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Predicting β-decay rates of radioisotopes embedded in anisotropic ECR plasmas

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Summary. — Studying in-plasma decay rates as a function of ionic charge state distribution (CSD) is the fundamental objective of the PANDORA project. To this effect, we present here two theoretical models to calculate β-decay lifetimes of radionuclide ions embedded in an energetic electron cyclotron resonance (ECR) plasma, starting from anisotropic electron distributions. The first model —designed as separate modules to implement various atomic processes like electron-ion reactions, ion-ion charge exchange collisions and ion loss dynamics sequentially— serves as a predecessor to a more robust second model aimed at coupling ion population kinetics with complex transport phenomena in an ECR plasma. The outputs from the models —in the form of space-resolved CSD and level populations— can be fed to an appropriate code based on known theories connecting atomic level configurations to decay lifetime to calculate the position-dependent β-decay rate.

1. – Introduction

The PANDORA (Plasmas for Astrophysics, Nuclear Decay Observations and Radiation for Archaeometry) project is a new and upcoming facility at INFN-LNS, Catania, Italy, aimed at studying nuclear astrophysics using energetic and compact ECR plasmas [1]. The first phase of experiments will be devoted to the measurement of in-plasma decay rates of select isotopes like ^{176}Lu, ^{134}Cs and ^{94}Nb by tagging the secondary γ-emission from the decay event. This will require a precise knowledge of the space-resolved $t_{1/2}$ of the nuclei, which depends on the atomic configuration of the ions as a function of position in the plasma. We thus report here recent developments in studying the space-resolved properties of ions in an ECR plasma using two simulation models that couple ion population kinetics with transport dynamics. The outputs from the models can be benchmarked against beams extracted from ECRIS devices, potentially validating the method as useful tools for fundamental research in ECR devices as well.

2. – Basic formalism and composite model

The physics of plasma ion dynamics is contained in the balance equation

$$\frac{\mathrm{d}n_i}{\mathrm{d}t} = \sum_{j\neq i} n_j G_{ji} - \sum_{i\neq j} n_i L_{ij} - \frac{n_i}{\tau_i} + n_i^{pump} \tag{1}$$

where $n_{i,j}$ are level populations of states i and j, G_{ji} and L_{ij} represent the inter-level gain and loss rates respectively, τ_i is the characteristic confinement time and n_i^{pump} is the influx rate. The usual approach is to construct a rate matrix $\mathbf{R}$ from all atomic levels, discretise the differential equation $\frac{\mathrm{d}\mathbf{n}}{\mathrm{d}t} = \mathbf{R} \cdot \mathbf{n}$ and then solve it iteratively till steady state is reached. We designed a rough model composed of interlinked modules which, in principle, could balance complex ECR ion dynamics and population kinetics in the simplest manner. The general idea was to spatially-resolve the plasma into smaller regions of interest (ROIs), pass electron data coming from self-consistent steady-state (SS) PIC simulations for each ROI to a population kinetics code FLYCHK to calculate the part of $\mathbf{R}$ pertaining to electron-ion reactions, simulate the process for an appropriately chosen interval Δt and then feed the output to a second module designed to implement ion-ion charge exchange collisions. The output from this module would then be given to a final set of codes to emulate the ion diffusion between different ROIs as well as the pumping of neutrals. The processed population $\mathbf{n}$ would be fed back to FLYCHK, repeating the whole process up to the steady state.

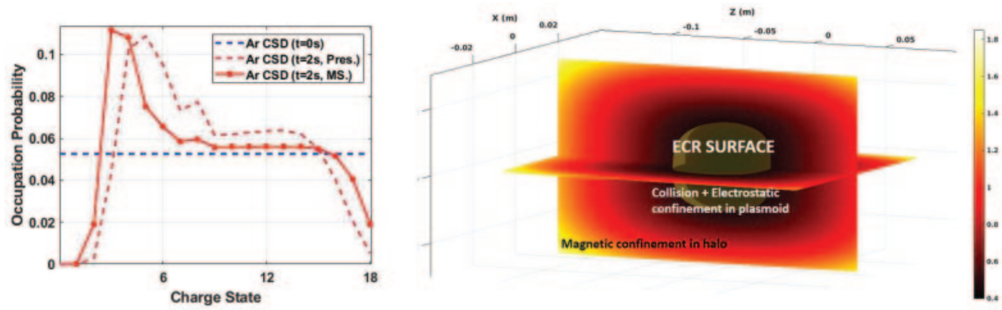
2·1. *Warm electron diagnostics.* – Owing to the importance of electron data in the simulation scheme, the anisotropic electron properties of the plasma were first carefully studied. 3D space-resolved maps of density and energy obtained from self-consistent simulations [2, 3] and based on algorithms detailed in previous work [4], the plasma was divided into ROIs assumed to contain quasi-independent electron populations. Analytical energy distribution functions (EDFs) were estimated for each ROI and experimental validation was made using space-resolved X-ray fluorescence imaging and soft X-ray spectroscopy [5].

2·2. *Modelling electron-ion reactions.* – FLYCHK is a popular 0D population kinetics tool capable of solving the collision-radiative (CR) model with a high degree of accuracy under both local and non-local thermodynamic equilibrium conditions [6]. The code could produce ion CSD and level populations at SS or as a function of time (TD).

