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

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

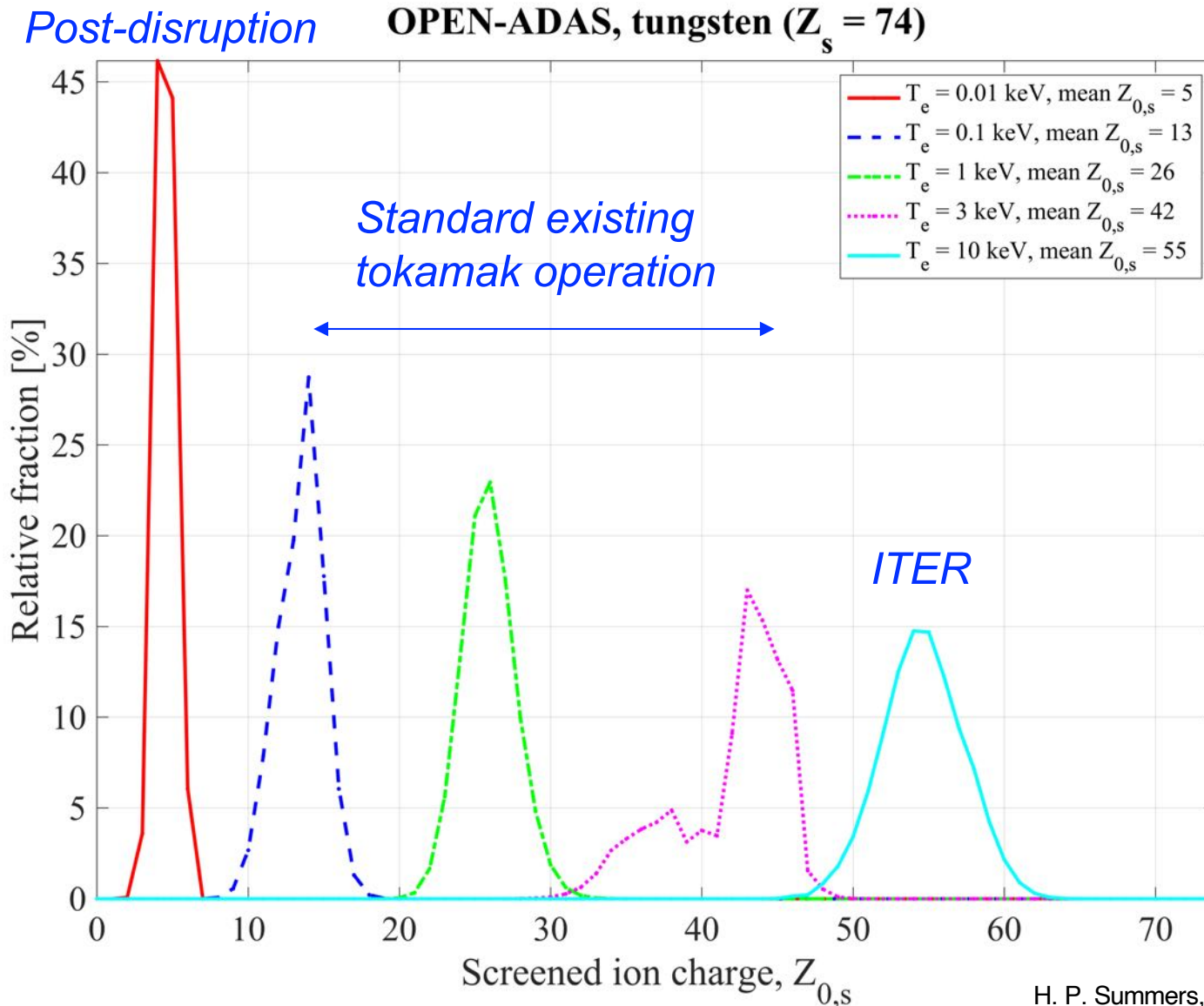
- **Passive sources** → **plasma-wall interactions**

- 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,...)

