DE LA RECHERCHE À L'INDUSTRIE

A unified description of the atomic physics for electron Fokker-Planck calculations

Y. Peysson[1*], D.Mazon[1]
J. Bielecki[2], D. Dworak[2], K. Król[2], A. Jardin[2], M. Scholz[2], J. Walkoviak[2], J. Decker[3]

[1]CEA/IRFM, F-13108, Saint-Paul-lez-Durance, France
[2]Institute of Nuclear Physics, Polish Academy of Sciences, PL-31342, Kraków, Poland
[3]EPFL, Swiss Plasma Center, CH-1015 Lausanne, Switzerland

* yves.peysson@cea.fr

www.cea.fr

Context

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

- ***Passive sources → plasma-wall interactions***
  - Tungsten-based plasma-facing components (planned to be used in the ITER tokamak reactor for reducing tritium retention)
  - Metallic objects in contact with the scrape-off layer like : RF antennas (Copper, Iron,…)
- ***Active sources → massive gas injection***
  - Mitigation of a runaway electron beam after a major disruption in the ITER tokamak reactor (Argon, Neon, …)

C. Bourdelle, et al., Nucl. Fusion, 55 (2015) 063017

A. Stahl, et al., Nucl. Fusion, 56 (20166) 112009

Partially ionized atoms in tokamak plasmas

- High-Z atoms have the property to be partially ionized from the core to the edge of the plasma.

- The distribution of the screened charge $Z_{0,s}$ (for an atom of species *s*) is therefore a function of the local plasma temperature.

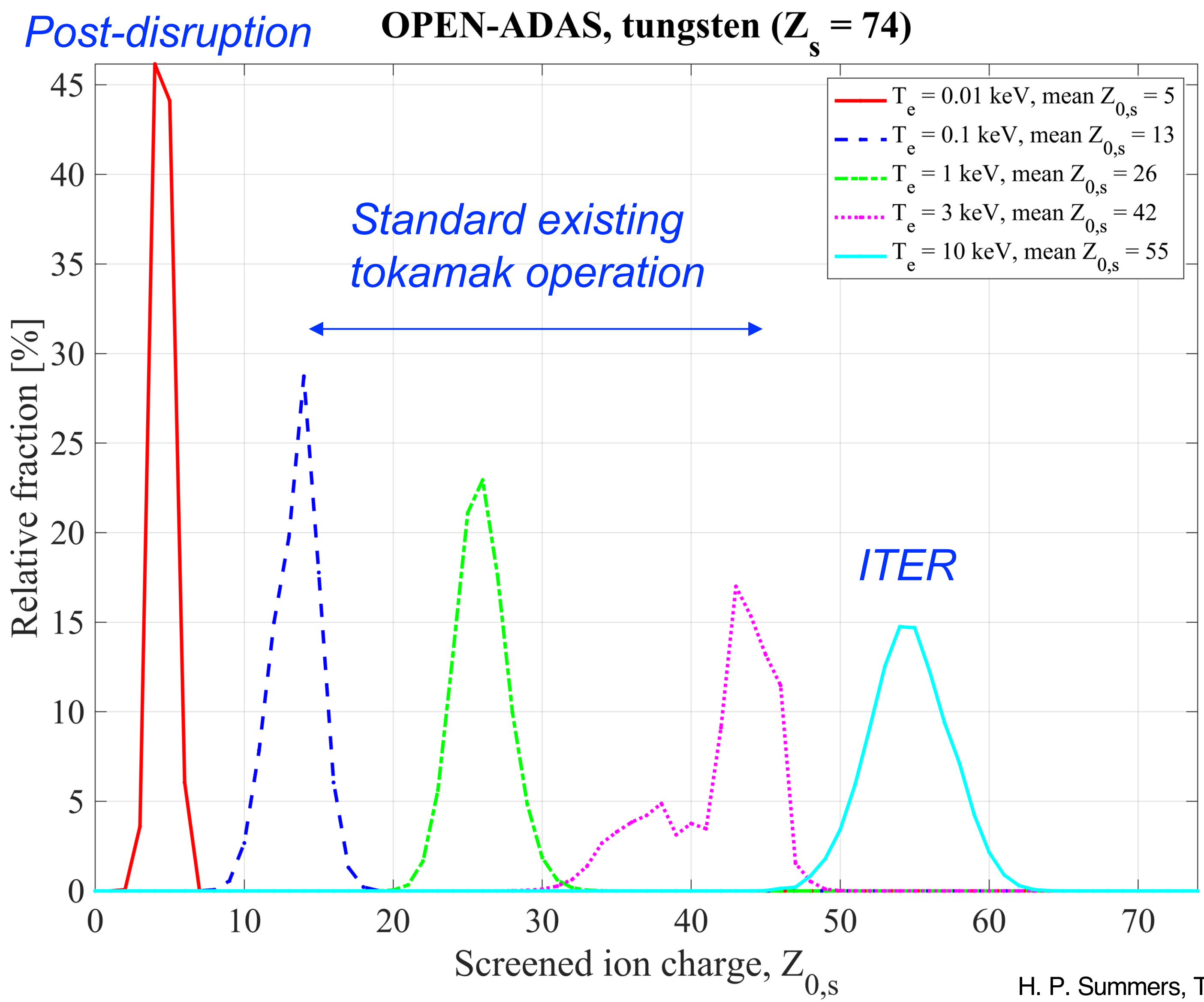
- Fast electrons will interact differently with bound electrons depending upon their kinetic energy → **the partial screening effect**.

- Calculations that describe the fast electron dynamics in momentum and configuration spaces must incorporate this new effect *in the electron-ion collision Fokker-Planck operator, <u>for all species present in the plasma and whatever their ionization state :</u>*

  - Very wide range of plasma temperatures : 10 eV *(disruption)* to 10 keV *(ITER)*

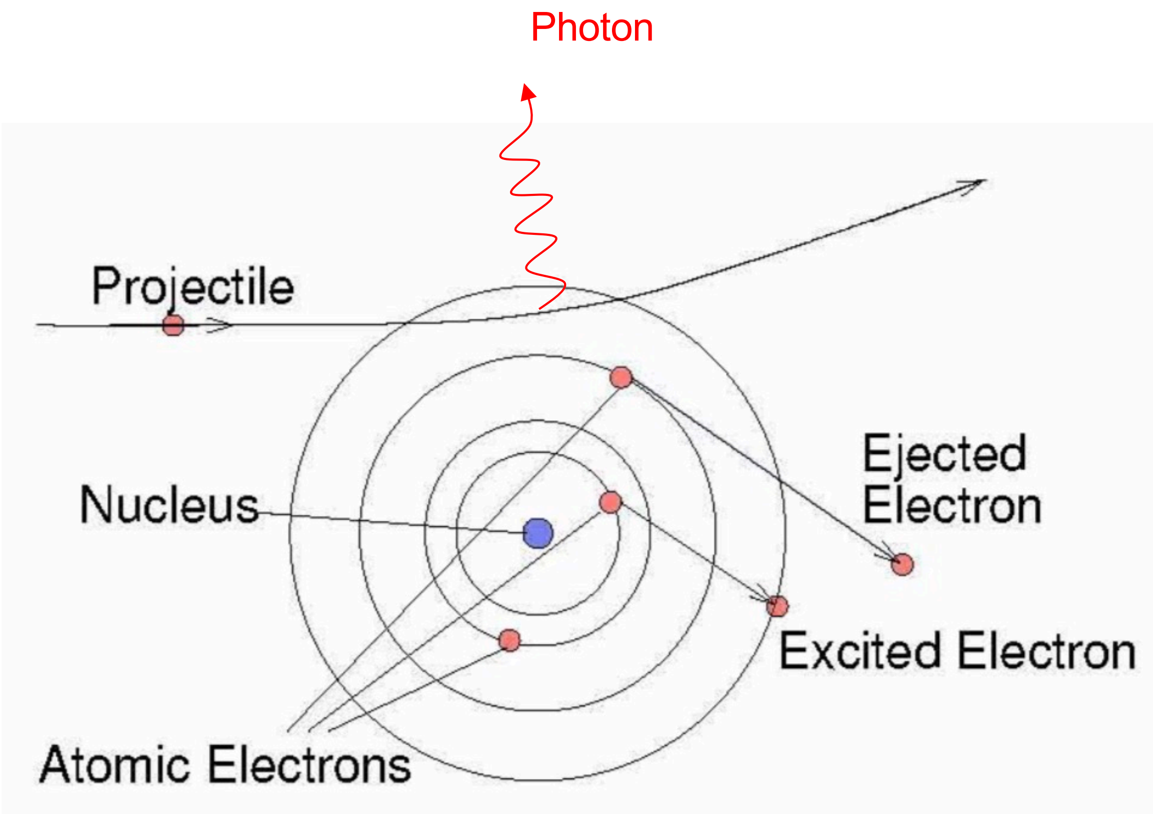
  - Very wide range of electron kinetic energies : 10-100 eV to ~10 MeV *(runaway electrons)*