2·3. *Modelling ion-ion collisions and charge exchange.* – Apart from the CR model, charge exchange collisions are the other major reactions affecting ion charge states. Since these were outside the scope of FLYCHK, a separate module was designed to implement them. The reaction rate was extended to the same matrix formulation, with each element defined as $R_{CEX} = \rho_i \rho_j \sigma_{CEX} v$ where $\rho_{i,j}$ represent the respective densities of colliding species (same ion in different charge states or different ions altogether), σ_{CEX} is the exchange cross section and v is the collision velocity in the centre-of-mass frame of reference. Only single-electron exchange were implemented, the cross-sections for which were modified from the work of Presnyakov [7] and Müller-Salzborn [8] as

$$\sigma_{CEX,i,i-1,j,j+1} = \pi a_0^2 i^2 (E_{Ry}/I_{j,j+1})^2, \qquad \text{modified Presnyakov,} \tag{2a}$$

$$\sigma_{CEXi,i-1,j,j+1} = A_1 i^{\alpha_1} I_{j,j+1}^{\beta_1}, \qquad \text{modified Müller-Salzborn.} \tag{2b}$$



(a) (b)

Fig. 1. – (a) Initial and final CSD of Ar after charge exchange reactions using modified Presnyakov (Pres.) and Müller-Salzborn (MS) cross sections (b) magnetic field profile and position of ECR layer with ion transport scheme (colourbar in T).

Here i represents the charge state of the electron-accepting ion, j is the charge state of the electron-donor, a_0 is the Bohr radius, E_{Ry} is the Rydberg energy, $I_{j,j+1}$ is the ionisation energy, and $A_1 = 1.43 \times 10^{-12}$, $\alpha_1 = 1.17$ and $\beta_1 = -2.76$ are fit coefficients. The differential equations for the population of each state could be discretised and solved iteratively up to SS or extracted prematurely for TD results (fig. 1(a)).

2˙4. *Ion transport in plasmas.* – Just like standard gaseous systems, particles in ECR plasmas are also subject to diffusion arising from density gradients and interparticle thermal collisions. However, owing to the presence of long-range EM forces, there are added elements of complexity in the charge particle transport discussed in detail in previous works [9]. In our model, we chose to consider diffusion and electrostatic effects in ROIs in the interior of the ECR layer and magnetic transport outside, and assume the particles as flowing between the ROIs (fig. 1(b)).

3. – Limitations and improved ion dynamics model

It was soon realised, however, that the simulation scheme suffered from a number of drawbacks. Despite relative simplicity, the formulation remained approximate and complicated in other ways. The time interval Δt could become prohibitively small for constantly shuffling between the modules, and space-resolution was limited by the shape and size of the ROIs. Additionally, the ion transport module was too imprecise for such a complex system and required a proper kinetics treatment, which is incompatible with a rate matrix approach.

A new and improved model was thus devised, which combined the modular nature and aspects of rate matrix formalism from the old scheme with a standard particle-in-cell (PIC) code. The idea now was to use PIC simulations to track the motion of macroparticles in i-th charge state while simultaneously checking for ionisation to $i+1$ or electron exchange to $i-1$. The use of macroparticles meant that reaction rates could no longer be calculated, so they were replaced with analogous probabilities $P_r = 1 - \mathrm{e}^{-\Delta t/\tau_r}$ where P_r is the probability of a certain reaction to occur, Δt is the time step per iteration and $\tau_r = 1/n_j \sigma_r v_r$ is the characteristic time for the reaction mediated by species n_j with cross section σ_r and collision velocity v_r.

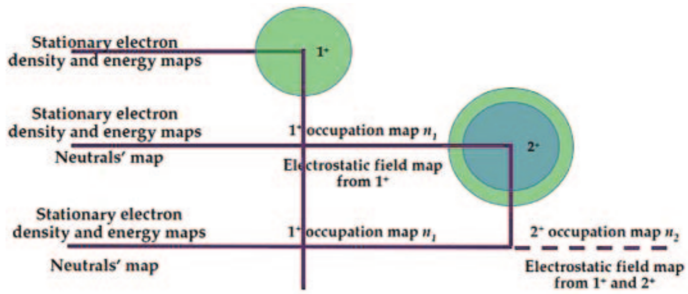


Fig. 2. – Simulation scheme of coupled population kinetics and ion dynamics PIC code.

The simulation would begin with a certain number of macroparticles in the 1^+ state distributed throughout the plasma according to the ionisation probability of neutrals. The plasma would be defined using electron density and energy maps in steady state, as well as parameters of the applied magnetic field. Each time step Δt, ionisation/charge exchange occurrence would be checked and particles still remaining in the 1^+ state would be evolved using equations of motion. The simulation would be continued till a sizeable number of 2^+ ions were generated, after which the 1^+ occupation map would be scaled to a density map and passed as input to 2^+ code where kinetics would be evaluated in the presence of electrons *and* the 1^+ ions. Each successive charge state would thus evolve in plasma consisting of ions of lower charges, and the results from each simulation would be absorbed into the following one, leading to a final steady state CSD neutral with the total electron density. Figure 2 shows a schematic of the algorithm.

4. – Conclusion

We have presented two models for evaluating space-resolved level population and CSD of ions in an ECR plasma for eventual application to the PANDORA project. The first model was quite simple and made use of pre-existing tools to simulate the plasma in a crude fashion, and consequently suffered from certain drawbacks. A second model was thus developed on the foundations of the first, which painted a detailed picture of ion dynamics while simultaneously capturing the most essential physics. The algorithm is robust, makes few assumptions about the state of the plasma and can potentially shed light on even fundamental ECR phenomena like the double layer generation [9], and we are presently working in this direction.

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