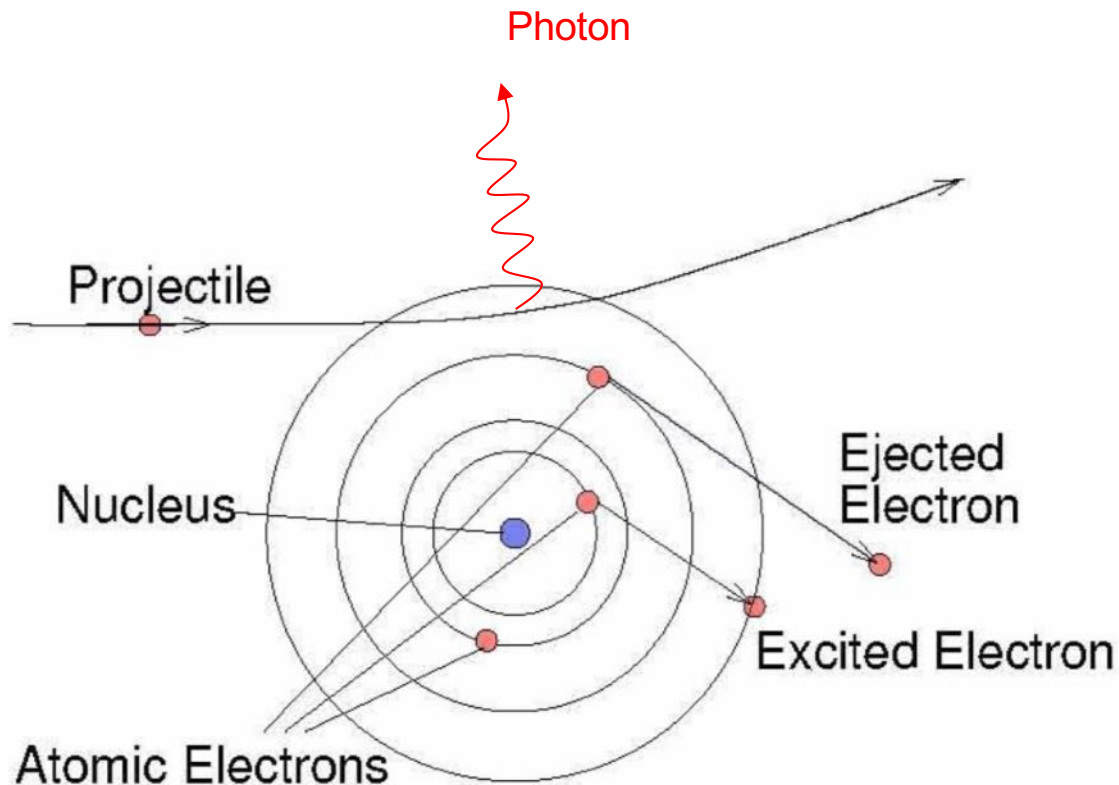
- **Active sources** → **massive gas injection**

