

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**
 - Mitigates edge plasma-facing components to reduce tritium retention
 - Objects like if 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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Impact of partially ionized atoms on fast electron dynamics and bremsstrahlung

- Atomic physics: Thomas-Fermi model $F(q)$
- Derivation of ionization states (Open-ADAS)
- Simple models (Thomas-Fermi, Yukawa)
- Exact models (DFT calculations)
- Impact of ionization state of any relevant high-Z atom on plasma physics (Ar, Ne, Cu, Fe, W,...) in the Born approximation
- Z = Z - F(q)** (atomic physics form factor F)
- Compton logarithm $\ln(p/\mu)$
- Impact of ionization state on cross-sections
- Cut-off approximation in collision integrals
- Plasma physics : elastic scattering**
 - e-i bremsstrahlung: $Z - Z - F(q)$
 - e-e bremsstrahlung: $n_e - n_e + \sum n_i N_i$
 - Ion scattering: $\lambda_{Debye}^2 \rho_{Debye}$
 - Electron scattering by fast electrons

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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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Elastic scattering by partially ionized atoms

- Weak perturbation theory (Ferry's Golden rule) for the transition probability
- $W = \frac{2\pi}{h} \left| \langle f | \hat{H} | i \rangle \right|^2 \rho_f$
- $\frac{d\sigma}{d\Omega} = \left| \langle f | \hat{H} | i \rangle \right|^2 \frac{\pi^2 N_e^2}{(2\pi)^2 \lambda^2}$
- 1st Born approximation (plane wave scattered from the free electron)

$$|f\rangle = \frac{1}{\sqrt{V}} \int_V \exp(-iq \cdot r) p_{Debye} dr$$

$$\text{Transferred momentum: } q = p_f - p_i = 2p \sin(\theta/2)$$

$$p_{Debye} = \hbar k_{Debye}$$

$$\text{Rutherford scattering cross-section: } \frac{d\sigma}{d\Omega} = \frac{1}{4\pi} \frac{q^2}{4p^2 \sin^2(\theta/2)} (Z_e - F_{Z_{Debye}}(q))^2$$

(pointless electron)

L Pitch-angle scattering in Fokker-Planck collision operator

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Elastic scattering by partially ionized atoms

- Perturbed Hamiltonian: $\hat{H} = \epsilon \hat{I}_{Z_e} + c \hat{U}_{N_e}$
- Bare nucleus potential: $U_{Z_e} = -\frac{Z_e e}{4\pi \epsilon_0 |\mathbf{r}|}$
- Bound electrons potential: $\nabla^2 U_{N_e} = -\frac{Z_e e}{4\pi \epsilon_0 |\mathbf{r}|}$

$$\text{Atomic form factor: } F_{Z_{Debye}}(q) = \int_V \exp(-iq \cdot r) p_{Debye} dr$$

Fourier transform of the bound electron density

$$\text{Rutherford scattering cross-section: } \frac{d\sigma}{d\Omega} = \frac{1}{4\pi} \frac{q^2}{4p^2 \sin^2(\theta/2)} (Z_e - F_{Z_{Debye}}(q))^2$$

(pointless electron)

L Pitch-angle scattering in Fokker-Planck collision operator

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Inelastic scattering by partially ionized atoms : e-i bremsstrahlung

- e-i bremsstrahlung (classical limit): $d^3\sigma = d\Omega B_{Debye} dE \frac{1}{4\pi} \frac{1}{\epsilon^2}$ Photon emission probability
- Full quantum relativistic differential cross-section (Bethe-Hellier, 1st Born approx.):

$$\frac{d^3\sigma_{Z_{Debye}}}{d\Omega dE d\Omega'} = \left(\frac{r_e}{2\pi} \right)^2 (Z_e - F_{Z_{Debye}}(q))^2 \sum_{k=1}^{k=4} B_k$$

$$q^2 = p_f^2 + p_i^2 - 2p_f p_i \cos \theta - 2p_f p_i \sin \theta \cos \phi$$

$$B_1 = \frac{1}{(Z_e - F_{Z_{Debye}}(q))^2} (4E_e^2 - q^2)$$

$$B_2 = \frac{p_f^2 \sin^2 \theta}{(Z_e - F_{Z_{Debye}}(q))^2} (4E_e^2 - q^2)$$

$$B_3 = 2E_e^2 (p_f^2 \sin^2 \theta + p_i^2 \sin^2 \theta - 2p_f p_i \sin \theta \cos \phi)$$