Distribution of ionization states in a Maxwellian plasma

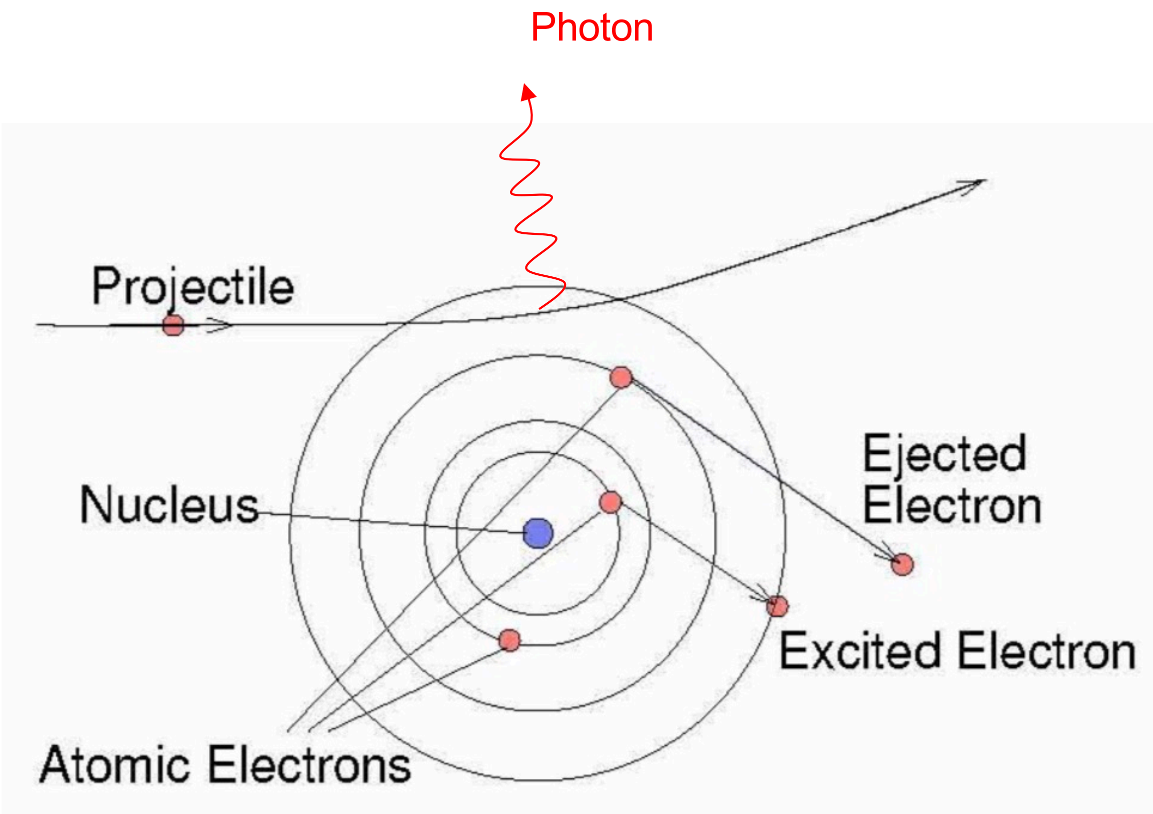


H. P. Summers, Technical report, ADAS (2004)

Impact of partially ionized atoms on magnetized tokamak plasma physics

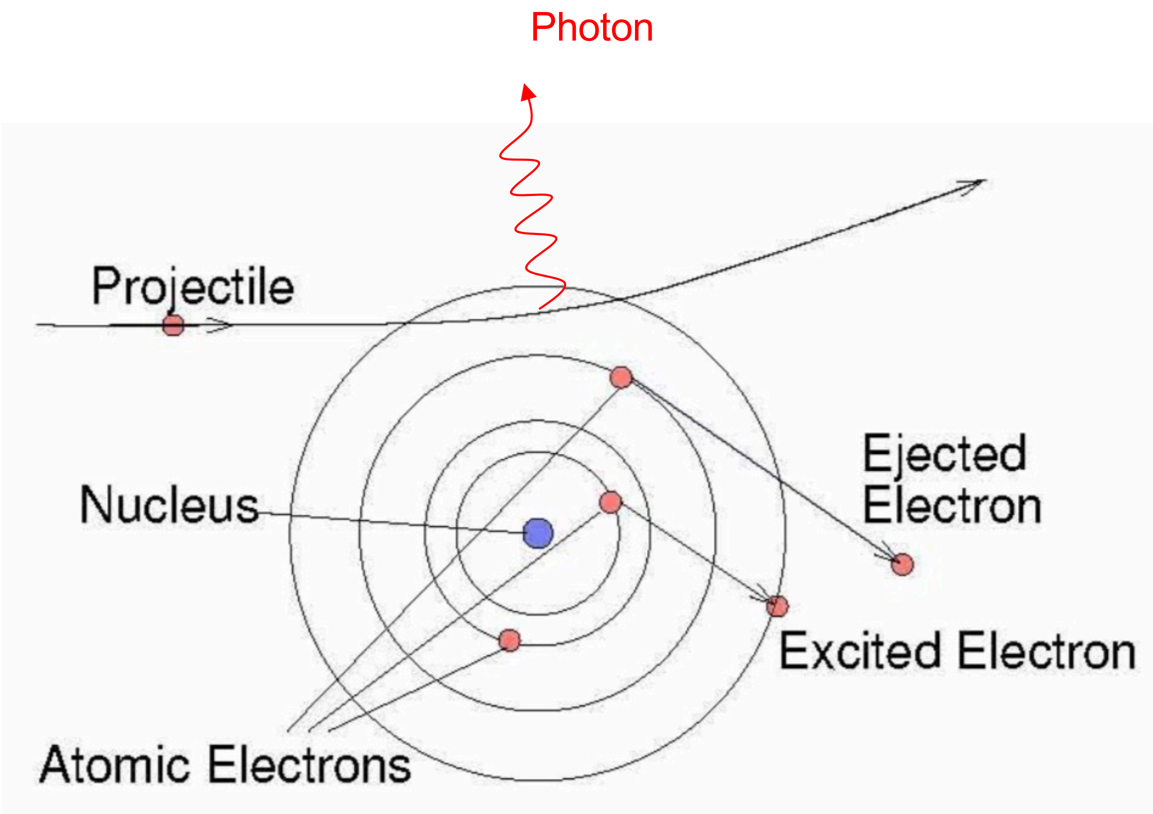


Impact of partially ionized atoms on magnetized tokamak plasma physics



Elastic scattering

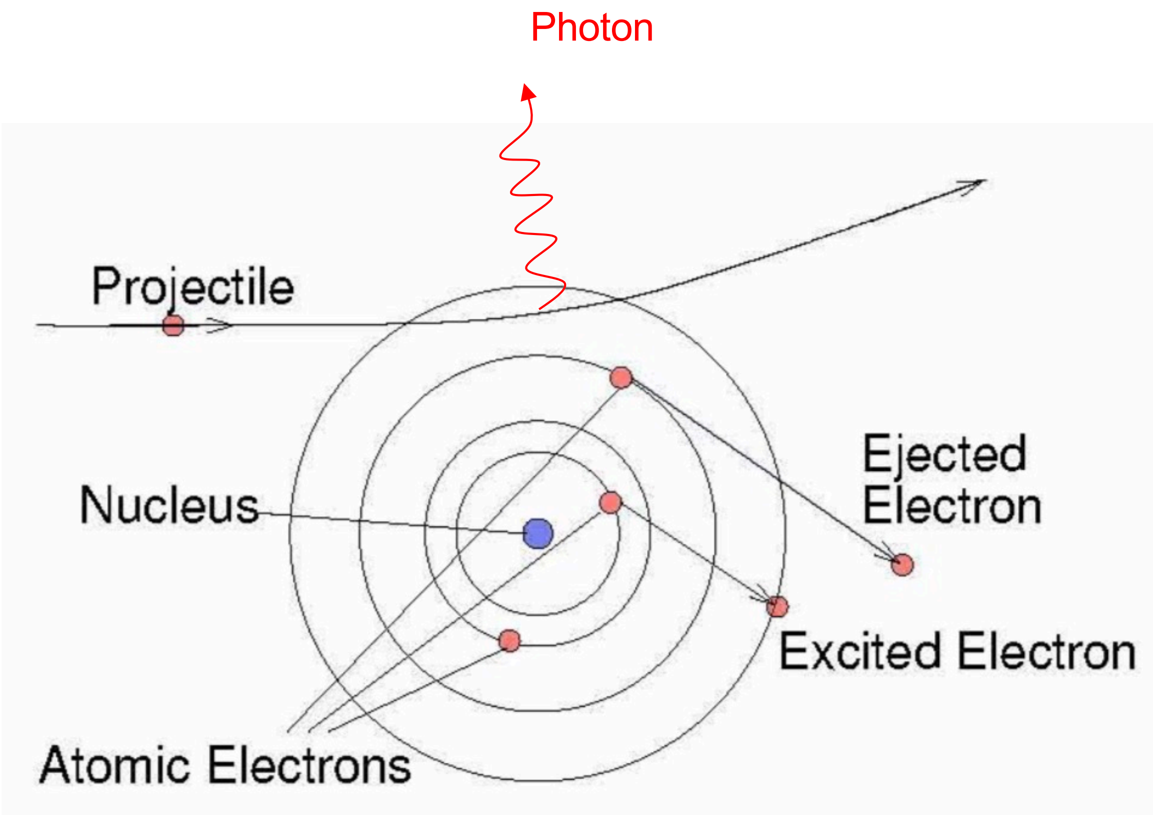
Impact of partially ionized atoms on magnetized tokamak plasma physics



