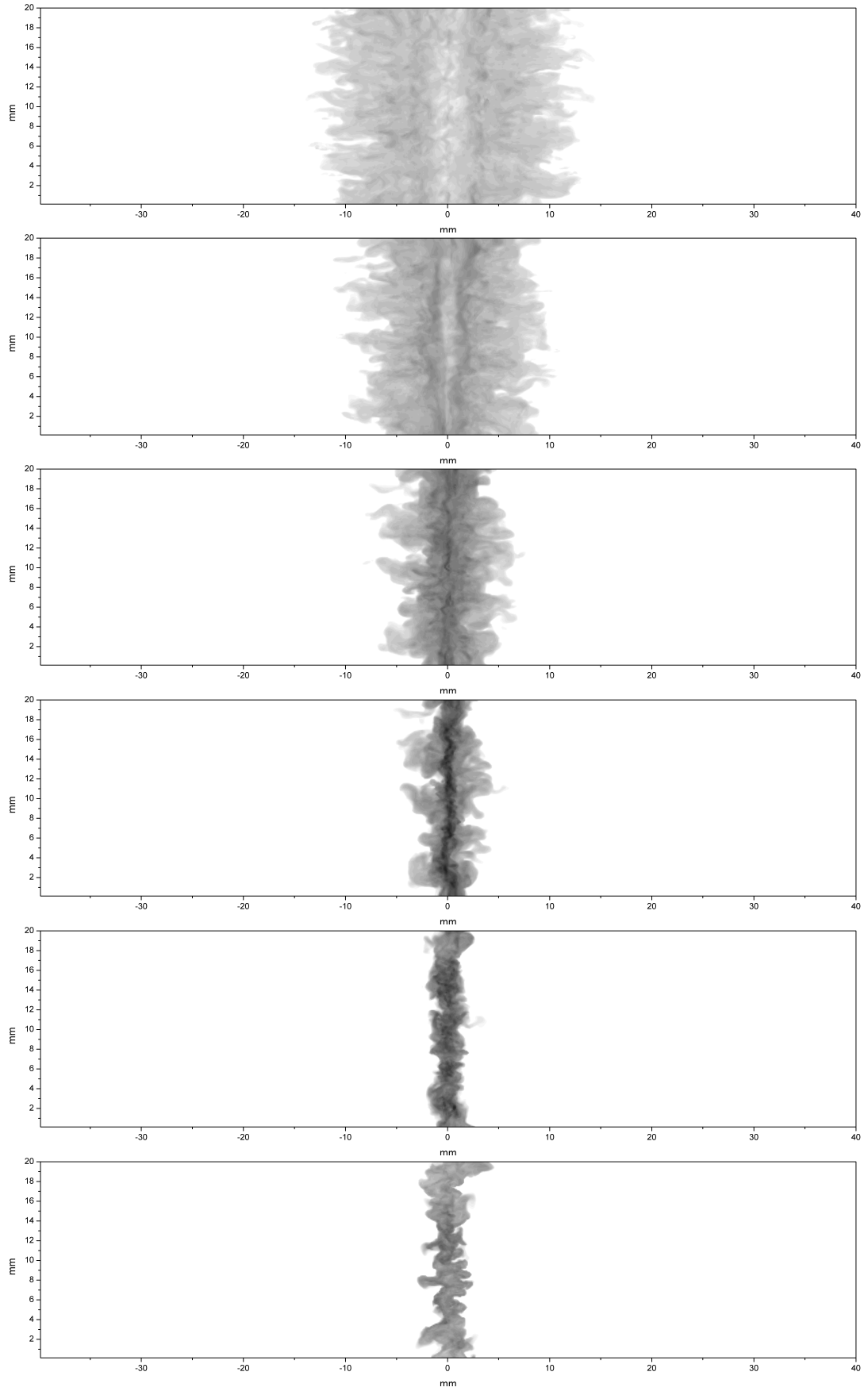


Figure 6.11: Unfiltered synthetic MCP pictures (from the top: -8ns, -5ns, -3ns, 0ns, +3ns, +5ns).