$$B_4 = (p_f^2 - p_i^2) (Z_e - F_{Z_{Debye}}(q))$$
- $\frac{d^3\sigma_{Z_{Debye}}}{d\Omega dE d\Omega'} = \int_{-1}^1 \sin \theta d\theta \int_{-1}^1 d\phi \frac{d^2\sigma_{Z_{Debye}}}{d\Omega' d\Omega}$ Radiation intensity is large but Abrahams-Oiticica reaction force is small

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Atomic physics

- Calculation of the bound electron density averaged over solid angle (form factor).
- Approximate models : Thomas-Fermi or Yukawa simplified atomic models.
- Exact models : numerical quantum calculations based on Density Functional Theory (DFT). Relativistic calculations must be carried out for high-Z elements using the Douglas-Kroll-Hess second order scalar relativistic Hamiltonian and the natural orbital-relativistic correlation basis set.
- Virtual theorem: $\frac{m_Z^2}{2} = \frac{Z_e^2 c^2}{4\pi r_{Debye}^2}$
- Quantum uncertainty principle: $m_Z h = \hbar / r$
- Ne (10) : 0.07, Ar (18) : 0.31, Cu (29) : 0.212, W (74) : 0.54

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Atomic physics: Thomas-Fermi model

- Poisson's equation: $\nabla^2 (\rho_{Debye} - V_{Debye}(r)) = 4\pi \rho_{Debye}(r)$
- Energy variational principle: $\rho_{Debye}(r) = \left(\frac{3}{2} \frac{C_{Thomas}}{r_{Debye}} \right)^{1/2} (V_{Debye}(r) - V_{Debye}(r_c))^{1/2}$
- Thomas-Fermi equation: $\frac{\partial^2 \rho}{\partial r^2} = \frac{\partial^2 \rho}{\partial Z_e^2} \mu_{Debye} - V_{Debye}(r) - \frac{Z_e^2 c^2}{r} \frac{\partial \phi}{\partial r} \quad \chi_e = r/r_{Debye}$
- Normalized Thomas-Fermi neutral atom radius: $a_0 = \frac{1}{4} \left[\frac{9\pi^2}{2Z_e^2} \right]^{1/3}$
- Ion ($Z_e < Z$): $\phi(x_{Debye}) = 0 = 1 - N_e / Z_e \quad x_{Debye} = r_{Debye} / (b_e a_0)$
- Form factor (numerical integration): $F_{Z_{Debye}}(q) = 4\pi \int_0^\infty \rho_{Debye}(r) \frac{q^2}{r^2} \sin \left(\frac{qr}{a_0} \right) dr$

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Plasma physics : elastic scattering

- Modified Rosenbluth potentials by screening effect
- Rutherford scattering cross-section: $\frac{d\sigma}{d\Omega} = \frac{r_e^2}{4p^2 \sin^2(\theta/2)} (Z_e - F_{Z_{Debye}}(q))^2$
- Screening effect
- Fully screening (ion = $F_{Z_{Debye}}(q) = N_e$)

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Partial screening for e-i bremsstrahlung

- Screening effects significant when $r_{max}/a_{Debye} \gg 1$ where $r_{max} = \frac{a_{Debye}}{q_e}$ (max. impact parameter)
- Equivalent to Bethe estimate (using Thomas-Fermi model) $\frac{E_0}{E} = \frac{1.088}{2 - \frac{1}{q_e}}$
- Screening effect on bremsstrahlung. Target (e-10)

$$HXR \propto Z_e^2 n_e^2 \text{ with fs} > 1$$

$$HXR \propto Z_e^2$$

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Fokker-Planck collision operator with partially ionized atoms

