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

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### Context

Growing interest for studying the impact of partially ionized high-Z atoms on fast electron dynamics in magnetized plasmas.

- Passive source : plasma-wall interaction**
  - Tungsten-based plasma-facing components to reduce tritium retention
  - Metallic objects like rf antennas in contact with the scrape-off layer (Copper, Iron, ...)
- Active source : massive gas injection** of Argon or Neon to mitigate the formation of a runaway electron beam after a major disruption.

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### Atomic physics

Calculation of the bound electron density averaged over solid angle (form factor).

- Simple models : Thomas-Fermi or Yukawa simplified atomic models.
- Exact models : numerical quantum calculations based on Density Functional Theory (DFT). Realistic calculations must be carried out for high-Z elements using the Douglas-Kroll-Hess second order scalar relativistic Hamiltonian and the natural orbitals-relativistic correlation basis set.
- Virial theorem :  $\frac{m v^2}{2} = \frac{Z e^2}{4 \pi \epsilon_0 r}$  →  $\frac{v}{c} = \frac{Z \alpha}{2} < 1$
- Quantum uncertainty principle :  $m v r = \hbar$  →  $\frac{v}{c} = \frac{\hbar}{2 m c r} < 1$
- Ne (10) : 0.07, Ar (18) : 0.131, Cu (29) : 0.212, W (74) : 0.54

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### Plasma physics : elastic scattering

- Modified Rosenbluth potentials by screening effect
- Rutherford scattering cross-section:  $\frac{d\sigma}{d\Omega} = \frac{r_D^2}{4 \pi^2 \sin^4(\theta/2)} (Z_1 - Z_2 - F_{sc})^2$
- Fully screening ion -  $F_{sc}(0) = N_e$

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### Partial screening for e- bremsstrahlung

- Screening effects significant when  $\frac{r_{max}(Z_{sc})}{r_{min}(Z_{sc})} \geq 1$  where  $r_{max} = \frac{2 \hbar^2}{m_e v^2}$  (max. impact parameter)
- Equivalent to Bethe estimate (using Thomas-Fermi model) :  $\frac{d\sigma}{d\Omega} \propto \frac{1}{k^2} \sum_{l=0}^{l_{max}} A_l^2$

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### Impact of partially ionized atoms on fast electron dynamics and bremsstrahlung

- Atomic physics : screening effect → F(q)**
  - Distribution of ionization states (Open-ADAS)
  - Simple models (Thomas-Fermi, Yukawa)
  - Exact models (DFT calculations)
  - Form factor F(q) for any ionized state of any relevant high-Z atom in plasma physics (Ar, Ne, Cu, Fe, W, ...) in the Born approximation.
- Plasma physics : elastic scattering**
  - Z - Z (Fq) (atomic physic form factor F)
  - Coupling together in F(q)
  - Validity of Fokker-Planck approximation
  - Cutoff approximation in collision integrals
- Plasma physics : isotropic scattering**
  - e- bremsstrahlung Z - Z (Fq)
  - e- bremsstrahlung  $N_e \rightarrow N_e + \sum_{i=1}^n N_i$
  - Ion excitation:  $\kappa_{ion} \propto Z^2$
  - Enhanced ionization by fast electrons

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### Atomic physics: Thomas-Fermi model