Elastic scattering

Inelastic scattering

Impact of partially ionized atoms on magnetized tokamak plasma physics

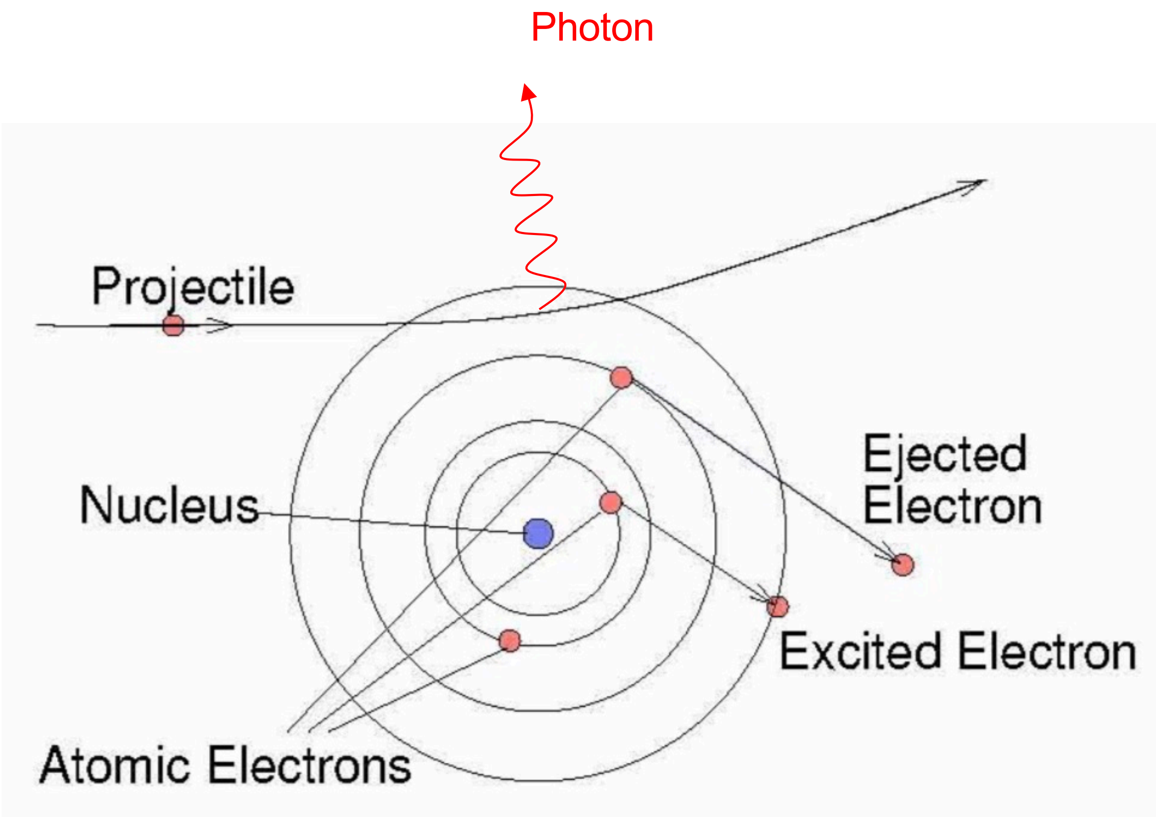


Elastic scattering

Ionization

Inelastic scattering

Impact of partially ionized atoms on plasma physics



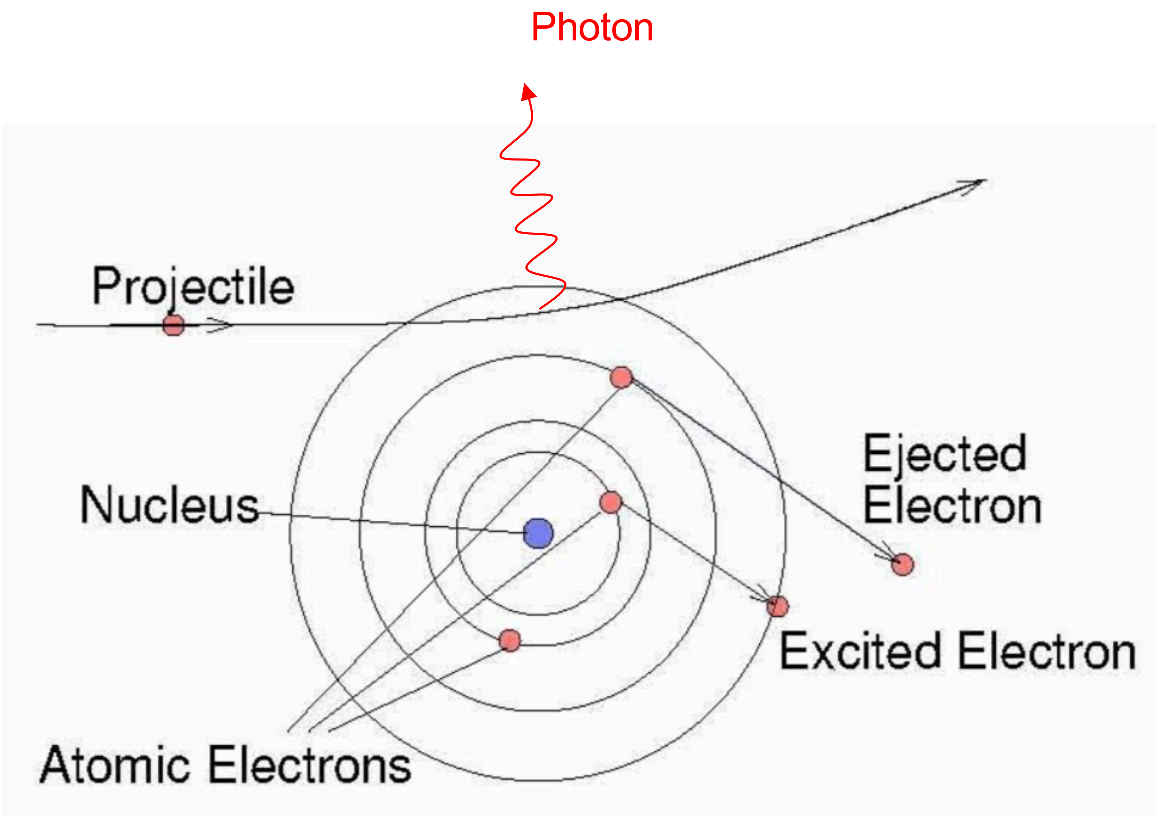
Bremsstrahlung

Elastic scattering

Ionization

Inelastic scattering

Impact of partially ionized atoms on magnetized tokamak plasma physics



Bremsstrahlung

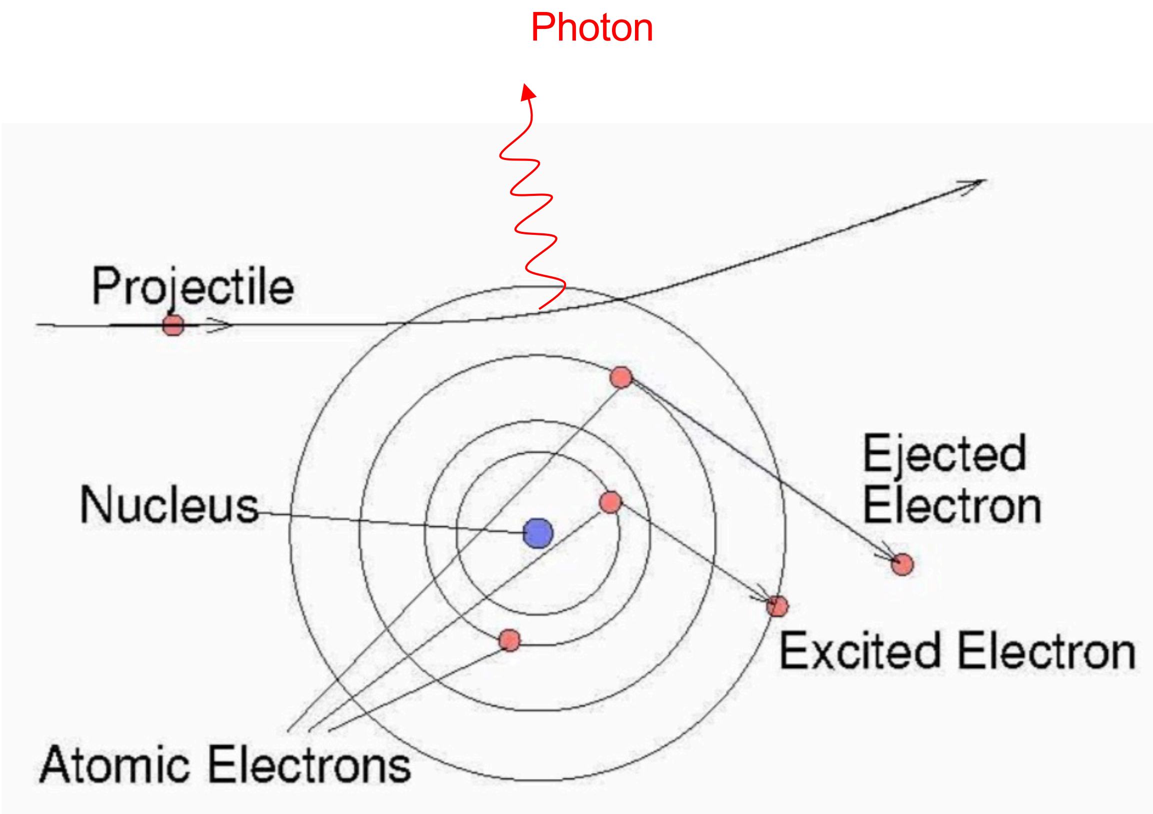
Elastic scattering

Ionization

Inelastic scattering

Line emission

Impact of partially ionized atoms on magnetized tokamak plasma physics



Bremsstrahlung

Elastic scattering

Ionization

Inelastic scattering

Line emission

- Partially ionized atoms are like in vacuum : $\langle r \rangle \ll n_e^{-1/3}$
- Partially ionized atoms are principally in the ground state : $\nu_{coll} \times \tau_{lifetime} \ll 1$

Partially ionized high-Z atoms and electron-ion collisions

Elastic scattering and screening effect

- e-i collisions dominated by small angle deflections → 1st Born approximation
- Screening effect : $Z_{0,s} \rightarrow Z_{0,s} - F(\mathbf{q})$ where $F(\mathbf{q})$ is the *atomic form factor* ($\mathbf{q}$ is the recoil momentum)
- $F(\mathbf{q})$ is the Fourier transform of the *density of bound electrons* $\rho(r)$

$$\boxed{F_{Z_{0,s}}(\mathbf{q}) \equiv \int_V \exp\left(-i\mathbf{q}\cdot\mathbf{r}/\hbar\right)\rho_{Z_{0,s}}d\mathbf{r}}$$

Inelastic scattering by atomic excitation

- Bethe's stopping-power for energy losses
- *Mean excitation energy* $\langle\hbar\omega_s\rangle$, function of the *density of bound electrons* $\rho(r)$

$$\boxed{\left\langle \hbar\omega_{Z_{0,s}}\right\rangle = \left(1/Z_{0,s}\right)\sum_{ik} f_{ik}\ln\left(\hbar\omega_{ik}\right)}$$

U. Fano and J. W. Cooper, Rev. Mod. Phys., 40(3) (1968) 441-507

The density of bound electrons ρ(r)

- Incorporating the physics of partially ionized high-Z atoms in Fokker-Planck calculations requires to know *the density of bound electrons for each species and each ionization state.*

- Fast and accurate time-dependent Fokker-Planck calculations for wide parameter ranges, $T_e \in \{10\text{-}10^4\}$ eV and $E_c \in \{10^{-2}\text{-}10^3\}$ keV, requires analytical expressions for the partial screening in the collision operator → *simplified analytic atomic models*

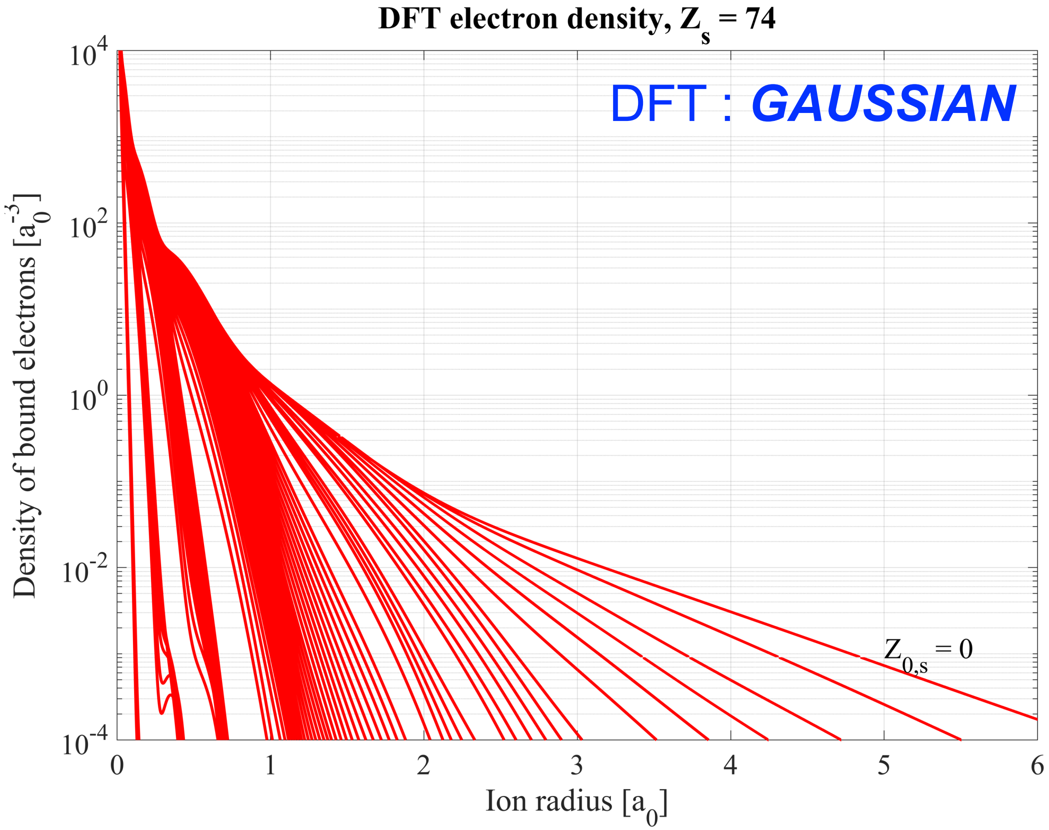
- **Density of bound electrons** :

  - *Ab initio quantum relativistic calculations* : (DFT) Density Functional Theory or (MCDHF) Multi-Configuration Dirac-Hartree-Fock model

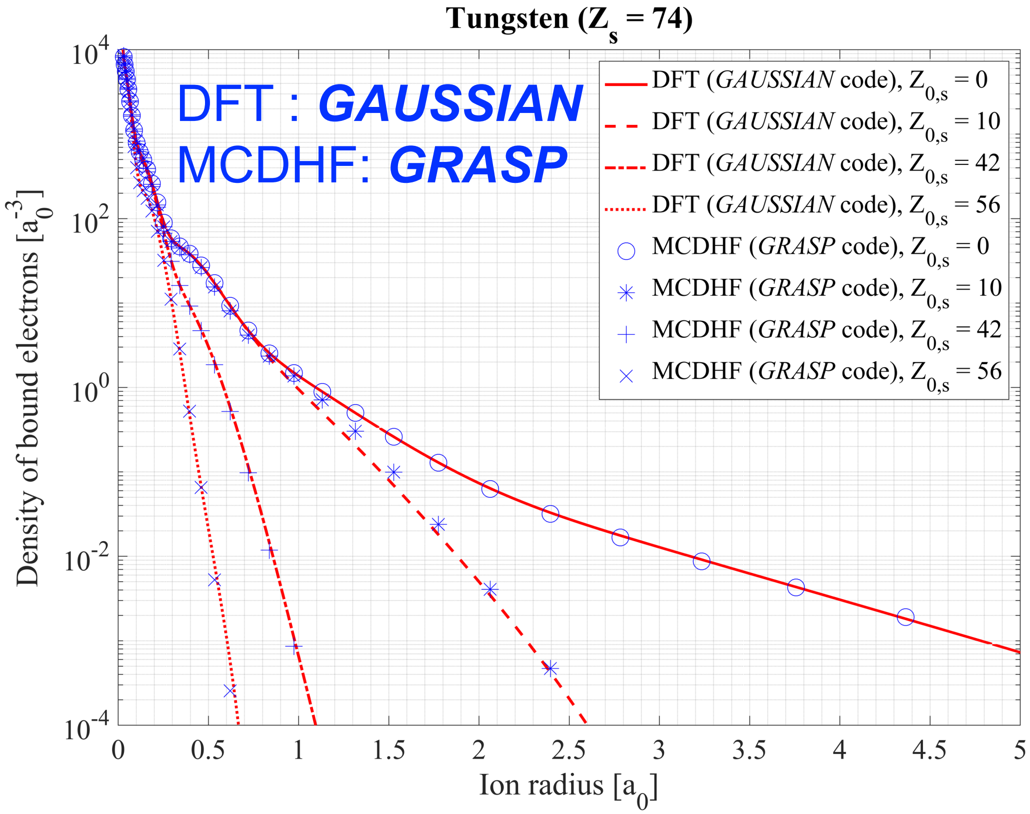
  - *Simplified analytic atomic models* : Thomas-Fermi or Yukawa models → **Problem** : **none of them able to describe consistently the density of bound electrons for all possible ionization states present in the plasma, depending on the tokamak operating regime.**

The density of bound electrons : ab initio codes

DFT : Density functional theory
MCDHF : Multi-Configuration Dirac-Hartree-Fock model