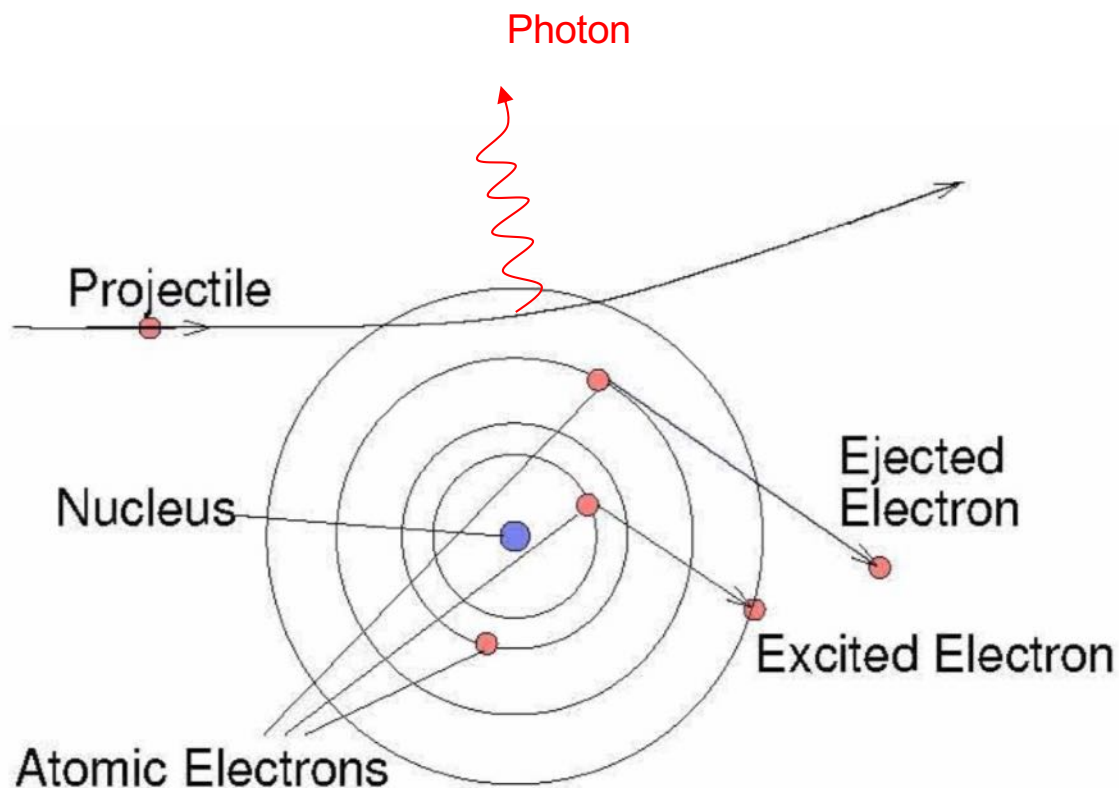
- Mitigation of a runaway electron beam after a major disruption in the ITER tokamak reactor (Argon, Neon, ...)

- 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, for all species present in the plasma and whatever their ionization state :
  - 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)