- Poisson's equation :  $\nabla^2 (\mu_{sc} - V_{sc}) = -4 \pi e^2 n_{sc}(r)$
- Energy variational principle :  $\mu_{sc}(r) = \left( \frac{3}{2} C_{TF} \right)^{-2/3} (\mu_{sc} - V_{sc}(r))^{2/3}$
- Thomas-Fermi equation  $\frac{d^2 \mu_{sc}}{dr^2} - \frac{2 \mu_{sc}}{r^2} = -\frac{Z e^2}{4 \pi \epsilon_0 r^3} \phi(x)$  ;  $x = r/r_D$
- Normalized Thomas-Fermi neutral atom radius  $\mu_{sc} \rightarrow \frac{1}{4} [9 \eta^2]^{1/3}$  ;  $r_D = \frac{1}{4} [9 \eta^2]^{1/3} r_D$
- Ion ( $N_i < Z_i$ ) :  $\phi(x_{0i}) = 0$  ;  $x_{0i} = 1 - N_i / Z_i$  ;  $x_{0i} = r_{0i} / r_D$
- Form factor (non-relativistic integration) :  $F_{sc}(q) = 4 \pi \int_0^{x_{0i}} \mu_{sc}(r) \frac{\sin(qr)}{qr} r^2 dr$

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### Fokker-Planck collision operator with partially ionized atoms

Fokker-Planck screening function →  $\int_{-\infty}^{\infty} |Z_1 - Z_2 - F_{sc}(q)|^2 \frac{dZ_2}{dZ_1} \ln A_1 + g_{sc}(p)$

which reduces to  $g_{sc}(p) = \frac{2 \pi^2}{N_e} \left( \ln(1 + (p r_D)^2) - \frac{(p r_D)^2}{1 + (p r_D)^2} \right)$

for simplified atomic models with  $n = 3/2$  for Thomas-Fermi-Kirillov model or  $n = 2$  for Yukawa (Tseng-Pratt) model. Condition of validity always fulfilled:  $\beta \ll \frac{A_1}{A_2} \frac{r_D}{r_{D2}}$

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### Partial screening for e- bremsstrahlung

Three methods (matlab script for RS-X2 code) for integrating the five differential bremsstrahlung cross-section (IES Koehn Most formula) on the scattered electron emission angles to obtain 2Bn formula with screening effects

$\int \frac{d^2 \sigma}{d\Omega d\Omega'} = \int \frac{d^2 \sigma}{d\Omega d\Omega'} \left( \frac{Z_1 - Z_2 - F_{sc}(q)}{Z_1 - Z_2} \right)^2 \frac{dZ_2}{dZ_1} \sum_{l=0}^{l_{max}} A_l^2$

- Integration of full 5-D blocks (k, B, p, B) : arbitrary form factor, slow but very memory demanding.
- Integration of full 4-D blocks (k, B, p, B) + loop for B integration : arbitrary form factor, slow but accurate.
- Integration of full 4-D blocks (k, B, p, B) : analytical integration in azimuthal angle φ. Tseng-Pratt-Botto form factor only, fast and accurate (12 complex integrals to evaluate analytically) → Table of Legendre polynomials cross-section for each element and ionization state with linear kinetic energy interpolation in RS-X2 code.

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### Extended work of atomic physics in hot plasmas

- Generalize screening effects to partially ionized high-Z atoms in hot plasmas (Copper, Iron, Tungsten, ...)
- Calculate a Fokker-Planck collision operator (elastic + inelastic terms) in presence of partially ionized high-Z atoms with screening effects for LUKE code.
- Consider screening effects for the quantum relativistic bremsstrahlung cross section differential in photon energy and angle in RS-X2 code.

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### Atomic physics: Thomas-Fermi-Kirillov model

- Approximate formulation of the form factor (Kirillov, Trubnikov et al, 1975)
- Two limits :  $\xi_{TF} \ll 1 \rightarrow F_{sc}^{TK}(\xi) = N_e$  ;  $\xi_{TF} \gg 1 \rightarrow F_{sc}^{TK}(\xi) = \frac{N_e}{2 \sqrt{\xi}}$
- Approximate neutral atom radius :  $N_e = Z_e$

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### Fokker-Planck collision operator with partially ionized atoms

Exact DFT calculations with  $N_e = Z_e - Z_{ion}$

$g_{sc}(p) = [Z_1^2 - Z_2^2] \ln(2 \eta / \alpha) + 7 \ln \eta - 1 + 2 Z_1 N_e I_{1,sc} + N_e^2 \left( \frac{1}{2} - I_{2,sc} \right)$

