Modeling of partial redistribution in high-density divertor plasmas

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1. Introduction

The preparation of ITER (tokamak under construction in Cadarache, France) and the numerical simulations supporting its design have prompted a renewal of interest in atomic line radiation models. The plasma in the divertor can be very optically thick to the hydrogen resonance lines, so that the resulting photon trapping can affect the ionization-recombination balance (e.g., [1] for a recent review). Estimates show that the photon mean free path λ_{mfp} of the first resonance lines can be shorter than 1 mm. Opacity effects have been demonstrated experimentally (from line ratio measurements) in C-Mod operating at high density regime [2] and numerically using coupled radiation transport / atomic kinetic codes [3,4]. Up to now, all of the numerical investigations of line radiation opacity done in the framework of magnetic fusion research were made assuming complete redistribution, i.e., the frequency and the direction of a photon outgoing from a scattering process were assumed independent of those of the incoming photon. In this work, we address the redistribution of the first resonance line of hydrogen (Lyman α) and we examine the role of partial redistribution on the collisional-radiative balance. A one-dimensional transport model is considered and addressed with a kinetic Monte-Carlo simulation routine.

2. Radiative transfer modeling with partial redistribution

Details on the formalism presented hereafter can be found in [5] and Refs. therein. We write a transport equation of Boltzmann-type for the radiation specific intensity $I(\omega,\vec{n},\vec{r},t)$:

$$\left(\frac{1}{c}\frac{\partial}{\partial t}+\vec{n}\cdot\vec{\nabla}+\chi(\omega,\vec{n})\right)I(\omega,\vec{n})=\eta^{*}(\omega,\vec{n})+\frac{\sigma_0}{4\pi}\int d\omega'\int d\Omega' R(\omega,\vec{n},\omega',\vec{n}')I(\omega',\vec{n}')\,. \quad (1)$$

Here ω denotes the radiation frequency, $\vec{n}$ is the unit vector along the propagation direction, the solid angle Ω' corresponds to $\vec{n}'$, χ and η^* are the extinction coefficient and the thermal emission coefficient, respectively, σ_0 is the scattering coefficient, and R is the so-called redistribution function (joint probability density function for photon absorption and emission). The $\vec{r}$ and t dependences have not been written for the sake of simplicity. For each atomic transition $u \to l$ between upper and lower levels u and l, the extinction and thermal emission coefficients are given by

$$\chi(\omega,\vec{n}) = \frac{\hbar\omega_0}{4\pi} B_{lu} N_l \phi(\omega,\vec{n}), \qquad \eta^*(\omega,\vec{n}) = \frac{\hbar\omega_0}{4\pi} A_{ul} N_u^* \phi(\omega,\vec{n}), \tag{2}$$

where $\omega_0 = \omega_{ul}$ is the Bohr frequency of the transition, B_{lu} and A_{ul} are the Einstein coefficients for absorption and spontaneous emission, N_l is the density of atoms in the lower level, N_u^* is the density of atoms in the upper level due to processes other than radiation absorption (e.g. collisional excitation), and $\phi(\omega,\vec{n})$ is the one-photon line profile. Here, we have adopted the convention $\int d\omega \int d\Omega \phi(\omega,\vec{n})/(4\pi) = 1 = \int d\omega \int d\Omega \int d\omega' \int d\Omega' R(\omega,\vec{n},\omega',\vec{n}')/(4\pi)^2$. The one-photon line profile is related to the redistribution function by $\phi(\omega,\vec{n}) = \int d\omega' \int d\Omega' R(\omega,\vec{n},\omega',\vec{n}')/(4\pi)$. In the case where only two levels are considered in the scattering process, the amplitude σ_0 is given by

$$\sigma_0 = \frac{A_{ul}}{\Gamma_u^{tot}} \times \frac{\hbar\omega_0}{4\pi} B_{lu} N_l = \frac{A_{ul}}{\Gamma_u^{tot}} \times \frac{\chi(\omega,\vec{n})}{\phi(\omega,\vec{n})}, \tag{3}$$

where Γ_u^{tot} is the total depopulation rate of the upper level u including both the radiative and collisional processes. The importance of scattering relative to the thermal emission is measured by the ratio A_{ul}/Γ_u^{tot}. This ratio is controlled by N_e and T_e. A rough estimation (e.g., from [6]) shows that this ratio is close to unity for Lyman α for typical conditions of dense divertor plasmas.

The approximation of complete redistribution consists in neglecting correlations between the incoming and outgoing photons, and leads to factorize the redistribution function as $R(\omega,\vec{n},\omega',\vec{n}') = \phi(\omega,\vec{n})\phi(\omega',\vec{n}')$. In tokamak plasmas, this assumption is questionable because of the Doppler effect (due to the atom motion) [7]. Non-trivial correlations between the frequencies and directions of the absorbed and reemitted photons induced by the Zeeman and Stark effects have also been reported in a recent work [8]. In the following, we address partial redistribution effects on the collisional-radiative balance with a simplified model.

