Effect of partially ionized high-Z atoms on fast electron dynamics in tokamak plasmas

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EFFECT OF PARTIALLY IONIZED HIGH-Z ATOMS ON FAST ELECTRON DYNAMICS IN TOKAMAK PLASMAS

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Abstract

The dynamics of fast electrons driven inductively or by resonant interactions with radio-frequency waves is known to be highly sensitive to the presence of impurities in hot magnetized hydrogen plasmas. The possibility to use tungsten for the ITER divertor, thanks to its low tritium retention and high melting temperature, has raised the question of the impact of partially ionized high-Z atoms on current drive efficiency by enhancing pitch-angle scattering but also collisional slowing-down and inelastic scattering. Pioneering work on the impact of the screening effect of partially ionized atoms in kinetic calculations was carried out primarily for the problem of runaway electron mitigation in very cold post-disruptive plasmas [1]. In the present paper, this approach is adapted and extended to regular plasma regimes, allowing to take into account any type of high-Z metallic impurity in the plasma core on the fast electron dynamics and the non-thermal bremsstrahlung. This work has been implemented in LUKE Fokker-Planck solver [2] and the quantum relativistic radiation code R5-X2 [3] and the impact of partially ionized high-Z impurities on Lower Hybrid driven current in the WEST tokamak has been investigated.

1. INTRODUCTION

The ability to efficiently generate all or part of the toroidal plasma current in tokamaks and to control its profile by radio frequency (RF) sources to achieve a steady-state high performance burning plasma has been a long-standing problem. So far, the methods based on the use of the waves at the Electron Cyclotron (EC) and Lower Hybrid (LH) frequencies are the most studied for this purpose [4,5]. While the former can drive a very localized current that can contribute to stabilize deleterious neoclassical tearing modes (NTM), the latter has the highest experimentally demonstrated current drive efficiency, allowing to investigate plasma properties during long pulse operation at zero loop voltage in existing machines [6].

In this context, the possibility to use tungsten for the ITER divertor [7], thanks to its low tritium retention and high melting temperature, has raised the question of the impact of partially ionized high-Z atoms on current drive efficiency by enhancing pitch-angle scattering but also collisional slowing-down. Indeed, it is well-known that the dynamics of fast electrons driven inductively or by resonant interactions with radio-frequency waves is highly sensitive to the presence of impurities in hot magnetized hydrogen plasmas. In addition, the possible presence of partially ionized high-Z atoms may also change considerably the properties of the non-thermal bremsstrahlung, one of the most powerful tools for diagnosing the suprathermal electron population and for a quantitative quantitative comparison between first principles modelling and observations.

The initial work on this experimental subject has been carried out for the problem of runaway electron dynamics in post-disruptive discharges, in which the critical field and the avalanche process by knock-on collisions are highly sensitive to the high-Z atoms [1]. Taking into account of partially screened atoms is indeed particularly critical in this case, because of the extremely low plasma temperature after the thermal quench (few eV). For high-power RF current drive experiments in tokamak plasmas, the problem is significantly different because the temperature of the plasma is much higher (up to several keV), and so only very high-Z atoms like tungsten but also other heavy elements like copper or iron, which are present in the plasma due to interactions with metallic structures of RF antenna, are still partially ionized in this regime. Nevertheless, the remaining large number of bound electrons may contribute significantly to the change in the dynamics of the RF-driven fast electrons as compared to the fully screened approximation used so far, since their binding energies fall in the range of the kinetic energies of the tail electrons, which lies usually up to 200 keV approximately, close to the highest binding energy in tungsten of 75 keV for example. In this case, scattering processes by bound electrons must be consistently taken into account in kinetic calculations, while the effect of bound electrons on the electron-ion non-thermal bremsstrahlung must be also fully considered, this radiation being a powerful tool for diagnosing the fast electron population in the plasma.