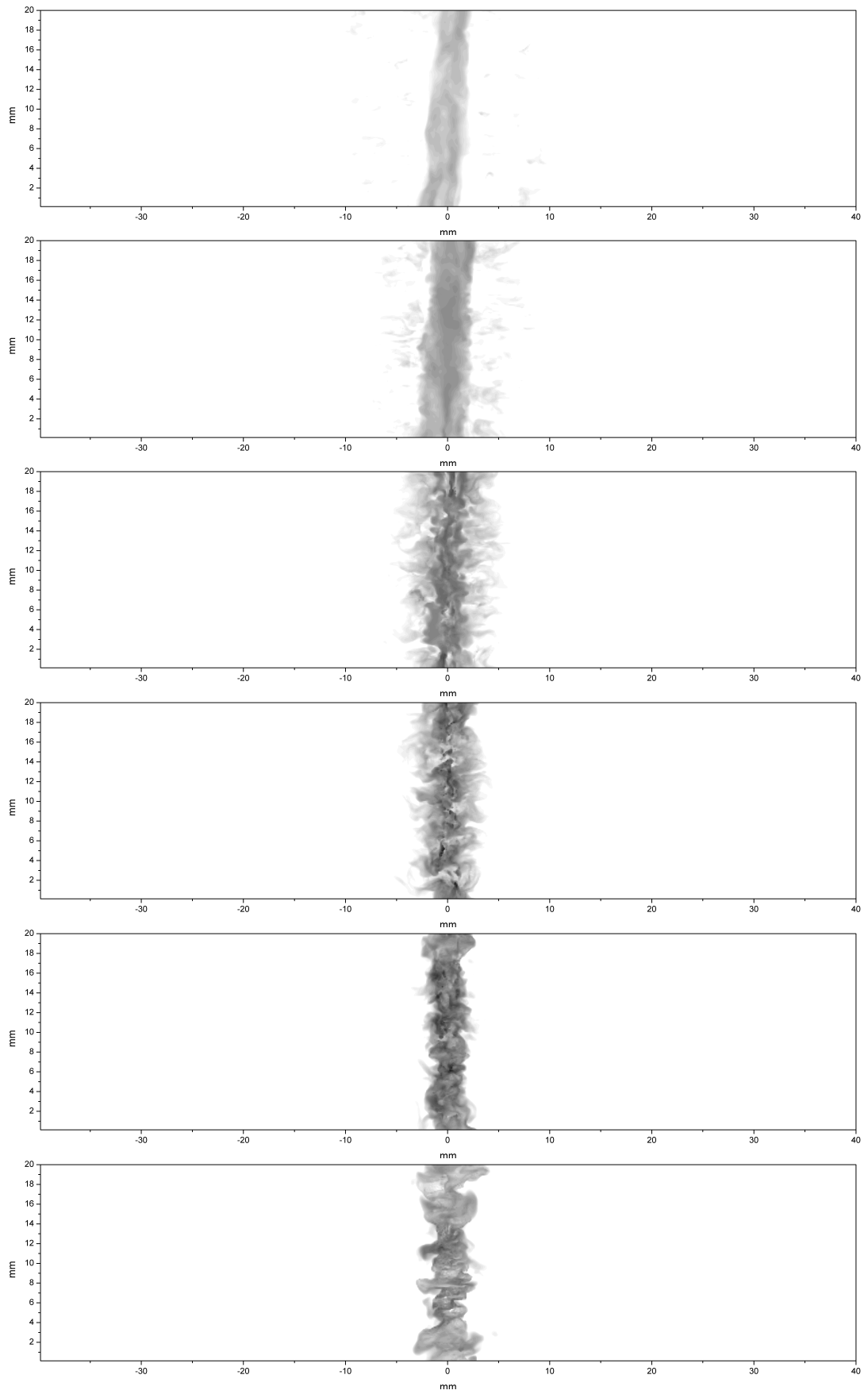


Figure 6.12: Synthetic MCP pictures filtered by 254 μm of polyimide (from the top: -8ns, -5ns, -3ns, 0ns, +3ns, +5ns).¹²⁷

Chapter 7

Conclusion

We have laid down the foundations of a new and fast pseudo NLTE model based on a Screened Hydrogenic approach that can be run in-line with a three-dimensional resistive Eulerian magnetohydrodynamic solver or as a post processing tool with synthetic spectra capabilities.