M. J. Frisch, et al., Technical report, Gaussian, Inc., Wallingford CT (2016)

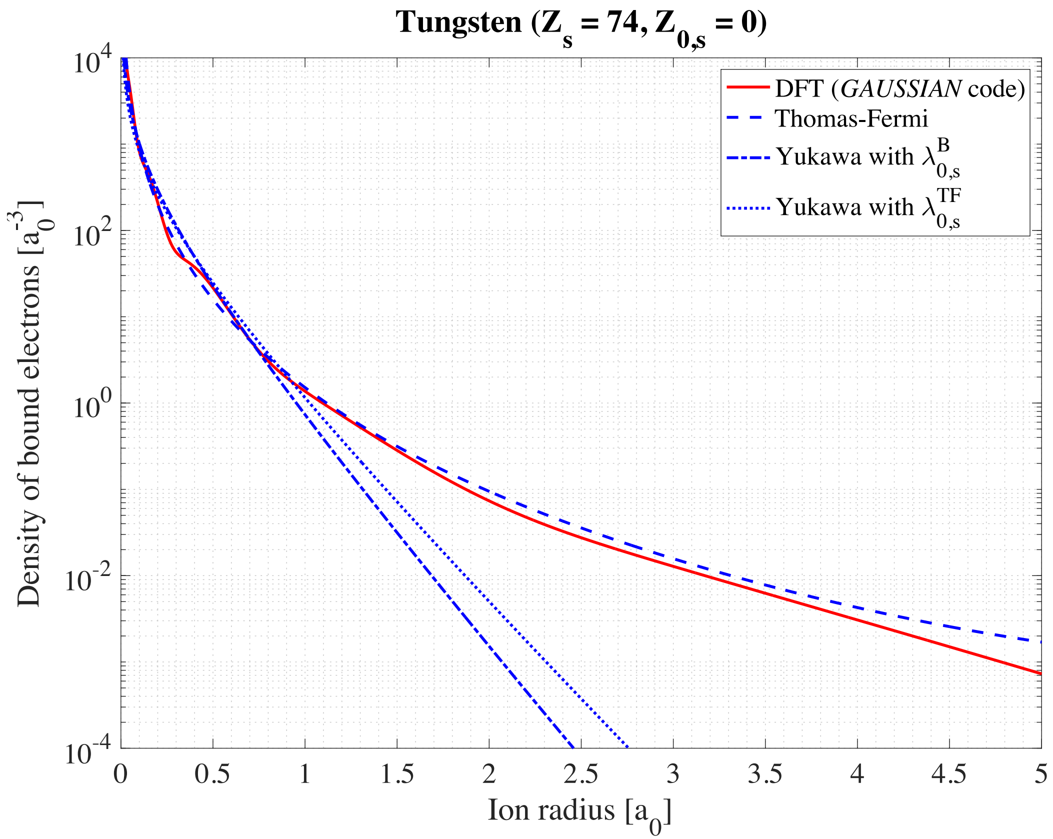


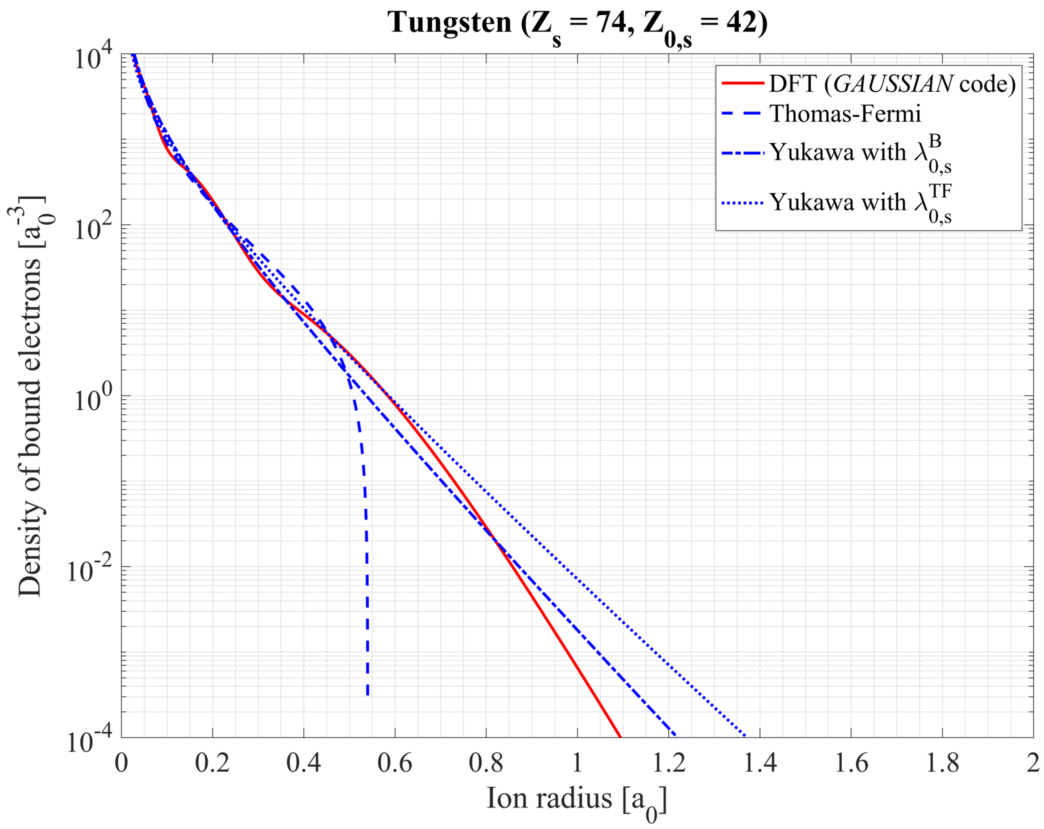
C. Froese Fischer, et al., Computer Physics Comm., 237 (2019) 184–187

Simple atomic models for Fokker-Planck calculations in magnetized tokamak plasmas

Weakly ionized atoms
↓
Thomas-Fermi model

Strongly ionized atoms
↓
Yukawa model





P. Amore, et al., . Applied Math. and Comp., 232 (2014) 929–943

The Multi-Yukawa model for a unified description of the atomic physics

Generalization of the Molière's method initially developed for the Thomas-Fermi model

- **Atomic potential** : $4\pi\epsilon_0 r U_{Z_{0,s}}(r) = -Z_{0,s} - \sum_i A_{Z_{0,s,i}} \exp\left(-\lambda_{Z_{0,s,i}} r\right)$
- Bound electron density by solving the Poisson equation $\nabla^2 U_{Z_{0,s}} = -\rho_{Z_{0,s}}/\epsilon_0$:

$$\boxed{\overline{\rho}_{Z_{0,s}}(\overline{r}) = \frac{Z_s - Z_{0,s}}{4\pi\overline{r}} \sum_i \overline{\lambda}^2_{Z_{0,s,i}} \overline{A}_{Z_{0,s,i}} \exp\left(-\overline{\lambda}_{Z_{0,s,i}}\overline{r}\right)}$$

$$\overline{r} = r/a_0 \qquad \overline{\rho}_{Z_{0,s}}(\overline{r}) = \rho_{Z_{0,s}}(\overline{r})\, a_0^3 \qquad \overline{\lambda}_{Z_{0,s,i}} \equiv \lambda_{Z_{0,s,i}} a_0 \qquad \overline{A}_{Z_{0,s,i}} = A_{Z_{0,s,i}}/\left(Z_s - Z_{0,s}\right)$$

- **Analytic atomic form factor** :

$$\boxed{F_{Z_{0,s}}(\overline{q}) = \left(Z_s - Z_{0,s}\right) \sum_i \frac{\overline{A}_{Z_{0,s,i}}}{1 + \left(\overline{q}\,\overline{a}_{Z_{0,s,i}}/2\right)^2}}$$

$$\overline{q} = q/\left(m_e c\right)$$

$$\overline{a}_{Z_{0,s,i}} \equiv 2\overline{\lambda}^{-1}_{Z_{0,s,i}}/\alpha$$

$\sum_i \overline{A}_{Z_{0,s,i}} = 1$ guarantees that $F_{Z_{0,s}}(0) = Z_s - Z_{0,s} = N_s$

Von Gert Moliere. Zeitschrift Naturforschung, 2a (1947) 133–145

Absolute Multi-Yukawa model calibration

- **Determination of** $\left(\overline{A}_{Z_{0,s,i}}, \overline{\lambda}_{Z_{0,s,i}}\right)$ **is an ill-posed problem.** Standard non-linear regression techniques are useless.

- **Method of moments** : $\boxed{\left\langle \overline{r}^l \right\rangle = \left\langle \overline{r}^l \right\rangle^{num}}$ where $\left\langle \overline{r}^l \right\rangle^{num}$ is determined from ab initio quantum numerical calculations (DFT or MCDHF) → Uniqueness of the solution if it exists.

- Defining $\mathcal{R}_l \equiv \left\langle \overline{r}^l \right\rangle / (l+1)!$ where

$$\mathcal{R}_l = \sum_i \overline{A}_{Z_{0,s,i}} \overline{\lambda}_{Z_{0,s,i}}^{-l}$$

$$\mathcal{R}_l^{num} = \frac{1}{(l+1)!} \frac{4\pi}{(Z_s - Z_{0,s})} \int_0^\infty \overline{r}^{l+2} \overline{\rho}_{Z_{0,s}}^N (\overline{r})\, d\overline{r}$$

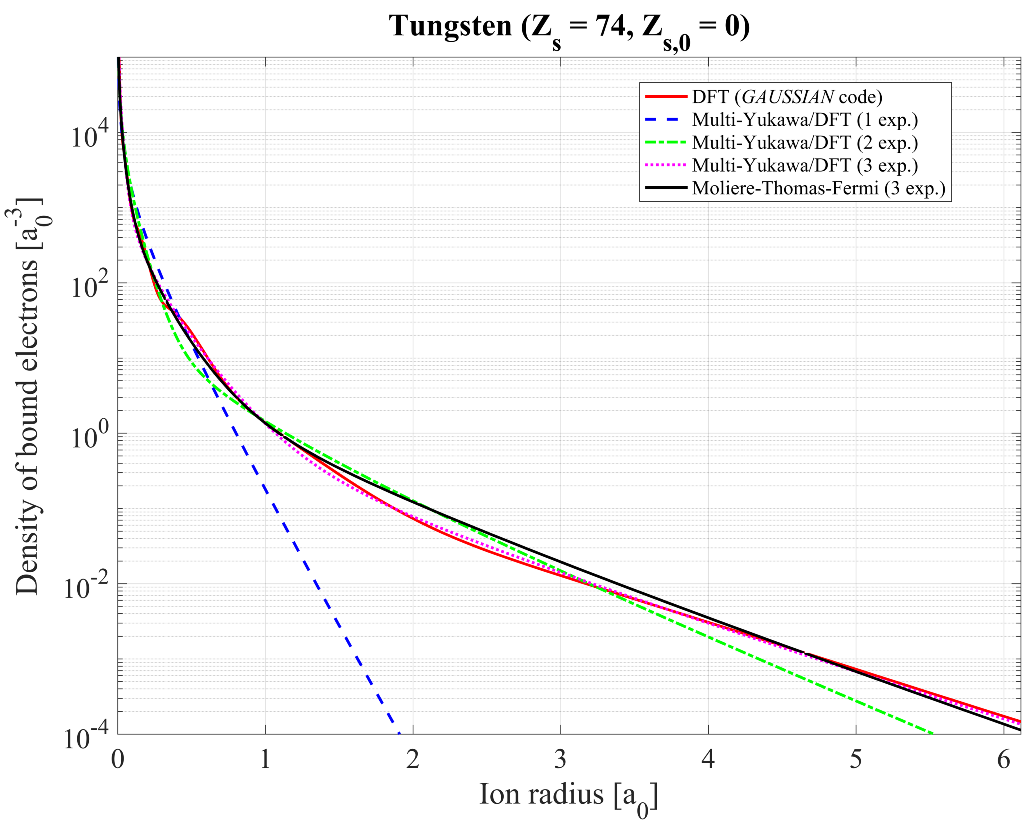
- *2l* equations to be solved, where *l* is the number of exponentials

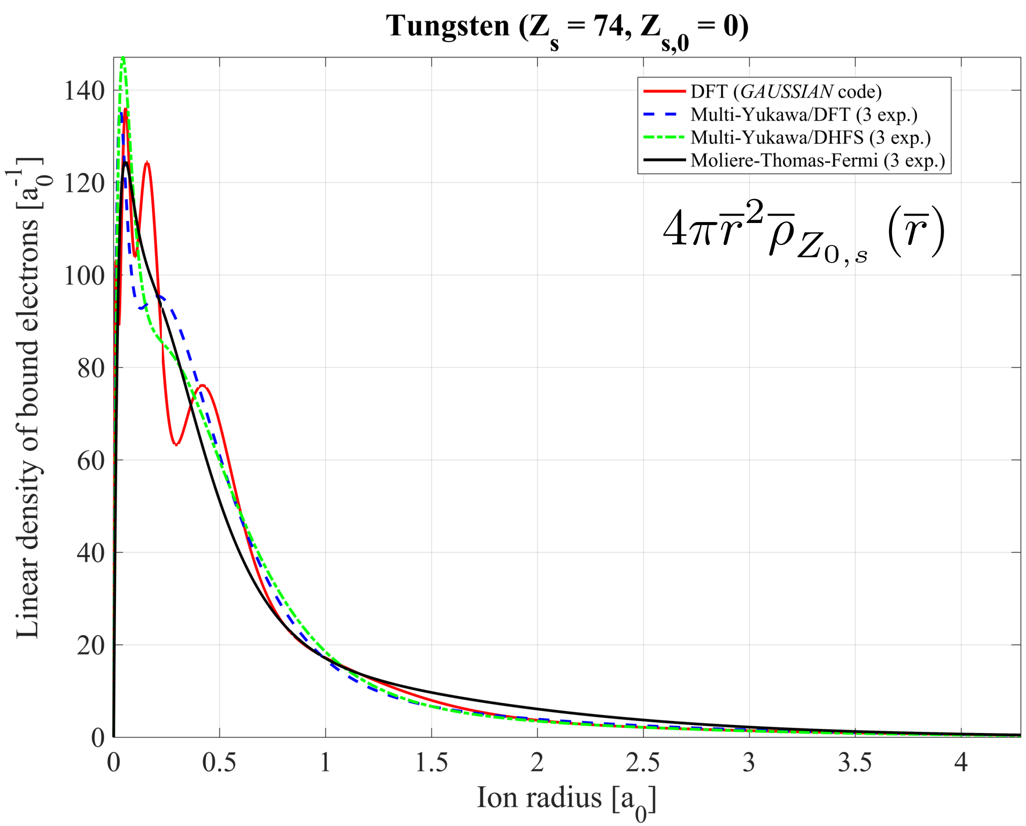
- If no solution found *l* → *l - 1*

F. Salvat, et al., Phys. Rev. A, 36(2) (1987) 467–474

Density of bound electrons (up to 3 exponentials)