In this context, the LUKE Fokker-Planck solver [2] and the quantum relativistic radiation code R5-X2 [3] have been upgraded to incorporate the contribution of partially ionized high-Z atoms in RF current drive calculations, and simulate high LH power discharges in the WEST tokamak equipped with tungsten divertors [7]. In Sec. 2, the modelling of the partial screening is first investigated, in the framework of the Born approximation by calculating the atomic form factor to account for the spatial extent of the high-Z ions using atomic electron densities calculated by different models. The modified collision operator used in Fokker-Planck calculations is derived in Sec. 3 from first principles, since the introduction of a form factor in the spinless relativistic Rutherford elastic scattering cross-section leads to significant modifications of its usual formulation. The inelastic scattering is then considered in Sec. 4. The differential cross-section of the electron-ion bremsstrahlung taking into account partial screening is studied in Sec. 5. The conditions in which the presence of bound electrons is modifying the properties of this radiative process are discussed. Finally, in Sec. 6, the impact of partially ionized high-Z atoms on RF current drive efficiency are investigated for the LH wave and an example of integrated simulation for a representative WEST discharge is shown, in which a significant fraction of tungsten impurities is present.

2. ATOMIC PHYSICS: MODELLING OF PARTIAL SCREENING

In order to calculate screening effects on electron scattering in tokamak plasma or bremsstrahlung radiation in tokamak plasmas, it is necessary to choose the most appropriate atomic model for describing the cloud of bound electrons around the nucleus. The ab-initio approach based on Density Functional Theory (DFT) requires full quantum relativistic calculations [8], taking into account accurately the many-body exchange and correlation interactions between electrons in the potential of the nucleus. In addition, for high-Z atoms, relativistic calculations must be carried out using the Douglas-Kroll-Hess second order scalar relativistic Hamiltonian and the natural orbital-relativistic correlation basic set [9]. For atoms whose condition $\alpha Z_s \ll 1$ is fulfilled (up to Argon), where $\alpha \approx 1/137$ is the fine structure constant, the classical limit holds, while relativistic corrections must be considered otherwise, in particular for copper and tungsten. This approach requires considerable numerical calculations, whose accuracy is usually beyond the purpose of the present work since simple approximate models provide useful frameworks to incorporate simply the screening effects in kinetic but also radiation calculations. What matters is the possibility to express the form factor, i.e., the Fourier transform of the bound electron density in the Born approximation, such that analytical calculations of the different cross-sections for collisions and radiations can be performed.

$a_0 \times \lambda_{0,s}$	He	Be	C	N	Ne	Ar	W
TF [10]	1.42	1.79	2.05	2.26	2.43	2.96	4.74
TF-K [11]	1.68	2.11	2.42	2.66	2.87	3.49	5.60
Y (HFS) [12]	1.2	1.61	1.91	2.15	2.36	3.03	5.48
DFT [9]	1.58	1.72	1.90	2.02	2.46	2.85	4.64

***Table 1**: Comparison of the inverse of the neutral atom size between different atomic models for Helium, Beryllium, Carbon, Nitrogen, Neon, Argon and Tungsten elements.*

So far, two models are appropriate for this purpose, one developed by Kirillov et al (TF-K), based on an interpolation between asymptotic limits of the exact Thomas-Fermi (TF) atomic model [10,11] and the Yukawa-like (Y) model based upon the expansion of the potential in the core of the atom as a series of exponentials [12]. Here, only the first correction term is considered to describe the screening effects. Both models lead to a simple formulation of the form factor, $F_{Z0,s}(q) = N_s/(1+[q\times\tilde{a}_{Z0,s}/2]^n)$, where n=3/2 for TF-K and n=2 for Y models respectively, N_s being the number of bound electrons. Here q is the usual transferred momentum between the free incoming electron and the bound ones, and $\tilde{a}_{Z0s} = 2a_{Z,0s}/\alpha$ where $a_{Z0,s}$ is the effective radius of the screened ion of type s and whose net charge is $Z_{0,s} = Z_s - N_s$. The neutral atom corresponds to $Z_{0,s} = 0$ and $N_s = Z_s$. For the Yukawa-like model, $a_{Z,0s} = a_0\times\lambda_{Z0,s}$ where a_0 is the classical Bohr radius, and the $\lambda_{Z0,s}$ is the inverse of the ion radius, which is related to the neutral atom radius $\lambda_{0,s}$ by the relation $(\lambda_{Z0,s}/\lambda_{0,s})^2 = f_s(Z_{0,s}/Z_s)$, with $f_s(x) = (1-x^{ns+1})/(1-x)^2$ which differs slightly from the expression $f_s(x)$ in Ref. [13] and gives a much better agreement with DFT calculations