7.1 A new atomic model

Originally conceived to improve the treatment of radiation in Z-pinch simulations under LTE conditions, the code has evolved into a general-purpose software that yielded results in surprisingly good agreement with a commercial package while being more than 1000 times faster on average. By using a simple modification of the Boltzmann-Saha equations, we have been able to approach the NLTE population distributions for low to moderate Z plasmas in various conditions of temperature and density.

In order to handle the amount of data generated by the spectral treatment of the billions of numerical cells constituting the simulation grids, an original data structure derived from a self-balancing binary search tree has been developed. Providing a fast and efficient access to the memory, it allows the generation of

filtered synthetic X-UV images and the dynamic spectral evolution during the transport of radiation through the simulation volume. This flexible component, contained in a library module, can be reused in different atomic codes.

The inline implementation of the model, relying on a simple approximation of the lines opacities and the tabulation of the Voigt profiles, has demonstrated its ability to reproduce with a good agreement the x-ray yields emitted by an aluminium wire array experiment carried out on the SPHINX generator. Model-related discrepancies in the dynamics of the implosion have been observed between simulations running in LTE and NLTE. Encouraging results have also been obtained for the synthetic yields of a nested stainless steel wire array on ZR, although we are still far from claiming predictive capabilities. At the beginning of the simulation, the initially small deposition of energy in the cold plasma slowly increases the ionization degree and the excited level populations of the lower charge states. As more energy is deposited, the low frequency region of the spectrum rapidly becomes optically thick, trapping some of the radiation in the plasma.

Several issues are yet to be addressed. One of the main concerns is related to the simple approach adopted for the opacity calculation. The different plasma parameters being evaluated locally, the method leads to grid size dependent results. The quality of the circuit models and their interaction with the synthetic pinch are another point of concern. As was mentioned in the previous chapters, a good circuit model is essential to obtain the correct amount of energy deposition and thus the correct amount of radiation stemming from the pinch. Similarly, the absence of the photoexcitation-stimulated emission terms from the population balance equations may strongly influence the emission in the L-shell and above region in the case of high radiative energy density plasmas (typically relevant for moderate to high Z materials).

7.2 Future improvements and applications

From the last considerations, it appears in the first place crucial to address the questions related to the opacity evaluation. Many advanced methods already exist to simulate the dynamics of the radiation field in the plasma. One of the most popular approach, the Monte Carlo Radiative Transfer (MCRT) scheme, mimics the behaviour of the real field by tracking individual photons through the grid, scattering and absorbing them when necessary.

While this probabilistic method makes reliable predictions of the experimental outcome, its computational cost is for the moment prohibitive in regards to the dimensions of our current Z-pinch simulations.

For instance, one can roughly estimate when the Moore's law (stating that the processing speed doubles approximately every two years) will allow us to perform a full scale ZR simulation using a Monte Carlo approach for the radiation transfer part. The number of floating point operations related to transport and required to complete one timestep (from the emission of the photons to their absorption) can be approximated by:

$$N_{flop} \sim N_c N_{\gamma/c} N_{steps} N_{flop/steps}$$

with N_c the number of cells in the simulation volume, $N_{\gamma/c}$ the number of Monte Carlo photons emitted in each cell, $N_{steps} \sim \langle \tau_v \rangle / dx$ the average number of steps required to describe the life of a photon (defined by the ratio of the average optical depth $\langle \tau_v \rangle$ to the grid spatial resolution dx) and $N_{flop/steps}$ the number of floating point operations per steps.

Assuming that the Moore's law will remain valid in the future, we can predict that MCRT methods will be applicable in

$$T_{years} = 2 \times \log 2(P_{MC}/P_{today}) \quad (7.1)$$

with $P_{MC} = N_{flop}/\Delta t$ the computing power (in floating-point operations per second or flops) required to perform the task and $P_{today} = 5 \times 10^{12}$ flops the computing power currently provided by our university cluster (512 CPUs, 10 Gflops per CPU).