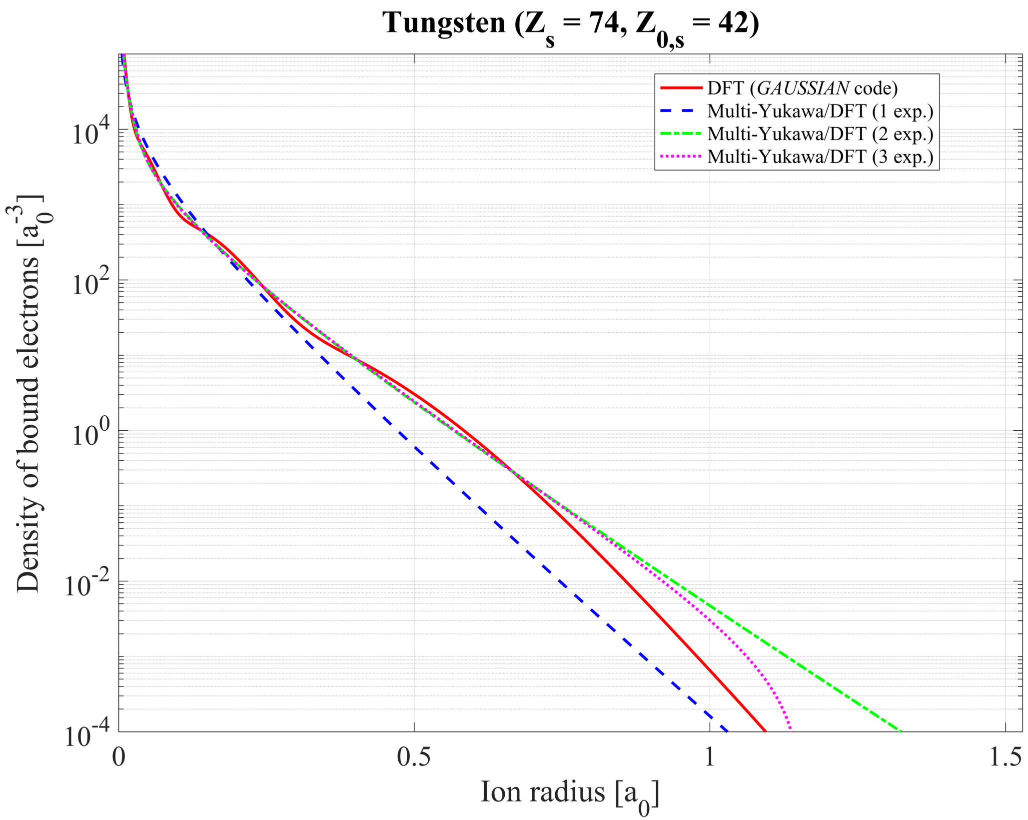
Neutral tungsten $Z_{0,s} = 0$

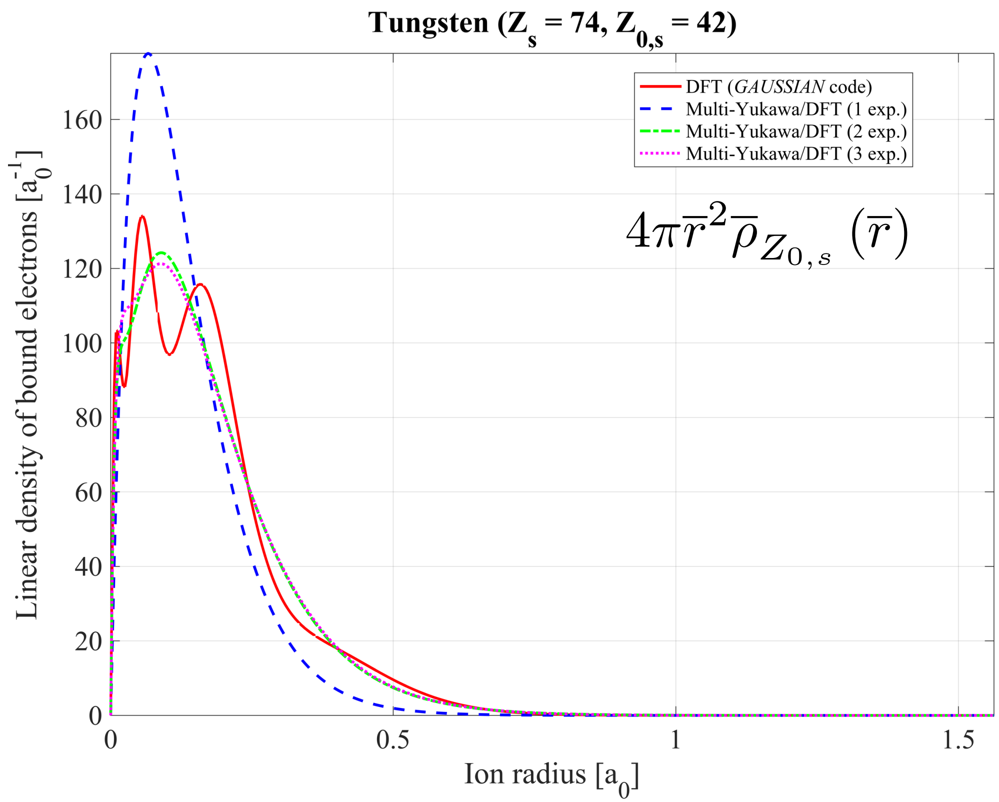




Density of bound electrons (up to 3 exponentials)

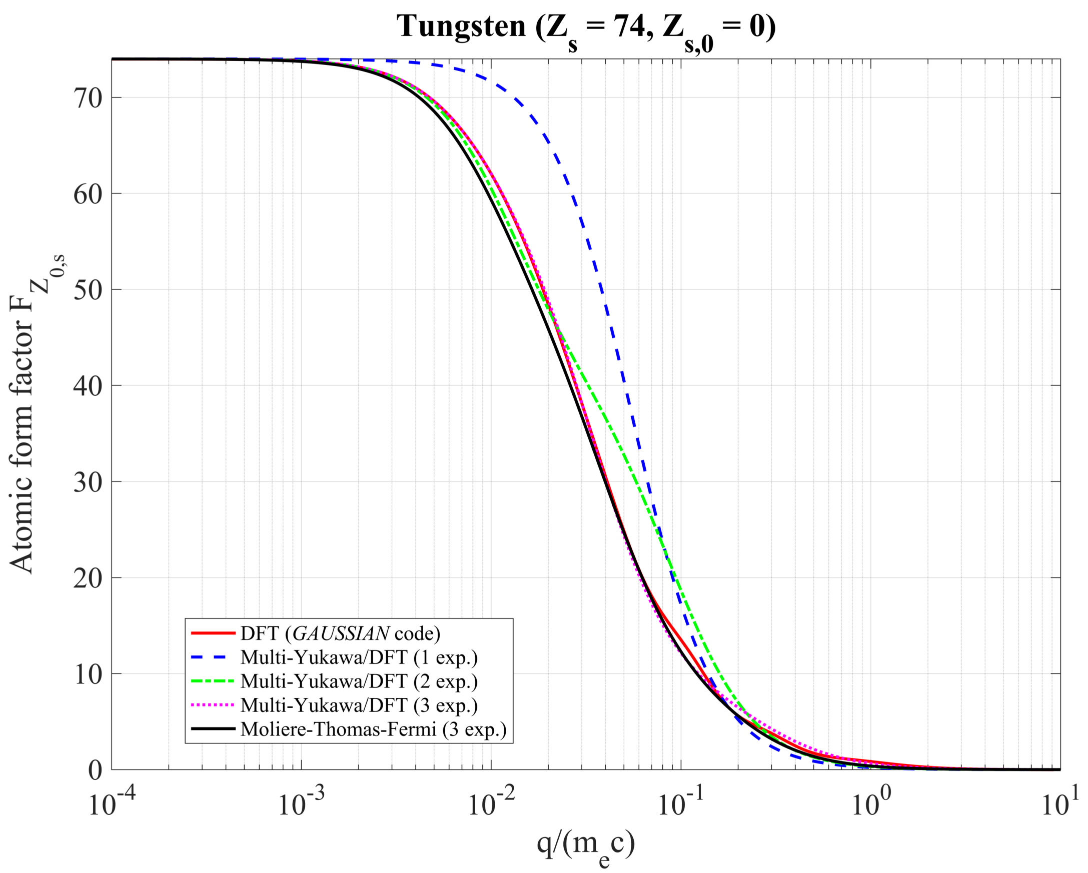
Partially ionized tungsten $Z_{0,s} = 42$



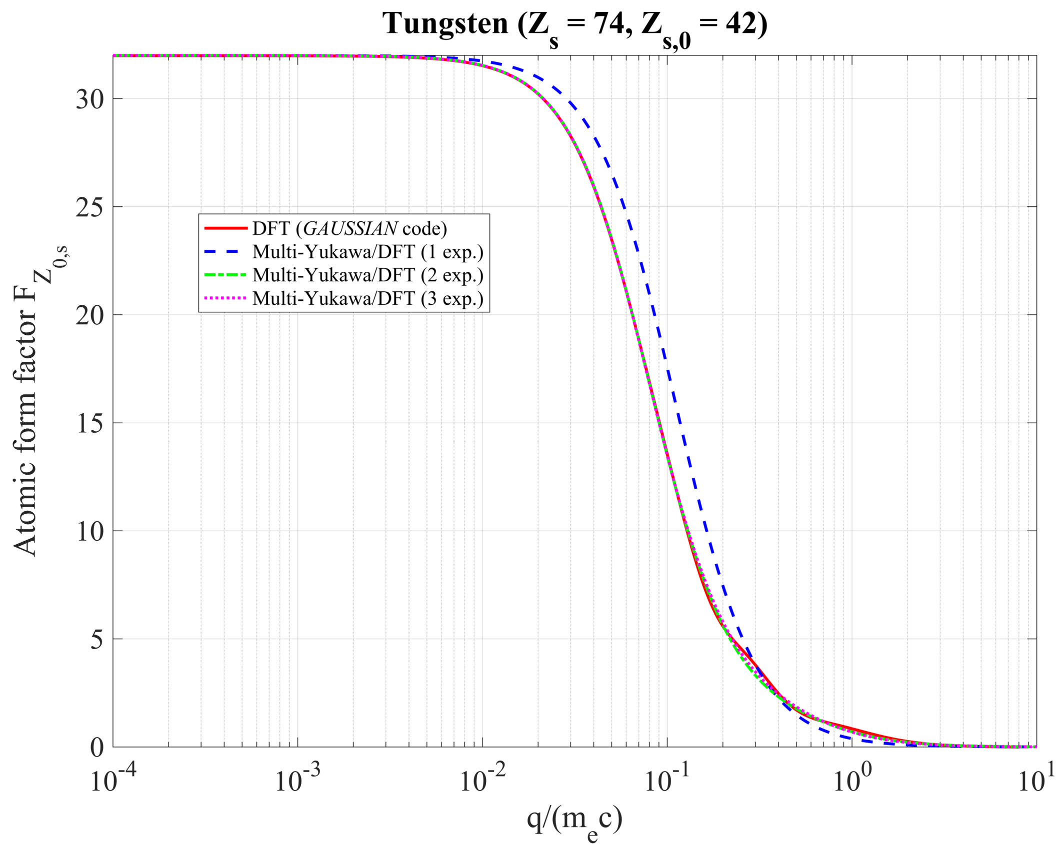


Atomic form factor (up to three exponentials)

Neutral tungsten $Z_{0,s} = 0$

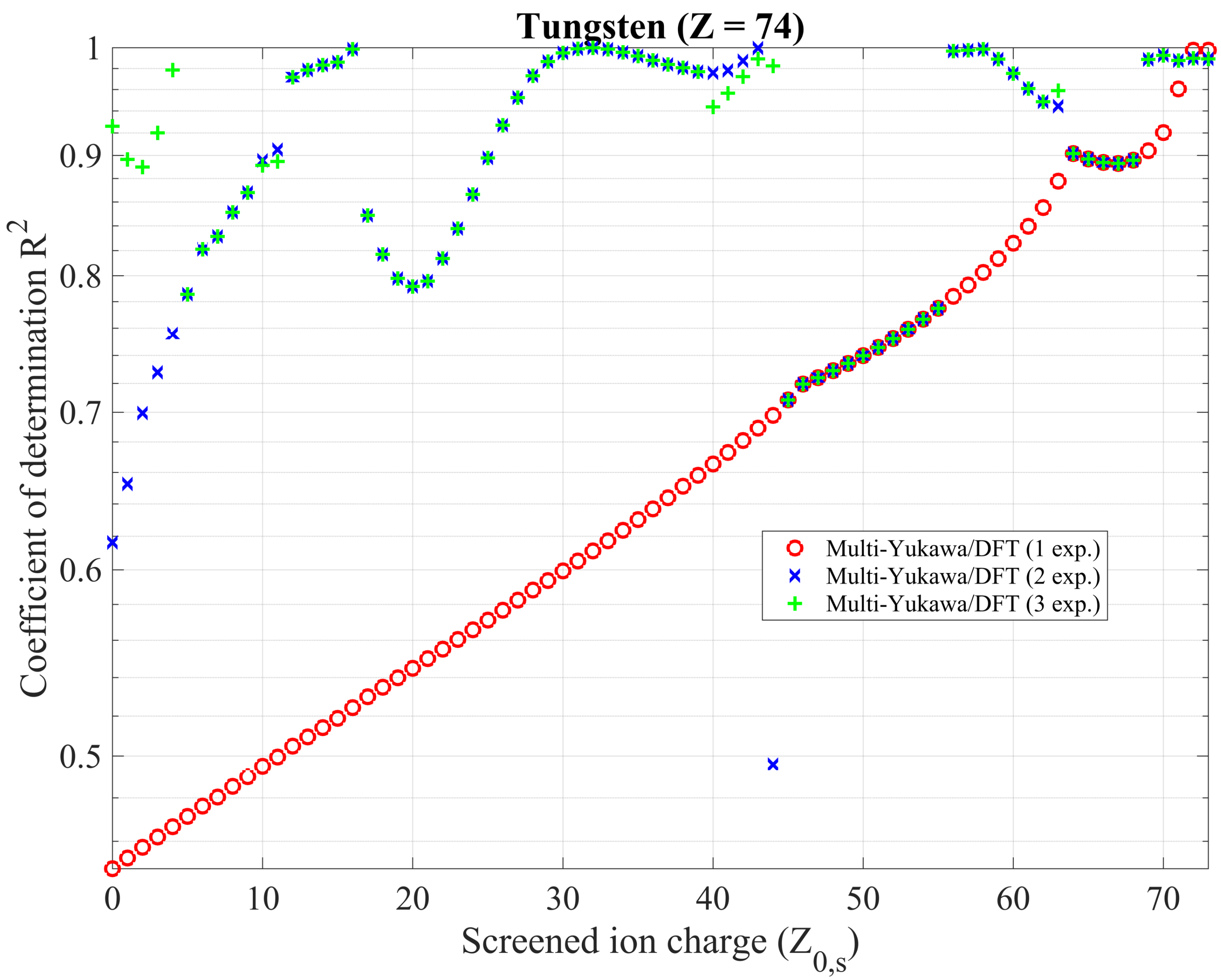


Partially ionized tungsten $Z_{0,s} = 42$



$$F_{Z_{0,s}}(0) = Z_s - Z_{0,s} = N_s$$

Coefficient of determination R^2 for tungsten



The atomic physics in Fokker-Planck calculations

Electron-ion Fokker-Planck collision operator :

$$\boxed{\mathbf{C}_{e,Z_{0,s}}\left(f_e, f_{Z_{0,s}}\right) \simeq -\nabla_p\left(\mathbf{A}_{Z_{0,s}} f_e\left(t,\mathbf{x},\mathbf{p}\right)\right) + \nabla_p\nabla_p\left(\mathbb{D}_{Z_{0,s}} f_e\left(t,\mathbf{x},\mathbf{p}\right)\right)}$$