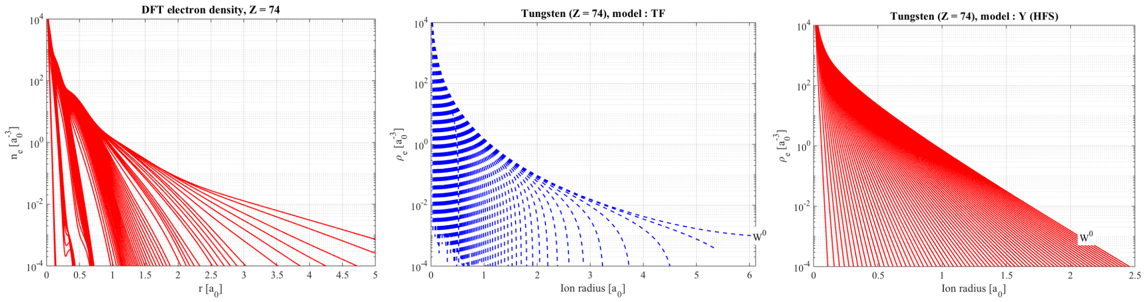

Fig. 1: Density of bound electrons averaged over solid angle for tungsten as a function of ion radius. Left: DFT model (code Gaussian, model PBE1PBE/gen/Auto (ANO-RCC) Integral= DKH2) [9], middle: TF model [10] and right: Y (HFS) model [12].

whatever the type of atoms and their ionization states using the Gaussian code [9]. Here, $n_s = Z_s \times (1/3 - 0.0020 \times Z_s)$ [13]. The value $\lambda_{0,s}$ may be given by the Thomas-Fermi model $a_0 \times \lambda_{0,s} \approx 1.13 \times Z_s^{1/3}$, but more accurately from a fit of Hartree-Fock-Slater (HFS) potentials, leading to $a_0 \times \lambda_{0,s} \approx 0.9 \times Z_s^{0.42}$ [12]. As shown in Table 1, the values of $\lambda_{0,s}$ for different elements are close to the reference DFT models which have been carried out with the GAUSSIAN code [9].

In Fig. 1, the electron densities spherically averaged over the solid angle for all ionization states of tungsten obtained with the DFT, TF and Y (HFS) models are shown. While general dependencies are similar, some details associated to deep atomic shells are missing in simplified models. Despite these differences, both give reasonable agreement of $\tilde{a}_{Z0s}$ which enters into the form factor. With the form factors deduced from TF-K and Y (HFS) models, accurate best fits of DFT calculations may be obtained, as shown in Fig. 2. The agreement is better with TF-K model for weakly ionized atoms, while both models give good agreement at higher ionized states, as expected from theory. Since post-disruptive plasmas are very cold, the TF-K is therefore more appropriate in this regime for describing the screening effects, as shown in Ref. [14], while Y (HFS) model is preferred for hot plasmas, even near the plasma edge, since it gives very close values of $\tilde{a}_{Z0s}$ as compared to DFT calculations. Besides this physical justification for the Y (HFS) model, it offers also the possibility to obtain semi-analytical expressions for the fast electron bremsstrahlung thanks to the simple analytic form of F(q) with n = 2, thus speeding up considerably calculations of this quantity. A unified atomic model may therefore be used for Coulomb collisions and bremsstrahlung.