Let us further assume a typical cartesian grid of dimension $1000 \times 1000 \times 1000$ and the worst case scenario in which each photon has to travel an average distance equivalent to half the sidelength of the grid ($N_{steps} = 500$). If we want to keep the processing time reasonable ($\Delta t = 1$ s) and for $N_{flop/steps} \approx 10$, the expression in (7.1) reduces to:

$$T_{years} \approx 2 \times \log 2(N_{\gamma/c})$$

giving 20 years $\lesssim T_{years} \lesssim 60$ years for $10^3 \leq N_{\gamma/c} \leq 10^9$, and this only for one group of frequencies¹...

Although the current limitations on the radiative transfer capabilities prevent any accurate accounting for the effects of remote radiation sources, an evaluation of the local density, temperature and velocity gradients should provide a basis to approximate the optical depth in the three directions of the grid and therefore remove the resolution dependence of the results. The remaining issue related to the loss of spectral resolution when multi-group radiation methods are used could be in part addressed by the implementation of an adaptive algorithm [45].

It appears also important to improve the accuracy of the different circuit models. At the time this work was performed, some advanced current schemes modelling the parasitic losses in parallel with the load were available but their implementation in the last version of GORGON is not yet effective.

As the amount of radiation released in the high energy region of the spectra is strongly related to the history of the emission in the highest shells, the next improvement should come from the inclusion of the radiation temperature in the population calculation process. To limit the computational cost of such

¹Assuming $P_{today} = 10 \times 10^{15}$ flops (K computer, RIKEN Advanced Institute for Computational Science), $T_{years} < 10$ years for $N_{\gamma/c} = 10^3$ and 50 frequency groups.

an operation, this temperature might be evaluated locally (from the neighboring cells emission). In addition, by adjusting the initial wire temperature and level of perturbations, the experimental pulse widths might also be recovered.

In the context of the offline version, the accuracy of the line broadening mechanisms should be assessed (some effects are likely to be missing) and the selectivity of the spectral point filter function should be increased to prevent the generation of excessively large files.

Finally, to further check the validity of the model and benchmark the code, simulations should be performed considering other types of Z-pinch loads (gas puff, radial array) and the results compared to the experimental data.

Appendix A

Radiation Basics

Although the results of this document are generally expressed in S.I units, in this part it will be convenient to work in C.G.S, a system of units somehow more common in the field of spectroscopy.

Relations between units

Energy:	$1 \text{ eV} = 1.602176487 \times 10^{-19} \text{ J}$ $1 \text{ J} = 10^{-7} \text{ erg}$
Charge:	$1 \text{ C corresponds to } 2997924580 \text{ statC}$

Constants

Elementary charge:	$e = 4.80320427 \times 10^{-10} \text{ statC}$
Planck constant:	$h = 6.62606896 \times 10^{-27} \text{ erg.s}$
Speed of light:	$c = 2.99792458 \times 10^{10} \text{ cm.s}^{-1}$
Electron mass:	$m = 9.10938215 \times 10^{-28} \text{ g}$
Boltzmann constant:	$k = 1.3806504 \times 10^{-16} \text{ erg.K}^{-1}$
Stefan-Boltzmann constant:	$\sigma_{SB} = 5.670400 \times 10^{-5} \text{ erg.cm}^{-2}.\text{s}^{-1}.\text{K}^{-4}$

A.1 Some useful characteristics of the radiation field

Let $f(\nu, \mathbf{r}, \boldsymbol{\Omega}, t) d\nu d\mathbf{r} d\boldsymbol{\Omega}$ be the number of photons in the frequency interval $[\nu + d\nu]$, contained at the time t in the volume element $d\mathbf{r}$ about the point $\mathbf{r}$, and having a direction of motion within an element of solid angle $d\boldsymbol{\Omega}$ around the unit vector $\boldsymbol{\Omega}$. The function f is called the distribution function and its units are $\text{cm}^{-3}.\text{Hz}^{-1}.\text{sr}^{-1}$ [47].