Friction vector : $\mathbf{A}_{Z_{0,s}} = \int d^3\mathbf{p}_s f_{Z_{0,s}}\left(t,\mathbf{x},\mathbf{p}_s\right)\int d\Omega \boxed{\frac{d\sigma_{e,Z_{0,s}}}{d\Omega}} u_s \triangle\mathbf{p}$

Mott-Rutherford cross-section

Diffusion tensor : $\mathbb{D}_{Z_{0,s}} = \frac{1}{2}\int d^3\mathbf{p}_s f_{Z_{0,s}}\left(t,\mathbf{x},\mathbf{p}_s\right)\int d\Omega \boxed{\frac{d\sigma_{e,Z_{0,s}}}{d\Omega}} u_s \triangle\mathbf{p}\triangle\mathbf{p}^T$

Elastic scattering : Mott-Rutherford cross-section and partial screening effect

Coulomb collision (1st Born approximation) : $$\boxed{\frac{d\sigma_{e,Z_{0,s}}}{d\Omega} = Z_{0,s}^2 \frac{r_e^2}{4} \frac{\left(1-x^2\right)\overline{p}^2+1}{\overline{p}^4 x^4}}$$

Elastic scattering : $|\triangle \mathbf{p}| = 2\,|\mathbf{p}| \sin\frac{\theta}{2} = 2\,|\mathbf{p}|\, x$ $\longrightarrow$ $\bar{q} = 2\bar{p}\sin\left(\theta/2\right)$

Partial screening effect : $$\boxed{Z_{0,s}^2 \rightarrow \left|Z_s - F_{Z_{0,s}}\left(\bar{q}\right)\right|^2}$$

$$\int_{1/\Lambda_{e,Z_{0,s}}}^{1} Z_{0,s}^2 \frac{dx}{x} \longrightarrow \int_{1/\Lambda_{e,Z_{0,s}}}^{1} \left|Z_s - F_{Z_{0,s}}\left(\bar{q}\right)\right|^2 \frac{dx}{x}$$

Coulomb logarithm Screening function

$$\int_{1/\Lambda_{e,Z_{0,s}}}^{1} \left|Z_s - F_{Z_{0,s}}\left(\bar{q}\right)\right|^2 \frac{dx}{x} \equiv \boxed{Z_{0,s}^2 \ln\Lambda_{e,Z_{0,s}}} + \boxed{g_{Z_{0,s}}\left(\overline{p}\right)}$$

L. Hesslow, et al., J. Plasma Phys., 84(6) (2018) 905840605

Atomic physics in LUKE Fokker-Planck solver

Collision operator as a divergence of a flux in momentum space (LUKE code)

$$\boxed{\left.\mathrm{d}f_e/\mathrm{d}t\right|_{coll} \equiv \sum_{s}\sum_{Z_{0,s}} \mathbf{C}_{e,Z_{0,s}}\left(f_e, f_{Z_{0,s}}\right) + \mathbf{C}_{e,e}\left(f_e, f_e\right) \equiv \nabla_{\mathbf{p}} \cdot \mathbf{S}_{\mathbf{p}}^{coll}\left(f_e\right)}$$

Coordinate system

(p, ξ, φ)

$$\begin{cases} S_p^{coll} = -D_{pp}^{coll}\dfrac{\partial f_e}{\partial p} + \dfrac{\sqrt{1-\xi^2}}{p} D_{p\xi}^{coll}\dfrac{\partial f_e}{\partial \xi} + F_p^{coll} f_e \\ S_\xi^{coll} = -D_{\xi p}^{coll}\dfrac{\partial f_e}{\partial p} + \dfrac{\sqrt{1-\xi^2}}{p} \boxed{D_{\xi\xi}^{coll}}\dfrac{\partial f_e}{\partial \xi} + F_\xi^{coll} f_e \end{cases}$$

$D_{p\xi}^{coll} = D_{\xi p}^{coll} = F_\xi^{coll} = 0$ by local axisymmetry

Inelastic scattering

$$D_{pp}^{coll}(e-i) \ll D_{pp}^{coll}(e-e)$$

$$F_p^{coll}(e-i) \ll F_p^{coll}(e-e)$$

Elastic scattering

The transformation

$$Z_{0,s}^2 \ln \Lambda_{e,Z_{0,s}} \rightarrow Z_{0,s}^2 \ln \Lambda_{e,Z_{0,s}} + g_{Z_{0,s}}(\overline{p})$$

is applied to $D_{\xi\xi}^{coll}(e-i)$ only.

J. Decker and Y. Peysson. Report EUR-CEA-FC-1736, Euratom-CEA (2004)

Screening function using the multi-Yukawa model

$$g_{Z_{0,s}}\left(\bar{p}\right) = Z_s\left(Z_s - Z_{0,s}\right)\sum_i \overline{A}_{0,s,i}\ln\left(1+\left(\bar{p}\bar{a}_{Z_{0,s,i}}\right)^2\right)$$

$$-\frac{\left(Z_s - Z_{0,s}\right)^2}{2}\sum_i \overline{A}_{0,s,i}^2\left(\frac{\left(\bar{p}\bar{a}_{Z_{0,s,i}}\right)^2}{1+\left(\bar{p}\bar{a}_{Z_{0,s,i}}\right)^2} + \ln\left(1+\left(\bar{p}\bar{a}_{Z_{0,s,i}}\right)^2\right)\right)$$

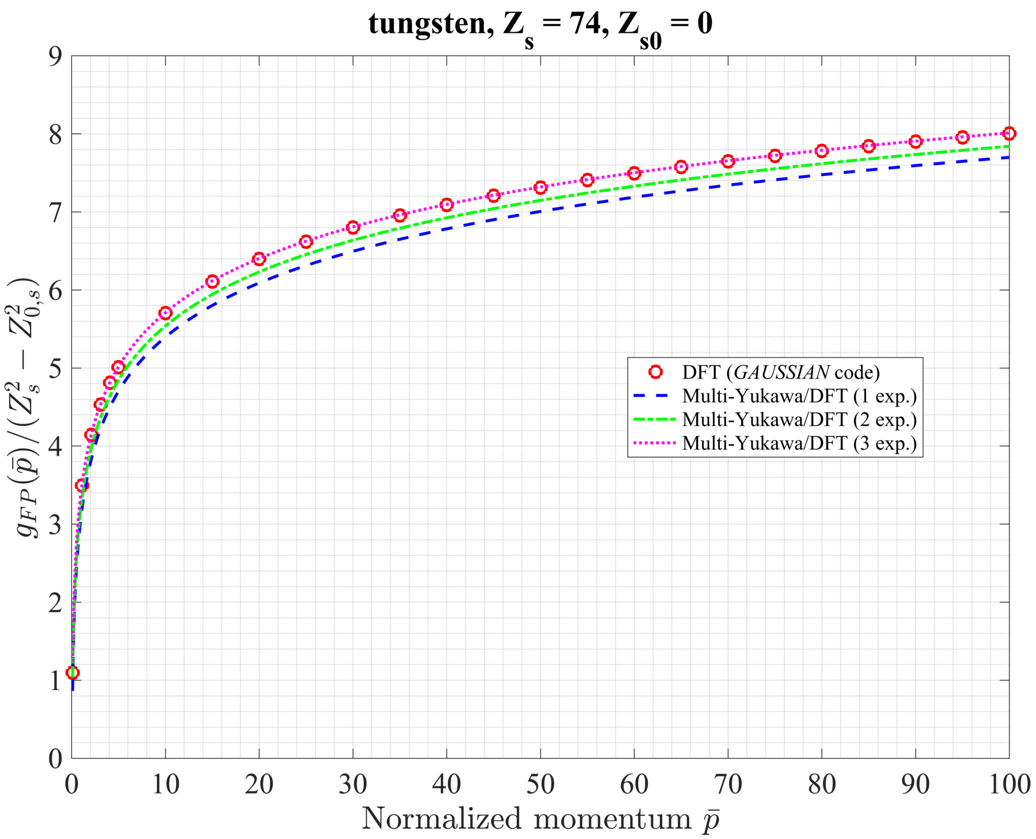
$$+2\left(Z_s - Z_{0,s}\right)^2\sum_i\sum_{j>i}\overline{A}_{0,s,i}\overline{A}_{0,s,j}\boxed{\widetilde{g}_{Z_{0,s},2,i,j}\left(\bar{p}\right)}$$

$$\begin{aligned}
\widetilde{g}_{Z_{0,s},2,i,j}\left(\bar{p}\right) = & \quad -\frac{1}{2}\frac{a^2_{Z_{0,s,i}} + a^2_{Z_{0,s,j}}}{a^2_{Z_{0,s,j}} - a^2_{Z_{0,s,i}}}\ln\left|\frac{1+\bar{p}^2\bar{a}^2_{Z_{0,s,j}}}{1+\bar{p}^2\bar{a}^2_{Z_{0,s,i}}}\right| \\
- & \quad \frac{1}{4}\ln\left|1+\bar{p}^2\left(\bar{a}^2_{Z_{0,s,i}} + \bar{a}^2_{Z_{0,s,j}}\right) + \bar{p}^4\bar{a}^2_{Z_{0,s,i}}\bar{a}^2_{Z_{0,s,j}}\right| \\
+ & \quad \frac{\bar{a}^2_{Z_{0,s,i}} + \bar{a}^2_{Z_{0,s,j}}}{4\left|\bar{a}^2_{Z_{0,s,i}} - \bar{a}^2_{Z_{0,s,j}}\right|} \\
\times & \quad \left[\ln\left|\frac{2\bar{a}^2_{Z_{0,s,i}}\bar{a}^2_{Z_{0,s,j}}\bar{p}^2 + \left(\bar{a}^2_{Z_{0,s,i}} + \bar{a}^2_{Z_{0,s,j}}\right) - \left|\bar{a}^2_{Z_{0,s,i}} - \bar{a}^2_{Z_{0,s,j}}\right|}{2\bar{a}^2_{Z_{0,s,i}}\bar{a}^2_{Z_{0,s,j}}\bar{p}^2 + \left(\bar{a}^2_{Z_{0,s,i}} + \bar{a}^2_{Z_{0,s,j}}\right) + \left|\bar{a}^2_{Z_{0,s,i}} - \bar{a}^2_{Z_{0,s,j}}\right|}\right|\right. \\
- & \quad \left.\ln\left|\frac{\left(\bar{a}^2_{Z_{0,s,i}} + \bar{a}^2_{Z_{0,s,j}}\right) - \left|\bar{a}^2_{Z_{0,s,i}} - \bar{a}^2_{Z_{0,s,j}}\right|}{\left(\bar{a}^2_{Z_{0,s,i}} + \bar{a}^2_{Z_{0,s,j}}\right) + \left|\bar{a}^2_{Z_{0,s,i}} - \bar{a}^2_{Z_{0,s,j}}\right|}\right|\right]
\end{aligned}$$