- Fokker-Planck screening function: $\int_{-1/2}^{1/2} (Z_e - F_{Z_{Debye}}(q))^2 \frac{dx}{x} = Z_e^2 \ln A_e + g_{Z_{Debye}}(p)$
- $g_{Z_{Debye}}(p) = \int_{-1/2}^{1/2} (Z_e - F_{Z_{Debye}}(q))^2 \frac{dx}{x}$

which reduces to

$$g_{Z_{Debye}}(p) = \frac{Z_e^2}{n} \ln \left(1 + (p/a_{Debye})^2 \right) - \frac{1}{1 + (p/a_{Debye})^2}$$

for simplified atomic models with $n = 3/2$ for Thomas-Fermi-Killilow model or $n = 2$ for Yukawa (Tseng-Pratt) model. Condition of validity always fulfilled:

$$p \ll a_{Debye}/2$$

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Fokker-Planck collision operator with partially ionized atoms

- Exact DFT calculations with $N_e = Z_e - Z_{Debye}$
- $g_{Z_{Debye}}(p) = (Z_e^2 - Z_{Debye}^2) / (2p/\alpha + \eta_{EM} - 1) + 2Z_e N_e \tilde{I}_{Z_{Debye}} + N_e^2 \left(\frac{1}{2} - \tilde{I}_{Z_{Debye}} \right)$
- $\tilde{I}_{Z_{Debye}} = \frac{4\pi}{N_e} \int_{-1/2}^{1/2} \tilde{\rho}_{Z_{Debye}}(r_1) r_1^2 \ln dr_1$
- $\tilde{I}_{Z_{Debye}} = \frac{4\pi^2}{N_e^2} \int_{-1/2}^{1/2} \tilde{\rho}_{Z_{Debye}}(r_1) \tilde{\rho}_{Z_{Debye}}(r_2) r_1 r_2 dr_1 \int_{-1/2}^{1/2} \tilde{\rho}_{Z_{Debye}}(r_2) r_2 dr_2 \left((r_1 + r_2)^2 \ln(r_1 + r_2) - (r_1 - r_2)^2 \ln(r_1 - r_2) \right)$

In the high velocity limit: $\tilde{I}_{Z_{Debye}} = \frac{2}{\alpha} \exp \left(\eta_{EM} - \frac{2Z_e \tilde{I}_{Z_{Debye}} + N_e (1 - \tilde{I}_{Z_{Debye}})}{Z_e + Z_{Debye}} \right)$

may be obtained from DFT for simplified atomic models with $n = 7/6$ for Thomas-Fermi-Killilow model or $n = 1$ for Yukawa (Tseng-Pratt) model. (Consistent with direct fit of the form factor)

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Partial screening for e-i bremsstrahlung

- Three methods (matlab script for RS-X2 code) for integrating the five differential bremsstrahlung cross-section (IBS Koch & Motz formula) on the scattered electron emission angles to obtain ZBM formula with screening effects
- $\frac{d^2\sigma_{Z_{Debye}}}{d\Omega_1 d\Omega_2} = \alpha \left(\frac{r_e}{2\pi} \right)^2 (Z_e - F_{Z_{Debye}}(q))^2 \frac{p}{k_B T_e^2} \frac{1}{\sqrt{1 - \frac{p^2}{E_0^2}}}$
- $p^2 = p_f^2 + p_i^2 + k^2 - 2p_f k \cos \theta_0 - 2p_i k \cos \phi - 2(p_f \cos \theta_0 + p_i \sin \theta_0) \cos \phi$
- Integration of full 5-6 blocks (k, θ_0, p, ϕ) → arbitrary form factor, fast but very memory demanding.
- Integration of full 4-4 blocks (k, θ_0, p, ϕ) → loop for θ integration : arbitrary form factor, slow but accurate.

Integrations of full 4-4 blocks (k, θ_0, p, ϕ) → parallel integration in azimuthal angle ϕ . Photon energy and angle θ → parallel integration in θ . Numerical results to evaluate analytically → Table of Legendre polynomials cross-section for each element and ionization state with electron kinetic energy interpolation in RS-X2 code.

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

- The Coulomb logarithm term predominates over the screening term for weakly ionized Tungsten ($Z_e < 20$, $T_e = 0.3$ 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 (0.200-1000 keV, 10-100 kA)

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WEST LH (+ICRH) discharge #55539

$P_{RF} = 4.8 \text{ MW}$

$n_{Debye} = 2$

$J_{RFET}(\tau=10s) = 0.45 \text{ MA}$

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

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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 very 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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