- **Spectral radiation intensity**

Each photon possesses an energy $h\nu$ and moves with speed c . Therefore the quantity:

$$I_\nu(\mathbf{r}, \boldsymbol{\Omega}, t) d\nu d\boldsymbol{\Omega} = h\nu c f(\nu, \mathbf{r}, \boldsymbol{\Omega}, t) d\nu d\boldsymbol{\Omega} \quad (\text{A.1})$$

represents the radiant energy in the unit frequency interval $d\nu$, passing per unit time through a unit area, with a direction of propagation in $d\boldsymbol{\Omega}$. The quantity I_ν is called the spectral radiation intensity and its units are $\text{erg}.\text{cm}^{-2}.\text{s}^{-1}.\text{Hz}^{-1}.\text{sr}^{-1}$.

- **Spectral radiant energy density**

Radiant energy with a frequency ν included in $d\nu$ and contained at time t in a unit volume $d\mathbf{r}$:

$$U_\nu = h\nu \int_{4\pi} f d\boldsymbol{\Omega} = \frac{1}{c} \int_{4\pi} I_\nu d\boldsymbol{\Omega} \quad [\text{erg}.\text{cm}^{-3}.\text{Hz}^{-1}] \quad (\text{A.2})$$

- **Spectral energy density at equilibrium**

Amount of energy per unit volume $d\mathbf{r}$ and radiated at equilibrium with a frequency ν in $d\nu$:

$$U_{\nu p} = \frac{8\pi h\nu^3}{c^3} \frac{1}{(e^{h\nu/kT} - 1)} \quad [\text{erg}.\text{cm}^{-3}.\text{Hz}^{-1}] \quad (\text{A.3})$$

- **Spectral intensity for radiative equilibrium (Planck's law)**

$$I_{\nu p} = \frac{cU_{\nu p}}{4\pi} = \frac{2h\nu^3}{c^2} \frac{1}{(e^{h\nu/kT} - 1)} \quad [\text{erg.cm}^{-2}.\text{s}^{-1}.\text{Hz}^{-1}.\text{sr}^{-1}] \quad (\text{A.4})$$

represents the radiant energy at equilibrium in the frequency interval $d\nu$, passing per unit time through a unit area, with a direction of propagation in $d\Omega$. $I_{\nu p}$ is maximum for $h\nu \approx 2.82143 kT$

- **Integrated equilibrium radiant energy density**

$$U_p = \int_0^\infty U_{\nu p} d\nu = \frac{4\sigma_{SB}T^4}{c} \quad [\text{erg.cm}^{-3}] \quad (\text{A.5})$$

with $\sigma_{SB} = 2\pi^5 k^4 / (15h^3 c^2)$ the Stefan-Boltzmann constant.

- **One-sided spectral radiant energy flux**

The amount of radiant energy in the frequency interval $d\nu$, passing per unit time from one side of a unit area with the normal unit vector $\mathbf{n}$ to the other is given by:

$$F_\nu(\mathbf{r}, t, \mathbf{n}) = h\nu c \int_{2\pi} f \cos(\theta) d\Omega = \int_{2\pi} I_\nu \cos(\theta) d\Omega \quad [\text{erg.cm}^{-2}.\text{s}^{-1}.\text{Hz}^{-1}] \quad (\text{A.6})$$

where θ is the angle between the surface normal $\mathbf{n}$ and the direction of propagation Ω . At equilibrium $I_\nu = I_{\nu p}$, therefore:

$$\begin{aligned} F_{\nu p} &= \int_{\theta=0}^{\pi/2} \int_{\phi=0}^{2\pi} I_\nu \cos(\theta) \sin(\theta) d\theta d\phi = I_{\nu p} \pi \\ \Rightarrow F_{\nu p} &= \frac{2\pi h\nu^3}{c^2} \frac{1}{(e^{h\nu/kT} - 1)} = c \frac{U_{\nu p}}{4} \quad [\text{erg.cm}^{-2}.\text{s}^{-1}.\text{Hz}^{-1}] \quad (\text{A.7}) \end{aligned}$$