3. A simplified model

The system of interest is a slab, infinite in the x and y directions and of size L in the z direction, containing a homogeneous and partially ionized deuterium plasma. The atoms are assumed to be composed of two levels only, the fundamental and first excited ones (i.e. with the principal quantum numbers n = 1, 2). Their velocity distribution function $f(\vec{v})$ is assumed Maxwellian, with $T_{at} = T_e = T_i$. The ground state is considered as a reservoir, as well as the ions and the electrons. Radiative transfer is considered in the stationary case (i.e. $\partial/\partial t \equiv 0$). The structure of the transport equation (1) makes it suitable for kinetic Monte-Carlo simulations. We follow the terminology used in the EIRENE code (which is used for simulations in magnetic fusion plasmas with realistic geometry [9]) and reported in the literature on neutron transport [10]. Let Σ be an arbitrary section over the x,y-plane and consider the volume $V = \Sigma \times L$. We define the collision density $\psi = \chi I/(\hbar\omega_0 A_{21} N_2^{*} V)$ and we write an integral equation for it, from integration of Eq. (1) along the characteristics:

$$\psi(X) = S(X) + \int dX' K(X,X')\psi(X'). \tag{4}$$

Here, X is a shortcut notation for $(\omega,\vec{n},\vec{r})$. The source and the kernel correspond to the thermal- and scattering-emission, respectively. These terms are given by

$$S(X) = \int_V \frac{d^3r'}{V} T(\vec{r}|\omega,\vec{n},\vec{r}')\frac{\phi(\omega,\vec{n})}{4\pi}, \quad K(X,X') = \frac{A_{21}}{\Gamma_2^{tot}} T(\vec{r}|\omega,\vec{n},\vec{r}')\frac{p(\omega|\omega',\vec{n},\vec{n}')}{4\pi}, \tag{5}$$

where $T(\vec{r}|\omega,\vec{n},\vec{r}') = H(\vec{n}\cdot(\vec{r}-\vec{r}'))\chi(\omega,\vec{n},\vec{r})\exp\left(-\int_0^{\vec{n}\cdot(\vec{r}-\vec{r}')} ds\chi(\omega,\vec{n},\vec{r}-\vec{n}s)\right)\delta(\vec{r}_\perp - \vec{r}_\perp')$ is the conditional probability of a photon being absorbed at $\vec{r}$ (H is the Heaviside function and $\perp$ refers to the plane perpendicular to $\vec{n}$) and $p(\omega|\omega',\vec{n},\vec{n}') = R(\omega,\vec{n},\omega',\vec{n}')/\phi(\omega',\vec{n}')$ is the conditional probability of reemitting a photon with frequency ω. The quantities $S(X)$, $K(X,X')$, and $p_{abs}(X) = 1 - \int dX' K(X,X')$ are directly interpretable as probabilities associated with a continuous random walk process ($X_1 \ldots X_k$). This allows one to evaluate physical observables by generating a set of random sequences and using an appropriate estimator. In the following, we use the Wasow estimator [10], i.e., for any detector function $g(X)$, we evaluate the integral $\int dX g(X)\psi(X)$ from the expectation value of the random variable $v = \sum_{m=1}^{k} g(X_m)$.

We have applied the Monte-Carlo procedure to the evaluation of the photoexcitation rate $W_{12} = B_{12}\int d\omega \int d\Omega \phi(\omega,\vec{n}) I(\omega,\vec{n})$ assuming various redistribution models: (i) perfect coherence, $p(\omega|\omega',\vec{n},\vec{n}') = \delta(\omega-\omega')$; (ii) complete redistribution; (iii) Doppler redistribution, i.e. $R(\omega,\vec{n},\omega',\vec{n}') = \int d^3v f(\vec{v})\delta(\omega-\omega_0-\omega_0\vec{n}\cdot\vec{v}/c)\delta(\omega'-\omega_0-\omega_0\vec{n}'\cdot\vec{v}/c)$ (see [7] for an analytical expression). A Doppler model has been assumed for the one-photon line profile. The following values have been set for the plasma parameters: $N_{n=1} = N_e = 10^{14}$ cm^{-3}, $T_{at} = T_e = T_i = 1$ eV. As can be seen in Fig. 1, the photoexcitation rate is sensitive to the redistribution mechanism. The case (i) indicates that neglecting the frequency change at a scattering event leads to a strong overestimate of the plasma's opacity. Furthermore, the small deviation (~10%) between the cases (ii) and (iii) suggests that the complete redistribution assumption can be used safely, at least in the plasma conditions considered here.

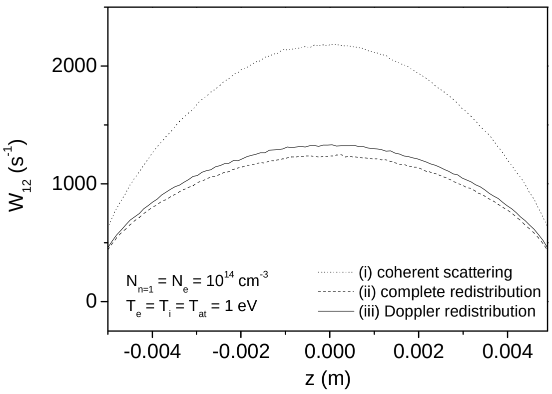

Figure 1 – Spatial dependence of the photoexcitation rate for the cases (i), (ii), and (iii). The model used for redistribution plays a critical role in the estimates.

5. Conclusion

We have examined the role of partial redistribution on the radiation transport and its consequence on the collisional-radiative balance in dense divertor conditions. With a simplified model, we have shown that the photoexcitation rate is sensitive to the redistribution mechanism. In the framework of ITER modeling, this suggests that a careful analysis of the radiation redistribution should be done if accuracy in transport simulations is required. An extension of the present work should be devoted to the investigation of the role of the Zeeman and the Stark effects. Other lines affected by opacity should also be examined.

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