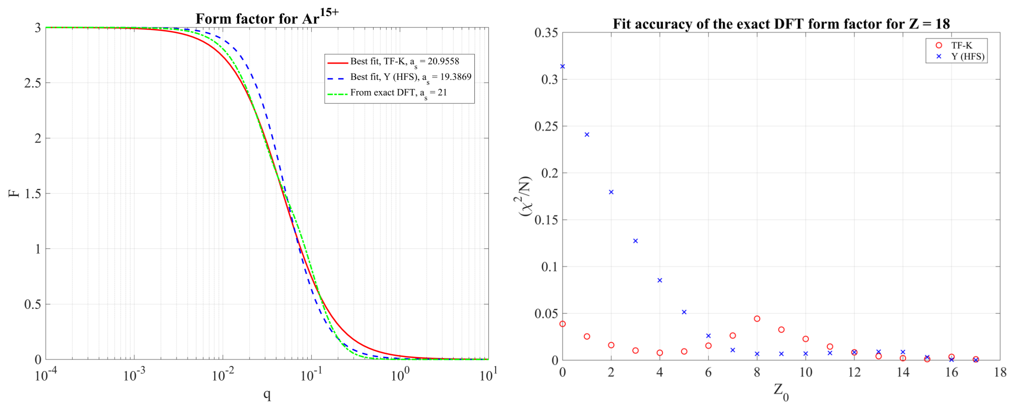

Fig. 2. Left: Form factor for Argon 15+, green: DFT calculations, dashed blue curve: best fit of DFT form factor with Y (HFS) model, full red curve : best fit of DFT form factor with TF-K model. Right: normalized chi-squared of the difference between form factor by DFT model and best fit using Y (HFS) model (blue crosses) and TF-K model (red circles).

3. PLASMA PHYSICS: ELASTIC SCATTERING

The introduction of partially ionized atoms in kinetic calculations leads to revisit completely the assumptions to derive the Fokker-Planck equation from first principle, since the usual spinless relativistic Rutherford elastic scattering cross-section used for calculating the diffusion and convection terms must be modified by replacing the ion charge Z_s by Z_s - $F_s(q)$ as shown in Eq. 1. The integration of the Rosenbluth potentials is then strongly modified [15]. While calculations have been initially performed in the ultra-relativistic limit, ion at rest of infinite mass and

$$\int_{1/\Lambda_s}^{1} \frac{dx}{x} Z_s^2 \rightarrow \int_{1/\Lambda_s}^{1} \left| Z_s - F_{Z_{0,s}}(q) \right|^2 \frac{dx}{x} = Z_{0,s}^2 \ln \Lambda_s + g_{Z_{0,s}}(p) \qquad (1)$$

zero temperature plasma for the problem of post-disruptive runaway electrons [14], it has been carried out in the present work in the classical or semi-relativistic limit, for thermal ions of finite mass and finite temperature plasmas for describing the effect of partially ionized high-Z impurities on the RF current drive. Regardless the assumptions, the impact of partial screening may be described by a similar formulation. It can be shown that the screening effect results in a change of the integral where Λ_s is the usual Coulomb factor for the species s. The first term is the usual pitch-angle effect in Fokker-Planck calculations, which is modified by the function $g_{Z0,s}(p)$ describing the partial screening effect [14]. This function may be obtained by a numerical integration of the bounded electron density from DFT calculations, or determined analytically for the TF-K or Y (HFS) models.

In that case, $\tilde{a}_{Z0,s}$ may be obtained explicitly, as shown in Eq. 2, where $I_{1,Z0,s}$ and $I_{2,Z0,s}$ are weighted integrals of the bound electron densities [14]. Here the *m* value is 7/6 for the TF-K model and one for the Y (HFS) one, so very close. Here, γ_{EM} is the Euler-Mascheroni constant. As shown in Fig. 3 for tungsten with a fully screened

$$\tilde{a}_{Z_{0,s}} = \frac{2}{\alpha} \exp\left[\gamma_{EM} - 1 + \frac{2Z_s I_{1,Z_{0,s}} + N_s\left(m - I_{2,Z_{0,s}}\right)}{Z_s + Z_{0,s}}\right] \qquad (2)$$