- **One-sided spectral radiant energy flux integrated over the frequency**
(Stefan-Boltzmann law)

$$F_p = \int_0^\infty F_{\nu p} d\nu \stackrel{\text{A.7}}{=} \int_0^\infty c \frac{U_{\nu p}}{4} d\nu \stackrel{\text{A.5}}{=} \sigma_{SB} T^4 \quad [\text{erg.cm}^{-2}.\text{s}^{-1}] \quad (\text{A.8})$$

A.2 Kirchhoff's law

Let us consider the absorption and emission of photons for a material placed in a radiation field of intensity I_ν :

$$\kappa_\nu I_\nu d\nu d\Omega = \text{energy absorbed per unit volume per unit time} \quad [\text{erg.cm}^{-3}.\text{s}^{-1}] \quad (\text{A.9})$$

$$j_\nu d\nu d\Omega = \text{spontaneous emission per unit volume per unit time} \quad [\text{erg.cm}^{-3}.\text{s}^{-1}] \quad (\text{A.10})$$

with j_ν and κ_ν respectively the emission and absorption coefficients. The quantum theory shows that the probability for the stimulated emission of a photon of a given frequency and direction is proportional to the number n of photons of the same frequency and direction present in the same phase cell. This implies that:

$$j_\nu(1 + n) d\nu d\Omega = \text{total emission per unit volume per unit time} \quad [\text{erg.cm}^{-3}.\text{s}^{-1}] \quad (\text{A.11})$$

The number of phase cells in a volume element of phase space $d\mathbf{p} d\mathbf{r}$ is $d\mathbf{p} d\mathbf{r}/h^3$, the number of photon in one cell is thus given by:

$$n_{/c} = f(\nu, \mathbf{r}, \boldsymbol{\Omega}, t) d\nu d\mathbf{r} d\boldsymbol{\Omega} h^3 / (d\mathbf{p} d\mathbf{r}) \quad (\text{A.12})$$

With $d\mathbf{p} = dS dp$ (dS being a surface element in the momentum space) and $d\boldsymbol{\Omega} = dS/p^2$, we obtain $d\mathbf{p} = p^2 dp d\boldsymbol{\Omega}$ or (knowing that $p = h\nu/c$, $dp = h d\nu/c$) :

$$d\mathbf{p} = \frac{h^3 \nu^3}{c^3} d\nu d\boldsymbol{\Omega} \quad (\text{A.13})$$

Injecting this last result in (A.12) and using (A.1):

$$n_{/c} = \frac{c^3 f}{\nu^2} = \frac{c^2}{h\nu^3} I_\nu \quad (\text{A.14})$$

The number of photons with a specific direction is equal to half this number, therefore $n = c^2 I_\nu / (2h\nu^3)$ and for (A.11) we have:

$$j_\nu \left(1 + \frac{c^2}{2h\nu^3} I_\nu\right) d\nu d\Omega = \text{total emission per unit volume per unit time} \quad [\text{erg.cm}^{-3}.\text{s}^{-1}] \quad (\text{A.15})$$

In thermodynamic equilibrium the absorption (A.9) and emission (A.15) balance, while the spectral radiation intensity I_ν is replaced by its value at equilibrium $I_{\nu p}$:

$$\frac{j_\nu}{\kappa_\nu} = \frac{I_{\nu p}}{1 + c^2 I_{\nu p} / (2h\nu^3)} = \frac{2h\nu^3}{c^3} \frac{1}{(e^{h\nu/kT} - 1)} \times \frac{1}{1 + (e^{h\nu/kT} - 1)^{-1}} = \frac{2h\nu^3}{c^3} e^{-h\nu/kT} \quad (\text{A.16})$$

This relation is one version of the Kirchhoff's law. It can be convenient to reformulate it as follows:

$$\frac{j_\nu}{\kappa'_\nu} = I_{\nu p} \quad (\text{A.17})$$

with here, $\kappa'_\nu = \kappa_\nu (1 - e^{-h\nu/kT})$ the absorption coefficient corrected for the induced emission. This law expresses the fundamental relation between the emission and absorption coefficients under LTE conditions.