In the high velocity limit :  $I_{1,sc} = \frac{4 \pi}{N_e} \int_0^{x_{0i}} \mu_{sc}(r) \frac{\sin(p r)}{p r} r^2 dr$  ;  $I_{2,sc} = \frac{4 \pi^2}{N_e^2} \int_0^{x_{0i}} \mu_{sc}(r) \frac{\sin(p r)}{p r} \mu_{sc}(r) \frac{\sin(p r)}{p r} r^2 dr$

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### Partial screening for e- bremsstrahlung

Z = 74, Tungsten ; Photon angle θ = 90 deg ; E<sub>e</sub> = 200 keV

Z = 74, Tungsten ; Photon angle θ = 45 deg ; E<sub>e</sub> = 200 keV

- Screening effect reduces progressively bremsstrahlung as compared to the fully stripped ion (Z<sub>e</sub> = Z)
- Screening decreases with kinetic electron energy.
- Screening are large for forward emission only and at low photo energies

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### Elastic scattering by partially ionized atoms

- Weak perturbation theory (Fermi's Golden rules) for the transition probability  $W = \frac{2 \pi}{\hbar} |\langle f | H | i \rangle|^2 \rho_f$
- 1<sup>st</sup> Born approximation (plane wave functions for the scattered free electron)
- Transferred momentum :  $q = p_f - p_i = 2 p_i \sin(\theta/2)$

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### Atomic physics: Yukawa (Tseng-Pratt) model

- Yukawa type model :  $\Delta \mu_{sc}(\xi) = Z_1 \mu_{sc}(\xi) + (Z_1 - Z_2) \exp(-\lambda_{sc} r) + \dots$
- By definition,  $N_e$  is considered as the neutral atom radius :
  - Thomas-Fermi :  $\lambda_{sc}^{TF} = Z_1^{3/2} / r_D = 1.13 Z_1^{3/2} / r_D$
  - Botto (fit of Hartree-Fock-Slater (HFS) potentials) :  $\lambda_{sc}^{B} = 0.92 Z_1^{3/2} / r_D$
- Best Z<sub>e</sub> dependence as compared to DFT
- Bound electron density :  $n_{sc}(r) = \frac{Z_1 N_e}{4 \pi r^2} \exp(-\lambda_{sc} r) \exp(-\lambda_{sc} r)$
- Form factor :  $F_{sc}^{TK}(q) = \frac{N_e}{1 + (\frac{q r_D}{2})^2}$  ;  $\frac{dF_{sc}^{TK}}{dZ_1} = 2 \mu_{sc}^{TK}(r_D)$  ;  $\frac{dF_{sc}^{TK}}{dZ_2} = -\lambda_{sc}^{TK}(r_D)$

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### Partial screening of high-Z elements and RF current drive

Open-ADAS ; Z<sub>ion</sub> = 20, 30, 40 ; 0.3 keV ; 3 keV ; Z keV

- The Coulomb logarithm term predominates over the screening term except for weakly ionized Tungsten (Z<sub>e</sub> < 20, i.e. < 0.3 keV, electrons lower than 50 keV)
- Partially ionized high-Z impurities may be considered as almost fully screened for RF current drive calculations → standard Fokker-Planck calculations holds for RF-driven discharge (IS-500 keV, T<sub>e</sub> = 1.0 keV)

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### WEST LH (HCRH) discharge #55539

P<sub>tot</sub> = 4.8 MW ; n<sub>0</sub> = 2 ; J<sub>parallel</sub>(@10s) = 0.45 MA

Large effect of partially ionized tungsten on bremsstrahlung level as compared to the fully screened approximation

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### Elastic scattering by partially ionized atoms