charge $Z_{0,s} = 20$, the partial screening term using the Y (HFS) model is exceeding the standard pitch-angle one $Z_{0,s}^2 \ln \Lambda_s$ corresponding to the fully screened limit when electrons have a kinetic energy exceeding 50 keV. This threshold is shifted to 500 keV when $Z_{0,s} = 30$. This means that only very energetic electrons are concerned by the effect of screening of partially ionized high-Z impurities on pitch-angle scattering, except possibly near the plasma edge. The plasma temperature and the ionization state are too high to have a considerable impact on RF current drive efficiency in the core plasma. This conclusion holds even if the energy dependence of the Coulomb logarithm is fully taken into account, which leads to a progressive rise of the pitch-angle with electron kinetic energy as shown in Fig. 3. From calculations using Open-ADAS code [16], the dominant fraction is corresponding to $Z_{0,s} = 20$ for tungsten when the local electronic temperature of the plasma is 0.3 keV, while it is $Z_{0,s} = 32$ and 43 when $T_e = 2$ and 3 keV respectively.

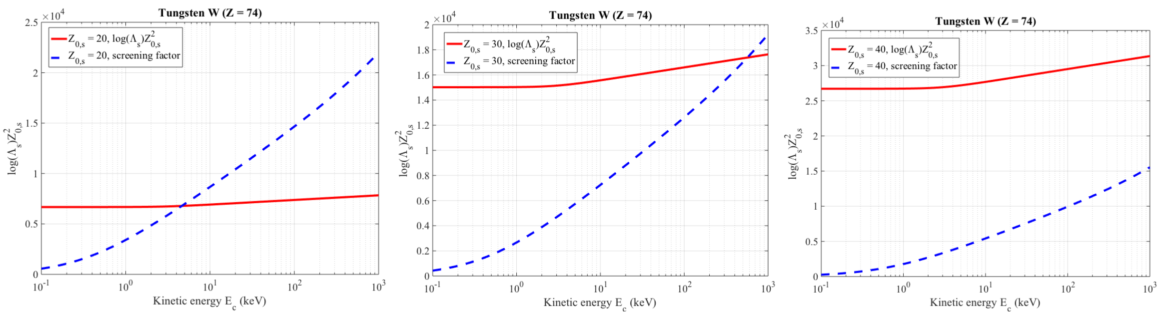

Fig. 3: Comparisons between fully screened Coulomb term (full red line) and screening term (blue dashed line) for three different ionization states (left: $Z_{0,s} = 20$, middle: $Z_{0,s} = 30$, right: $Z_{0,s} = 40$) using the atomic TF model. For the case of $Z_{0,s} = 20$, screening corrections become significant for electrons above 50 keV approximately.

4. PLASMA PHYSICS: INELASTIC SCATTERING

In the presence of partially ionized high-Z impurities, the interaction between the fast electrons and the cloud of bound electrons may lead to energy transfer. Several mechanisms may occur, like bremsstrahlung which is considered in the next section, but also ion excitation which is here detailed. The interesting question of enhanced ionization by fast electrons is not yet taken into account. The transfer of energy between free and bounded electrons requires a full quantum approach, and it is based on the standard Bethe's theory [14,17]. The atomic system is approximated by a charge bound in a simple harmonic well in the limit of a large impact parameter. The electric field of the passing electron is therefore uniform for the partially ionized atom. The total energy loss per unit length is proportional to the number of bound electrons N_s, and has a logarithm dependence with the mean excitation energy $I_{Z0,s}$ which incorporates all the atomic physics. Some relativistic correction factors are also taken into account, but their contributions are small as far as the fast electron kinetic energies are less than twice the electron rest mass energy.

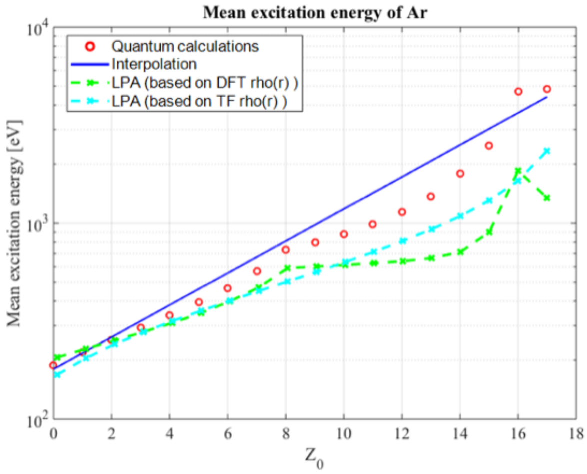

Fig. 4: Mean excitation energy for Argon. Blue full line: interpolation method, red circles from quantum calculations [18], cyan and green dashed lines: LPA approximation using atomic electron density from DFT and TF models respectively [20].