Appendix B

Screening constants

	1s	2s	2p	3s	3p	3d	4s	4p	4d	4f
1s	0.31	0.0135	0.0003	0	0	0	0	0	0	0
2s	0.7388	0.3082	0.2522	0	0	0	0	0	0	0
2p	0.9461	0.3481	0.3495	0.0392	0.021	0.0007	0.0097	0.006	0	0
3s	0.9511	0.8511	0.648	0.3106	0.2496	0.1676	0.0477	0.0245	0.029	0
3p	0.9696	0.855	0.7916	0.3002	0.3136	0.3226	0.0513	0.0338	0.0392	0
3d	0.9987	0.9865	0.9413	0.4847	0.323	0.3786	0.0743	0.0781	0.0188	0.0224
4s	0.934	0.7502	0.85	0.6718	0.6068	0.6547	0.2983	0.2881	0.1889	0.1276
4p	0.9886	0.9068	0.8899	0.676	0.677	0.6543	0.2988	0.3348	0.2663	0.2574
4d	0.9988	0.9973	0.9891	0.9856	0.9109	0.716	0.4474	0.3416	0.3438	0.2737
4f	0.9988	0.9983	0.9955	0.9891	0.982	0.9768	0.5507	0.4388	0.4126	0.3863
5s	0.999	0.9989	0.9966	0.9908	0.7852	0.7829	0.4829	0.6502	0.5692	0.673
5p	0.9991	0.999	0.9989	0.9978	0.8853	0.8282	0.5122	0.6828	0.5719	0.6902
5d	0.9992	0.9991	0.999	0.9988	0.9983	0.849	0.7665	0.7797	0.7494	0.6928
5f	0.9993	0.9992	0.9991	0.9989	0.9988	0.9936	0.9892	0.9761	0.9445	0.9156
5g	0.9994	0.9993	0.9992	0.999	0.9989	0.997	0.992	0.9865	0.945	0.938
6s	0.9995	0.9994	0.9993	0.9991	0.999	0.9987	0.9931	0.9873	0.9454	0.941
6p	0.9996	0.9995	0.9994	0.9992	0.9991	0.9989	0.9987	0.9924	0.9449	0.9447
6d	0.9997	0.9996	0.9995	0.9993	0.9992	0.999	0.9989	0.9947	0.9906	0.9806
6f	0.9998	0.9997	0.9996	0.9994	0.9993	0.9991	0.999	0.9989	0.995	0.99
6g	0.9999	0.9998	0.9997	0.9995	0.9994	0.9992	0.9991	0.999	0.9989	0.9988
6h	0.9999	0.9999	0.9998	0.9996	0.9995	0.9993	0.9992	0.9991	0.999	0.9989

Table B.1: Table of screening constants of the submatrix $\sigma_{1s \leq k \leq 6h, 1s \leq k' \leq 4f}$ of the screened hydrogenic model [18].

	5s	5p	5d	5f	5g	6s	6p	6d	6f	6g	6h
1s	0	0	0	0	0	0	0	0	0	0	0
2s	0	0	0	0	0	0	0	0	0	0	0
2p	0	0	0	0	0	0	0	0	0	0	0
3s	0	0	0	0	0	0	0	0	0	0	0
3p	0	0	0	0	0	0	0	0	0	0	0
3d	0.0269	0.0191	0.0024	0	0	0	0	0	0	0	0
4s	0.0507	0.0387	0.0245	0	0	0	0	0	0	0	0
4p	0.062	0.0433	0.062	0	0	0	0	0	0	0	0
4d	0.1002	0.0875	0.0533	0	0	0	0	0	0	0	0
4f	0.061	0.0544	0.0796	0.0121	0.0118	0	0	0	0	0	0
5s	0.2979	0.3183	0.1706	0.1309	0.0758	0	0	0	0	0	0
5p	0.2771	0.3341	0.2204	0.2022	0.1559	0	0	0	0	0	0
5d	0.3682	0.3247	0.3133	0.2945	0.2329	0.0038	0.0144	0	0	0	0
5f	0.6088	0.5321	0.4565	0.3602	0.3068	0.0063	0.0047	0	0	0	0
5g	0.7826	0.643	0.5645	0.4602	0.4119	0.0344	0.0279	0.026	0.0021	0	0
6s	0.9427	0.7263	0.6131	0.6026	0.59	0.3078	0.2722	0.1387	0.1196	0.0951	0.0405
6p	0.94	0.8387	0.7241	0.6548	0.65	0.2287	0.3379	0.1911	0.1516	0.1247	0.0675
6d	0.9527	0.9111	0.8994	0.8508	0.8	0.5106	0.4427	0.3155	0.2135	0.1744	0.1553
6f	0.9804	0.98	0.97	0.96	0.95	0.5754	0.5281	0.4519	0.3352	0.2475	0.2245
6g	0.9987	0.985	0.98	0.97	0.96	0.6717	0.6224	0.5513	0.4662	0.366	0.3023
6h	0.9988	0.9987	0.99	0.98	0.97	0.8789	0.8104	0.6756	0.5625	0.5204	0.4194