- Perturbed Hamiltonian :  $H = H_0 + V_{sc}$
- Bare nucleus potential :  $V_{sc} = -\frac{Z e^2}{4 \pi \epsilon_0 r}$
- Bound electrons potential :  $V_{sc} = -\frac{Z e^2}{4 \pi \epsilon_0 r} \phi(x)$  ;  $\phi(x) = 1 - \frac{3}{2} \sqrt{\frac{2}{\pi}} \int_0^x \frac{dx'}{x'^2} \exp(-x')$
- Form factor :  $F_{sc}(q) = \int_0^{x_{0i}} \mu_{sc}(r) \frac{\sin(qr)}{qr} r^2 dr$
- Rutherford scattering cross-section :  $\frac{d\sigma}{d\Omega} = \frac{r_D^2}{4 \pi^2 \sin^4(\theta/2)} (Z_1 - Z_2 - F_{sc}(q))^2$  ;  $\beta = v/c$
- Pitch-angle scattering in Fokker-Planck collision operator

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### Atomic physics : bound electrons density

Density of bound electrons averaged over solid angle for response to a plane wave

Thomas-Fermi ; Yukawa (HFS)

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### Inelastic scattering by partially ionized atoms : ion excitation

The energy loss by excitation of ions over a distance Δx is equivalent of the work of an effective force F<sub>exc</sub> over that distance

Modified Fokker-Planck term :  $F_{exc} = F_{exc}^{exc} + F_{exc}^{ion} = \frac{2 \pi^2}{N_e} \left( \frac{Z_1 - Z_2 - F_{sc}(q)}{q} \right)^2$

Neutral atoms :  $N_e \approx 10 Z_e$  ;  $N_e \approx 10 Z_e$

Hydrogen atom :  $N_e \approx 13.8 Z_e^2$

All ionization states :  $N_e(z_{ion}) \approx \exp\left(\frac{z_{ion}}{z_{ion,crit}} + \beta\right)$

Local Plasma Approximation (DFT or TF) → Z<sub>ion</sub>

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### Summary

- Screening effects of partially ionized high-Z impurities are fully implemented in LUKE kinetic solver and the quantum relativistic bremsstrahlung code RS-X2.
- These rules may be used for side-away (RF-driven) and runaway electrons (disruption) in cold or hot plasmas.
- Very small impact screening of partially ionized high-Z impurities on LH current drive efficiency confirmed by WEST discharge simulations → fully screened ion can be considered in RF calculations.
- Large effect of screening on bremsstrahlung at low photon energies → decoupling between the current density and bremsstrahlung profiles.

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### Inelastic scattering by partially ionized atoms : e- bremsstrahlung

- e- bremsstrahlung (classical limit) :  $\frac{d^2 \sigma}{d\Omega d\Omega'} = \frac{2 \pi^2}{3} \frac{Z_1^2 - Z_2^2}{\sin^4(\theta/2)} \phi(\cos \theta) \sin^2 \theta \sin \theta' \cos \theta'$
- Fully quantum relativistic differential cross-section (Bethe-Heitler, 1<sup>st</sup> Born approx.)
- Radiation intensity is large but Abraham-Lorentz-Dirac reaction force is small

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### Atomic physics : the form factor F(q)

Form factor  $F_{sc}(q) = \int_0^{x_{0i}} \mu_{sc}(r) \frac{\sin(qr)}{qr} r^2 dr$ 

Thomas-Fermi model → cold plasma, -10 eV (post-disruptive runaway electrons)

Yukawa-type model → hot plasma, >100 eV (RF current drive)

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### LH current drive efficiency

T<sub>e</sub> = 1 keV ; T<sub>e</sub> = 5.13 keV

LUKE ; V<sub>parallel</sub> = 4 kV ; V<sub>parallel</sub> = 40 kV ; V<sub>parallel</sub> = 70 kV

Screening effects are decreasing when plasma temperature is increased. Very small impact of screening effects for partially ionized high-Z impurities for LH current drive, confirmed by simulation of WEST LH discharges. Fully screened ions (Open-ADAS) can be used for RF calculations.

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