Since the energy loss by excitation of ions over a distance Δx is equivalent of the work of an effective force F_{ei} over that distance, this effect can be easily introduced in the Fokker-Planck code, by adding an electron-ion convection term to the usual electron-electron one. The parametric dependencies of $I_{Z0,s}$ with $Z_{0,s}$ is based on an heuristic interpolation from the neutral atom $I_{Z0,s}=10\times Z_s$ [eV] to the purely hydrogenoid ion $I_{Z0,s}=13.6\times Z_s^2$ [eV]. It is found that taking the law $I_{Z0,s} \approx \exp(aZ_{0,s}/(Z_s-1)+b)$, where coefficients a and b are determined from the two above limits of ionization, gives very reasonable agreement with refined quantum calculations for all ionization states [18,19]. An example is shown in Fig. 4 for Argon, and it is assumed to be valid up to tungsten.

An alternative approach is to use the so-called Local Plasma Approximation (LPA) model developed initially by Lindhard and Scharff [20]. The advantage is to consider consistently the density of cloud electrons for elastic and inelastic scattering from any atomic model. Within the LPA, the specific energy loss of a charged particle incident on a gas of free electrons at rest is determined by making a local approximation i.e., assuming that the stopping at any point **r** in an inhomogeneous gas is equivalent to the stopping in a homogenous gas of the density ρ(**r**) at that point. Averaging the expression over a single atom, $I_{Z0,s}$ can be written down as,

$$\ln I_{Z0,s} = \frac{1}{N_s} \int 4\pi r^2 \rho\left(r\right) \ln\left(\gamma \hbar \omega_0\right) d^3 r \qquad (3)$$

where ω_0 is the corresponding local-plasma frequency. Here $\rho(|\boldsymbol{r}|)$ is the electron density calculated from DFT, TF or any atomic model, r = |**r**| is the local radius in the atomic cloud of bound electrons and $\hbar$ is the reduced Plank constant. The γ factor is a free parameter whose value is √2, as suggested in Ref. [20].

When the mean excitation energy is calculated with the LPA, using electron density $\rho(r)$ taken either from DFT calculations or TF model, the results remain in good agreement for low Z_0 while LPA model underestimates $I_{Z0,s}$ for higher ionization states, as shown in Fig. 4.

5. FAST ELECTRON-ION BREMSSTRAHLUNG

The effect of partial screening of high-Z atoms on the electron-ion bremsstrahlung has been considered long time ago in the Born approximation [21]. The available formula is 1BS according to the standard nomenclature in Ref. [22], which corresponds to the triply differential cross-section in photon energy and in photon and electron emission angles. However, for calculating the line-integrated bremsstrahlung emission in the hard x-ray photon energy range, taking into account the magnetic field line curvature in a tokamak and the angular anisotropy of the fast electron distribution function, the doubly differential cross-section in photon energy and in photon emission angles is necessary, which requires to integrate the 1BS formula over all directions of the scattered electron. This represents an important numerical challenge, in presence of screening effect. Without screening, this angular integration leads to well-known formula 2BN of the bremsstrahlung cross-section, while formula 3BS for arbitrary screening is here useless.