Table B.2: Table of screening constants of the submatrix $\sigma_{1s \leq k \leq 6h, 5s \leq k' \leq 6h}$ of the screened hydrogenic model [18].

	7s	7p	7d	7f	7g	7h	7i
7s	0.2976	0.2908	0.2775	0.2595	0.2389	0.2172	0.1947
7p	0.3086	0.3018	0.288	0.269	0.2474	0.2247	0.2016
7d	0.3297	0.3238	0.3105	0.2895	0.2653	0.2405	0.2159
7f	0.3591	0.3546	0.3442	0.3243	0.2955	0.2664	0.2388
7g	0.3942	0.3912	0.3843	0.371	0.3447	0.3069	0.2731
7h	0.4335	0.4318	0.428	0.4209	0.407	0.3748	0.3256
7i	0.4762	0.4756	0.4744	0.4721	0.4679	0.4585	0.4253

Table B.3: Table of screening constants of the submatrix $\sigma_{7l,7l'}$ of the screened hydrogenic model for $0 \leq l, l' \leq 6$ [18].

	8s	8p	8d	8f	8g	8h	8i
8s	0.2976	0.2921	0.2815	0.2668	0.2498	0.2315	0.2125
8p	0.3061	0.3008	0.2898	0.2745	0.2566	0.2376	0.2181
8d	0.3229	0.318	0.3073	0.2907	0.271	0.2505	0.2297
8f	0.3463	0.3424	0.3336	0.3176	0.295	0.2713	0.2482
8g	0.3748	0.3719	0.3655	0.3537	0.3324	0.3031	0.2755
8h	0.4068	0.4049	0.4007	0.3931	0.3794	0.3529	0.3159
8i	0.4417	0.4406	0.4383	0.4341	0.427	0.4135	0.3821
8j	0.4793	0.479	0.4782	0.4768	0.4746	0.4705	0.4616

Table B.4: Table of screening constants of the submatrix $\sigma_{8l,8l'}$ of the screened hydrogenic model for $0 \leq l, l' \leq 7$ [18].

	9s	9p	9d	9f	9g	9h	9i	9j
9s	0.2975	0.2931	0.2843	0.2722	0.2578	0.2421	0.2258	0.2089
9p	0.3044	0.3	0.2911	0.2784	0.2635	0.2473	0.2305	0.2133
9d	0.318	0.314	0.3052	0.2916	0.2754	0.258	0.2402	0.2222
9f	0.3372	0.3338	0.3263	0.3132	0.2948	0.2752	0.2556	0.2362
9g	0.3607	0.3581	0.3523	0.3419	0.3244	0.3009	0.278	0.2562
9h	0.3874	0.3855	0.3813	0.374	0.3615	0.3396	0.3104	0.2841
9i	0.4166	0.4154	0.4126	0.4078	0.4	0.3864	0.3599	0.3239
9j	0.4481	0.4474	0.4458	0.4432	0.4389	0.4318	0.4187	0.3882
9k	0.4817	0.4815	0.4809	0.4801	0.4787	0.4765	0.4726	0.4642

Table B.5: Table of screening constants of the submatrix $\sigma_{9l,9l'}$ of the screened hydrogenic model for $0 \leq l, l' \leq 8$ [18].

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