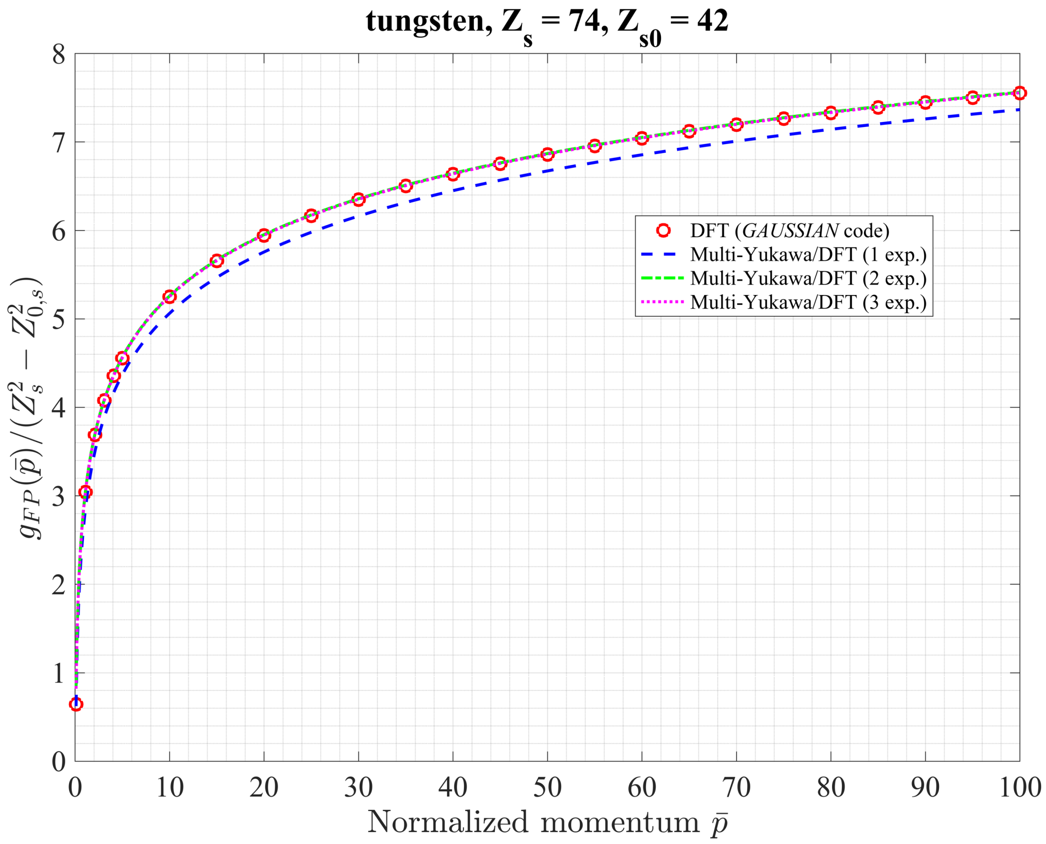
- Fully analytic expression
- Arbitrary number of exponentials

Screening function : comparison between multi-Yukawa model and numerical quantum calculations

Neutral tungsten $Z_{0,s}$=0



Partially ionized tungsten $Z_{0,s}$=42



Drag force by atomic excitation

- Bethe's stopping power formula where the energy E loss is :

$$-\left.\frac{dE}{dx}\right|_{Z_{0,s}} = 4\pi r_e^2 n_{Z_{0,s}} \left(Z_s - Z_{0,s}\right) \frac{m_e c^2}{\beta^2} \left[\ln B_{Z_{0,s}} - \beta^2\right]$$

$$B_{Z_{0,s}} = \frac{\sqrt{2}\gamma\beta\sqrt{\gamma - 1}}{\boxed{\left\langle \hbar\omega_{Z_{0,s}} \right\rangle} / m_e c^2}$$

Atomic physics is described by the mean excitation energy

- Since the energy loss over a distance Δx is equivalent of the work of an effective drag force,

$$\boxed{F_p^{excitation}(p) = -\sum_s \sum_{Z_{0,s}} \left.\frac{dE}{dx}\right|_{Z_{0,s}}}$$

- Incorporation in LUKE Fokker-Planck code : $\boxed{F_p^{coll} = \underbrace{F_p^{e-i} + F_p^{e-e} + F_p^{excitation}}_{\text{Dominant terms}} + F_p^{ALD}}$

$$S_p^{coll} = -D_{pp}^{coll} \frac{\partial f_e}{\partial p} + \frac{\sqrt{1-\xi^2}}{p} D_{p\xi}^{coll} \frac{\partial f_e}{\partial \xi} + \boxed{F_p^{coll}} f_e$$

H. Bethe and W. Heitler. Proceedings of the Royal Society of London, volume A146, (1934) 83–112

Mean excitation energy

- *Mean excitation energy* → $\boxed{\langle \hbar\omega_{Z_{0,s}} \rangle = (1/Z_{0,s}) \sum_{ik} f_{ik} \ln\left(\hbar\omega_{ik}\right)}$
  - f_{ik} : dipole oscillator strength of the transition
  - ω_{ik} : dipole frequency for the transition between |i> and |k> quantum states

Hydrogenoid mean excitation energy :14.99 x Z_s^2 eV

- **Exponential interpolation** : $\ln\langle \hbar\omega_{Z_{0,s}} \rangle \simeq \ln\left(\frac{\boxed{I_H}}{10} Z_s\right)\frac{Z_{0,s}}{Z_s - 1} + \ln\left(\boxed{10 Z_s}\right)$

Bloch relation

- **Local plasma approximation (LPA)** :

$$\ln\langle \hbar\omega_{Z_{0,s}} \rangle = \sum_i \overline{\lambda}^{2}_{Z_{0,s,i}} \overline{A}_{Z_{0,s,i}} \int_0^\infty \overline{r} \exp\left(-\overline{\lambda}_{Z_{0,s,i}}\overline{r}\right)$$
$$\times \ln\left(\sqrt{2}\alpha^2 m_e c^2 \sqrt{\frac{Z_s - Z_{0,s}}{\overline{r}} \sum_j \overline{\lambda}^{2}_{Z_{0,s,j}} \overline{A}_{Z_{0,s,i}} \exp\left(-\overline{\lambda}_{Z_{0,s,j}}\overline{r}\right)}\right) d\overline{r}$$

S. Rosendorff and H. G. Schlaile. Phys. Rev. A, 40(12) (1989) 6892–6896
J. Linhard and M. Scharff. Dan. Mat. Fys. Medd, 27(15) (1953)
W.K. Chu and D. Powers. Phys. Letters, 40A(1) (1972) 23–24, 1972

Mean excitation energy

- **Variational quantum description** : $\left\langle \hbar\omega_{Z_{0,s}} \right\rangle^2 = 2\frac{K_0}{\left\langle \overline{r}^2 \right\rangle}\alpha^2 m_e c^2$

The *averaged kinetic energy of the cloud of bound electrons* K_0 is determined using the virial theorem (non-relativistic limit) : $2K_0 \simeq \left\langle U_{Z_{0,s}} \right\rangle / N_s$

$$\left\langle \hbar\omega_{Z_{0,s}} \right\rangle = \frac{\alpha^2 m_e c^2 \sqrt{N_s}}{\sqrt{6\sum_i \overline{\lambda}^{-2}_{Z_{0,s,i}} \overline{A}_{Z_{0,s,i}}}} \times \sqrt{\sum_i \overline{A}^2_{Z_{0,s,i}} \frac{\overline{\lambda}_{Z_{0,s,i}}}{2} + \sum_i \sum_{j\neq i} \overline{A}_{Z_{0,s,i}} \overline{A}_{Z_{0,s,j}} \frac{\overline{\lambda}^2_{Z_{0,s,i}}}{\overline{\lambda}_{Z_{0,s,i}} + \overline{\lambda}_{Z_{0,s,j}}}}$$

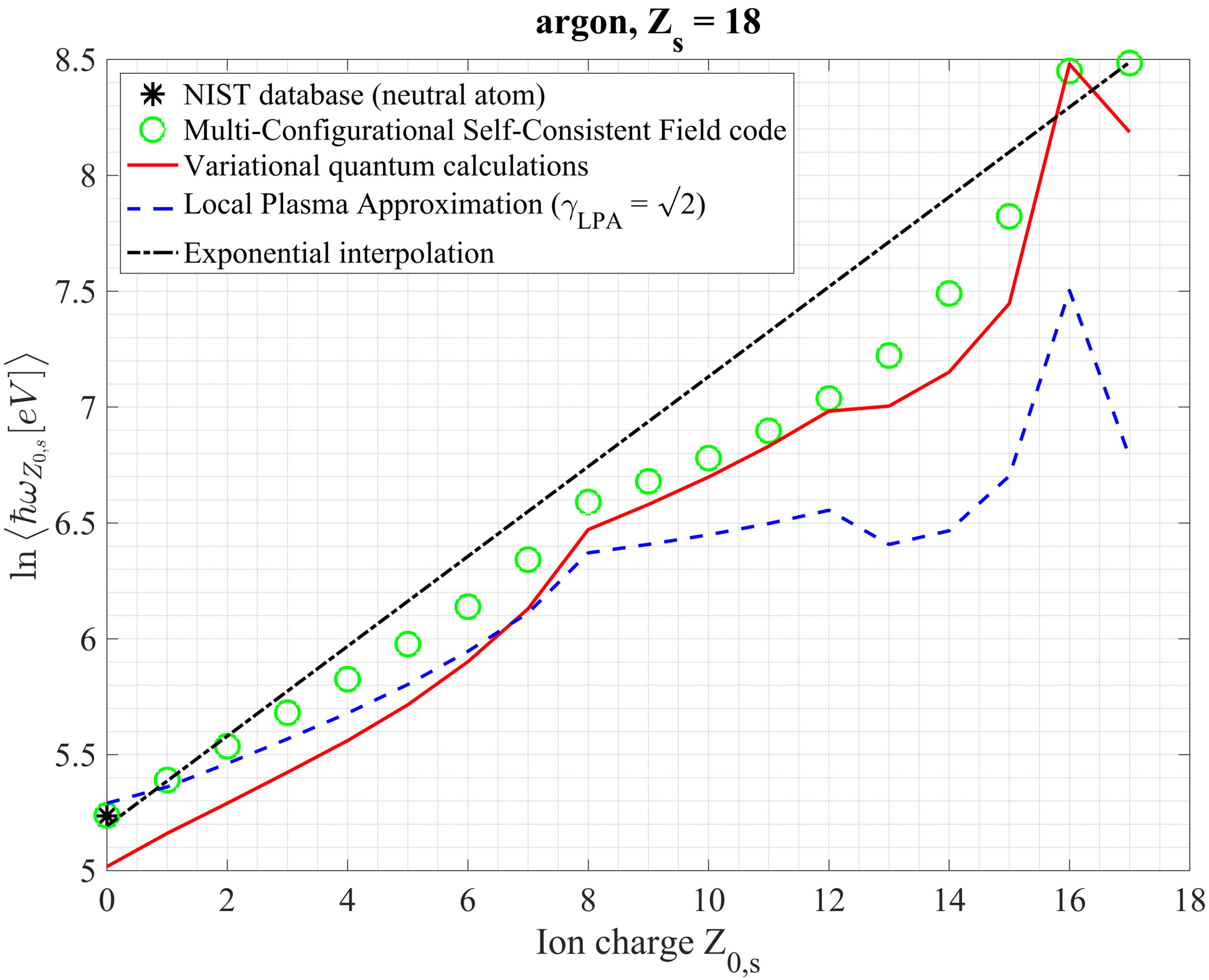
- Single exponential limit : $\left\langle \hbar\omega_{Z_{0,s}} \right\rangle = \alpha^2 m_e c^2 \sqrt{\overline{\lambda}^3_{Z_{0,s,1}} N_s / 12}$
- Thomas-Fermi model for neutral atoms : $\overline{\lambda}_{Z_{0,s,1}} = 1.13 Z_s^{1/3}$

$\left\langle \hbar\omega_{Z_{0,s}} \right\rangle = 9.44 Z_s\, eV$ → *Bloch relation ~ 10Z_s eV is well retrieved*

W.K. Chu and D. Powers. Phys. Letters, 40A(1) (1972) 23–24, 1972

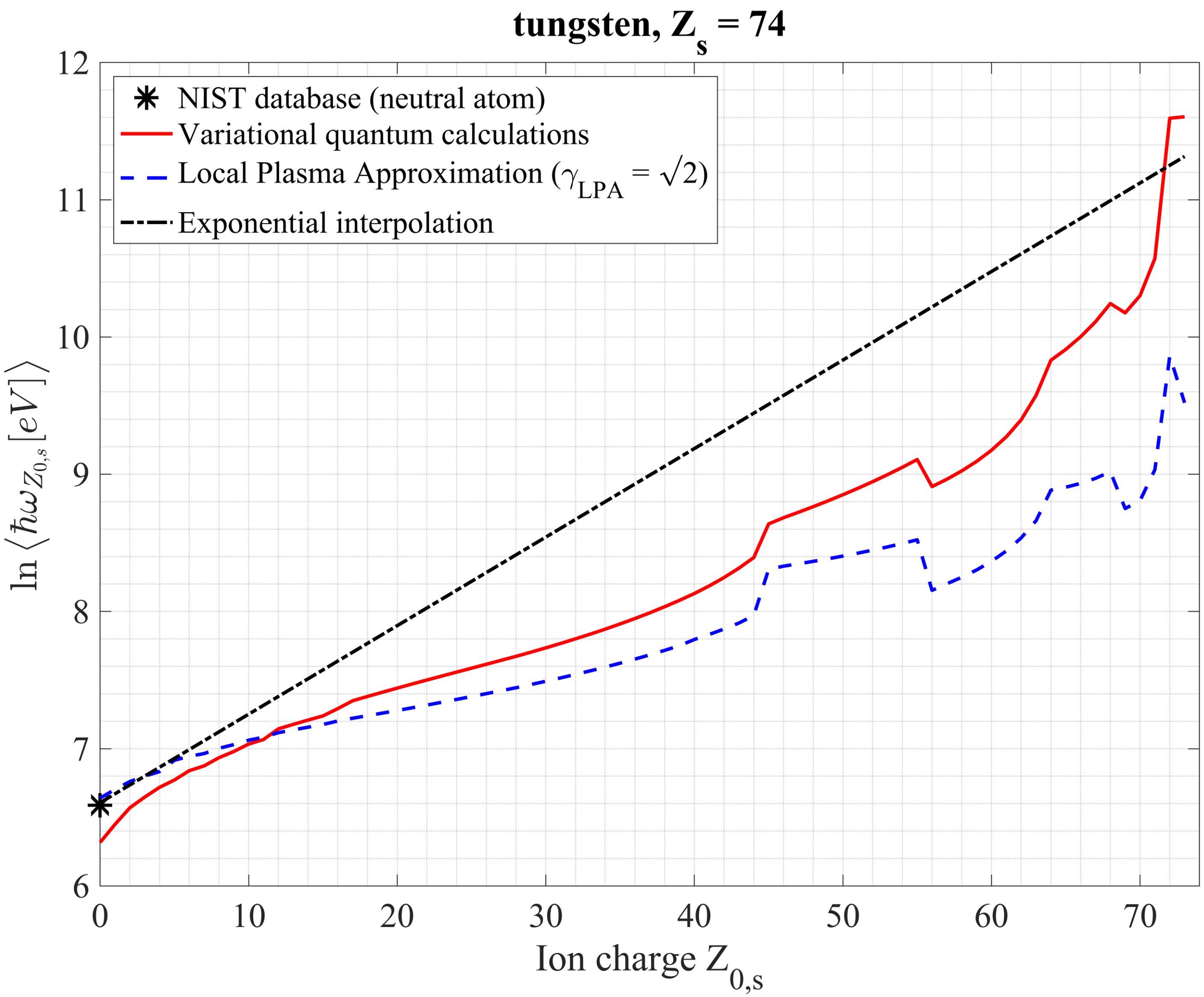
Xavier Garbet, et al., Journal of Applied Physics, 61 (1987) 907