Three methods have been considered to perform the numerical integration. By considering full 5-D blocks $(k,\theta_0,p,\theta,\varphi) \rightarrow (k,\theta_0)$ which are fast but very memory demanding calculations can be carried out for arbitrary form factors. However, the constraint on the required computing memory may be considerably reduced by considering a loop for the integration on the θ angle. In this case, the calculation remains accurate, but very slow. A more effective method is to perform first an analytical integration over the azimuthal angle φ, which can be only performed using the form factor of the model Y (HFS). In that case, the cross-section may be split in twelve integrals that can be all determined analytically. The calculation is therefore fast and weakly demanding for the computing memory. It remains valid as far as the model Y (HFS) may be applied, which is the case of high-Z atoms in hot plasmas. To speed up calculations, the cross-section for each element and ionization state is projected onto the Legendre polynomials basis, allowing to build a table of data. In the limit where the photon energy is close to the incoming electron, the standard Elwert correction is taken into account, without considering specific corrections due to the screening effect [23].

As expected, screening effects on fast electron bremsstrahlung becomes significant when the maximum impact parameter $r_{max} = \alpha a_0/q_{min}$ is much larger than $a_{Z,0s}$. Therefore, it takes place for rather low energy photons as compared to the incoming electron kinetic energy, as shown in Fig. 5, reducing significantly the e-i bremsstrahlung level from the charge of the bare nucleus only, which was usually considered in bremsstrahlung calculations (or increasing it for the fully screened ion). The effect tends to fade out when the emitted photon is more and more perpendicular to the incoming electron direction.

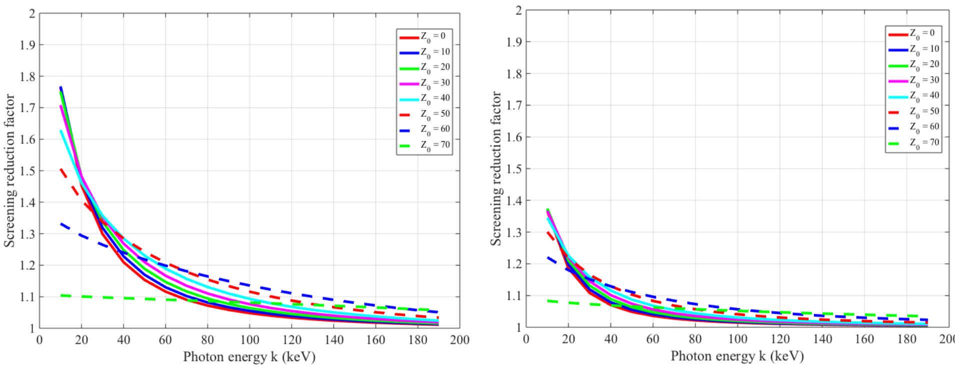

Fig. 5: Screening reduction factor (left: $\theta = 0$ deg.) and (right: $\theta = 60$ deg.) as function of the photon energy for various tungsten ionization states. The kinetic energy of the incoming electron is 200 keV. The reference cross-section is 2BN [22].

6. CURRENT DRIVE EFFICIENCY AND INTEGRATED SIMULATIONS

The impact of partially ionized high-Z atoms on the Lower Hybrid current drive efficiency has been first investigated in the theoretical limit as a function of Z_s. As shown in Fig. 6, in the case of the flat plateau in the fast electron distribution function between $v_{\|min}/v_{th} = 4$ and $v_{\|max}/v_{th} = 7$, where v_{th} is the local thermal velocity, the current drive efficiency is decreasing when Z_s is increased, consistently with the usual $4/(5+Z_s)$ dependence [24], up to $Z_s = 11$ where $T_e = 1$ keV and $Z_s = 40$ for $T_e = 5.11$ keV. For low temperature plasmas, the screening effect reduces the decrease of the current drive efficiency with Z_s, because the fully screened mean ion charge $Z_{0,s}$ is lower than Z_s of the bare nucleus. This effect is visible at higher T_e, but much weaker, because ions with higher Z_s are mostly fully stripped. Taking into account of the screening effect leads therefore to an intermediate situation between the cases of fully screened and fully stripped ions, principally visible for low temperature plasmas and high-Z elements.