Mean excitation energy for argon



S. P. A. Sauer, et al., J. Chem. Phys., 148 (2018) 174307

Mean excitation energy for tungsten



Conclusions

- A unified atomic model description allowing analytical formulations of the partial screening effect in Fokker-Planck calculations has been carried out, such that the impact of high-Z elements in hot tokamak plasmas on fast electron physics may be accurately described for any tokamak regimes.

- The atomic potential is expressed as a series of Yukawa potentials. *Extension of the Molière's method initially derived for the Thomas-Fermi model*. A general numerical procedure has been derived for the model calibration against ab initio quantum relativistic numerical calculations (DFT, MCDHF, …).

- The robustness of the multi-Yukawa description has been evaluated for tungsten element as a function of the number of exponentials → best results : 3 exponentials

- Analytic forms of the elastic and inelastic in diffusion and friction terms of the Fokker-Planck collision operators with the multi-Yukawa atomic model have been derived.

- A robust analytical estimate of the *mean excitation energy* has been obtained from non-relativistic quantum calculations, giving a consistent dependence with the ion charge. Applicable to any element including tungsten.

Absolute Multi-Yukawa model calibration (three exponentials case)

- Case of three exponentials expandable to any number of exponentials :

  - $\overline{\lambda}$ should be ***a real and positive solution*** of the polynomial equation :

$$\boxed{\overline{\lambda}^3 - X_1\overline{\lambda}^2 + X_2\overline{\lambda} - X_3 = 0}$$

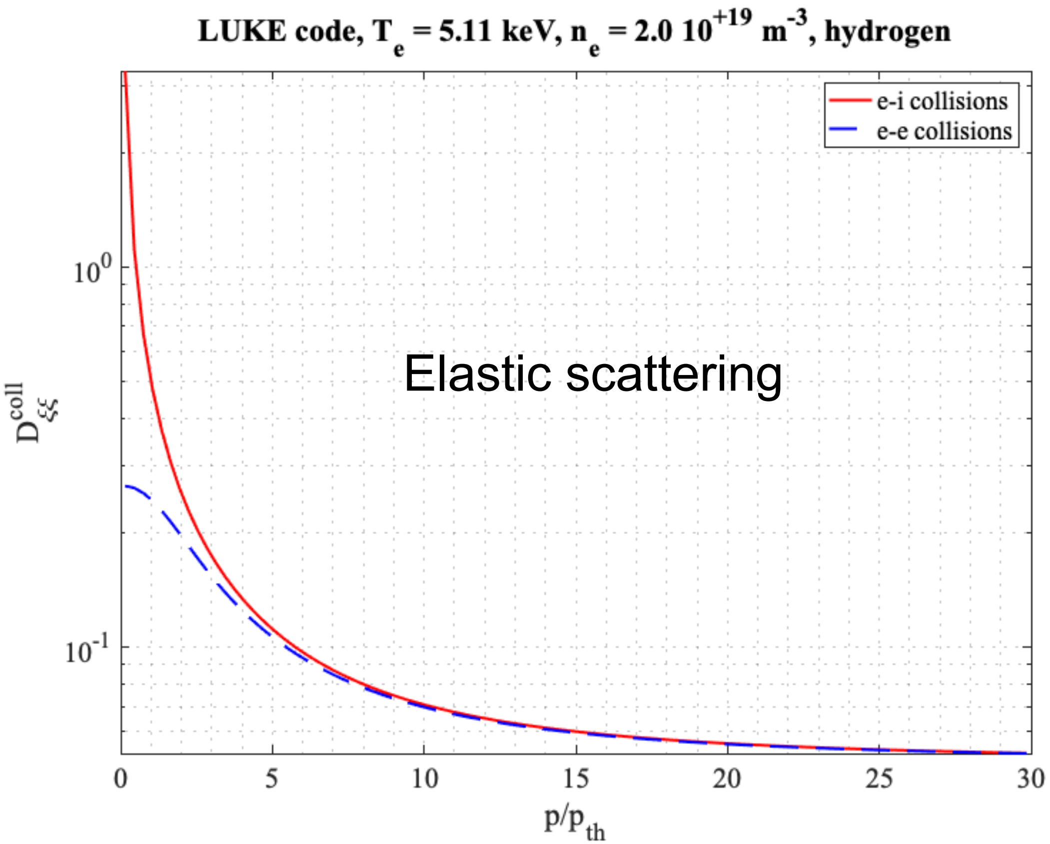
  - Defining $\mathbf{X} = \begin{bmatrix} X_1 \\ X_2 \\ X_3 \end{bmatrix} = \begin{bmatrix} \overline{\lambda}_{Z_{0,s,1}} + \overline{\lambda}_{Z_{0,s,2}} + \overline{\lambda}_{Z_{0,s,3}} \\ \overline{\lambda}_{Z_{0,s,1}}\overline{\lambda}_{Z_{0,s,2}} + \overline{\lambda}_{Z_{0,s,2}}\overline{\lambda}_{Z_{0,s,3}} + \overline{\lambda}_{Z_{0,s,1}}\overline{\lambda}_{Z_{0,s,3}} \\ \overline{\lambda}_{Z_{0,s,1}}\overline{\lambda}_{Z_{0,s,2}}\overline{\lambda}_{Z_{0,s,3}} \end{bmatrix}$

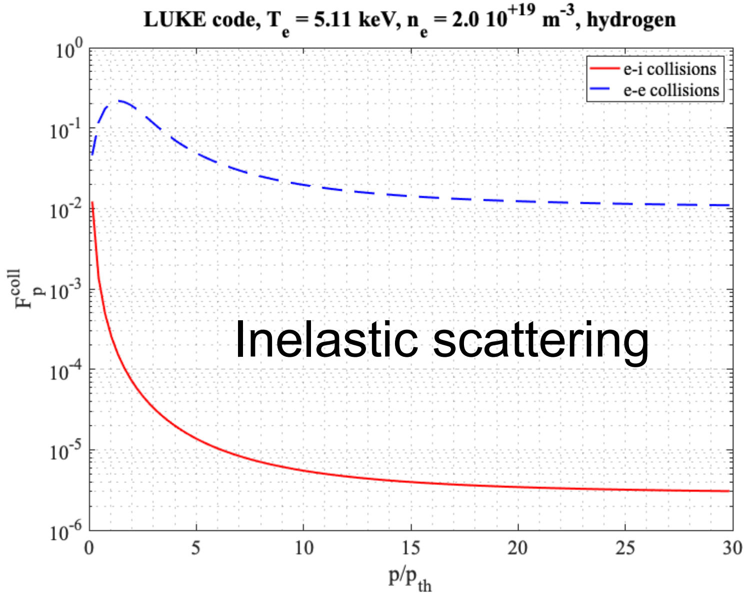
the coefficients $\overline{A}_{Z_{0,s,i}}$ are given by the matrix relation : $\boxed{\mathbf{A} = \mathbb{N}^{-1}\mathbb{M}\mathbf{X}}$
where

$$\mathbf{A} = \begin{bmatrix} \overline{A}_{Z_{0,s,1}} \\ \overline{A}_{Z_{0,s,2}} \\ \overline{A}_{Z_{0,s,3}} \end{bmatrix} \qquad \mathbb{M} = \begin{bmatrix} 1 & -\mathcal{R}_1^{num} & \mathcal{R}_2^{num} \\ \mathcal{R}_1^{num} & -\mathcal{R}_2^{num} & \mathcal{R}_3^{num} \\ \mathcal{R}_2^{num} & -\mathcal{R}_3^{num} & \mathcal{R}_4^{num} \end{bmatrix} \qquad \mathbb{N} = \begin{bmatrix} \overline{\lambda}_{Z_{0,s,1}} & \overline{\lambda}_{Z_{0,s,2}} & \overline{\lambda}_{Z_{0,s,3}} \\ 1 & 1 & 1 \\ \overline{\lambda}_{Z_{0,s,1}}^{-1} & \overline{\lambda}_{Z_{0,s,2}}^{-1} & \overline{\lambda}_{Z_{0,s,3}}^{-1} \end{bmatrix}$$

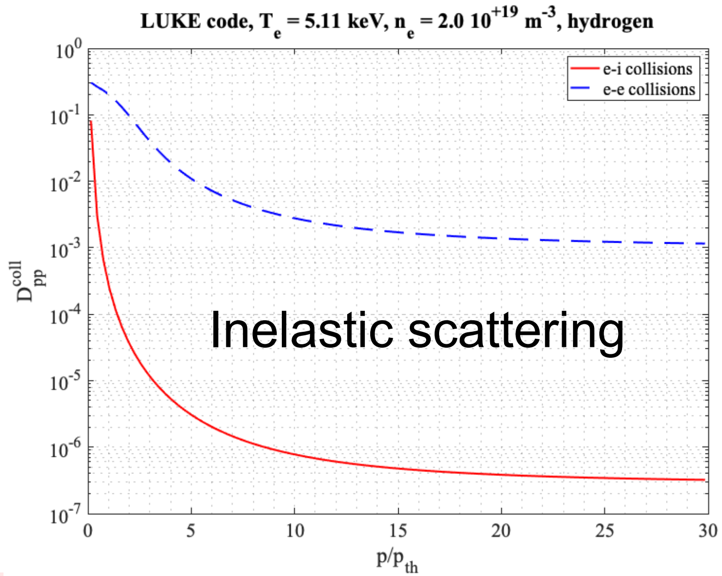
  - If no three real and positive $\overline{\lambda}$ solutions are found → less number of exponentials

Collision terms in LUKE Fokker-Planck solver





m_e/m_s



m_e/m_s

Screening function from numerical quantum calculations

$$g_{Z_{0,s}}^{num}\left(\bar{p}\right) = \left(Z_s^2 - Z_{0,s}^2\right)\left(\ln\left(2\bar{p}/\alpha\right) + \gamma_{EM} - 1\right) + 2Z_s N_s \hat{I}_{1,Z_{0,s}} + N_s^2\left(\frac{1}{2} - \hat{I}_{2,Z_{0,s}}\right)$$

$$\hat{I}_{1,Z_{0,s}} \equiv \frac{4\pi}{N_s}\int_0^\infty \boxed{\bar{\rho}_{Z_{0,s}}^{num}\left(\bar{r}_1\right)}\,\bar{r}_1^2 \ln \bar{r}_1 d\bar{r}_1$$

DFT

$$\hat{I}_{2,Z_{0,s}} = \frac{4\pi^2}{N_s^2}\int_0^\infty \boxed{\bar{\rho}_{Z_{0,s}}^{num}\left(\bar{r}_1\right)}\,\hat{J}_{2,Z_{0,s}}\left(\bar{r}_1\right)\bar{r}_1 d\bar{r}_1$$

$$\hat{J}_{2,Z_{0,s}}\left(\bar{r}_1\right) = \int_0^\infty \boxed{\bar{\rho}_{Z_{0,s}}^{num}\left(\bar{r}_2\right)}\,\bar{r}_2 d\bar{r}_2\left(\left(\bar{r}_1+\bar{r}_2\right)^2\ln\left(\bar{r}_1+\bar{r}_2\right) - \left(\bar{r}_1-\bar{r}_2\right)^2\ln\left|\bar{r}_1-\bar{r}_2\right|\right)$$

where γ_{EM} is the Euler-Mascheroni constant.

Calculation valid for $\overline{p} \gg 1$ only.

L. Hesslow, et al., J. Plasma Phys., 84(6) (2018) 905840605