Finally, simulations of a fully representative WEST discharge have been carried out, investigating the effect of tungsten impurities on the LH-driven current level and the fast electron bremsstrahlung. For the discharge #55539, 4.8 MW of LH power is injected in the plasma, and the launched power spectrum is peaked at $n_{\|0} \approx 2$ according to the antenna phasing. The plasma current is 0.45 MA. The simulations are studied at t = 6s where only the LH power is coupled to the plasma. The fraction of tungsten is estimated to be 3.6×10^{-4} from calculations of the radiated power consistently calculated by the METIS tokamak simulator [25]. From the toroidal MHD equilibrium provided by the METIS code, the LH driven current including a residual Ohmic electric field corresponding to a loop voltage of 0.1 V is very close to observations, including or not screening effect of partially ionized high-Z impurities in the calculations, a result that is consistent with theoretical expectations. However, including the contribution of high-Z impurities in the plasma and taking into account of the screening effect leads to a large increase of the calculated bremsstrahlung level, by a factor ×3 approximately. Nevertheless, the observed emission is still much larger than the calculated one, the tail of fast electrons being very sensitive to the residual electric field, even at a small level. Further investigations at zero loop voltage are in progress in order to estimate carefully the role of tungsten in bremsstrahlung.

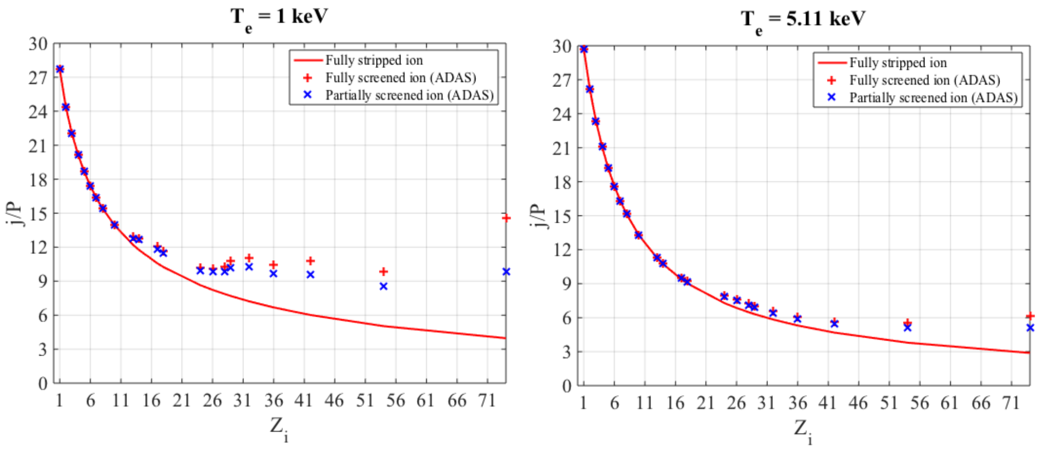

Fig. 6: Local current drive efficiency for the Lower Hybrid wave as function of the atomic number. Calculations are performed for a flat plateau in the distribution function between $v_{||min}/v_{th} = 4$ *and* $v_{||max}/v_{th} = 7$*. Left figure:* $T_e = 1$ *keV, Right figure:* $T_e = 5.11$*keV. On both figures, the full red line corresponds to the case of a fully stripped ion, the red crosses to a fully screened ion, and the blue crosses correspond to the case where partial screening is taken into account. This effect fades out at large temperature.*

7. CONCLUSION

The effect of partially ionized high-Z atoms has been studied and incorporated in the 3-D linearized bounce-averaged relativistic electron Fokker-Planck code LUKE and the quantum relativistic radiation code R5-X2. From theory, the reduction of the RF current drive efficiency by tungsten impurities should be small in hot plasmas, even if the density of impurities is quite large. The impact of inelastic scattering is also minor. These results are confirmed by numerical calculations of a realistic LH sustained discharge on WEST tokamak in which the fraction of tungsten is rather large. Conversely, the fast electron bremsstrahlung is very sensitive to partially ionized high-Z atoms, the screening effect leading to a decoupling between the hard x-ray emission profile and the current density profile driven by the fast electron population. The calculation of the fast electron bremsstrahlung requires therefore an accurate determination of the electron temperature profile, as well as the spatial distribution of the density of the different species in the plasma. This makes the interpretation of the fast electron bremsstrahlung more difficult in this context.

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