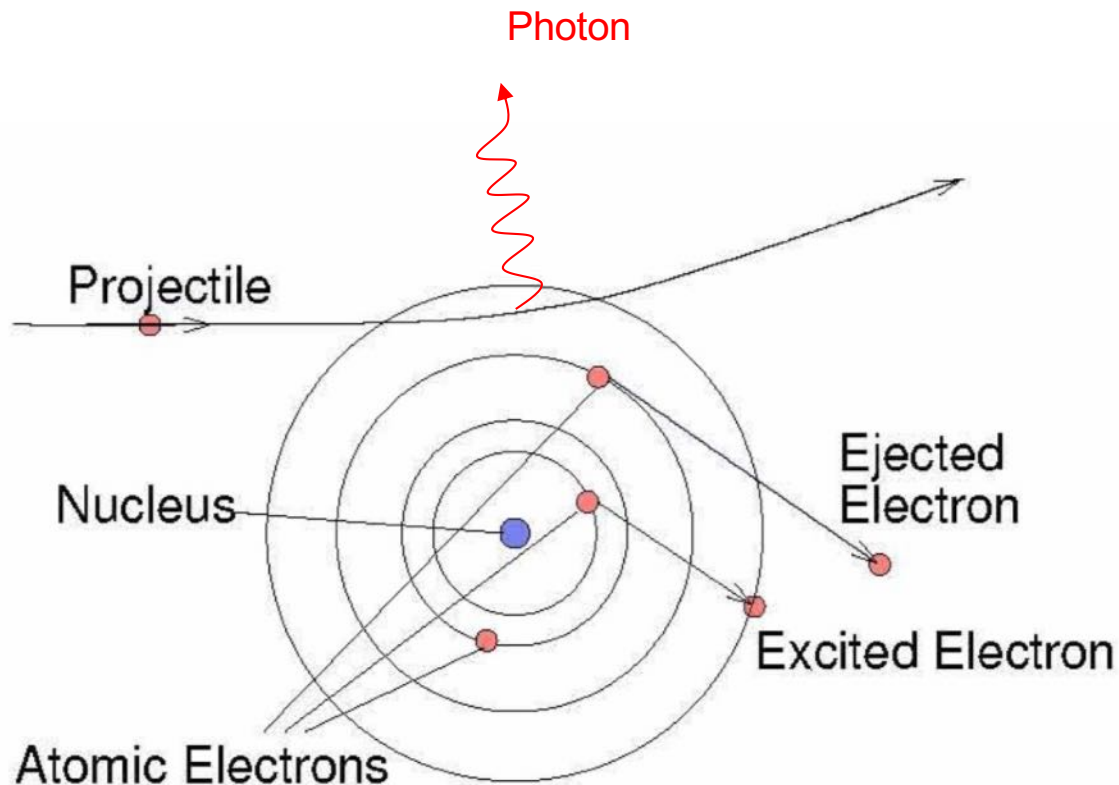


H. P. Summers, Technical report, ADAS (2004)





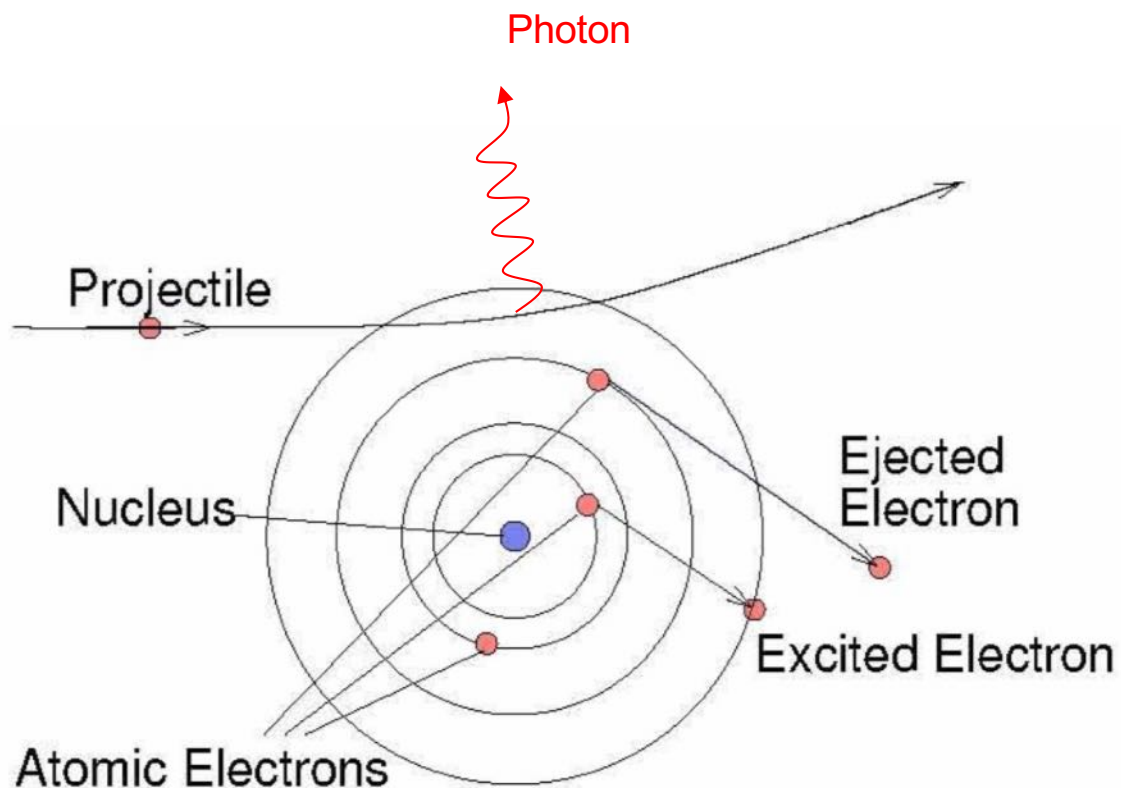
**Elastic scattering**



**Elastic scattering**

**Inelastic scattering**

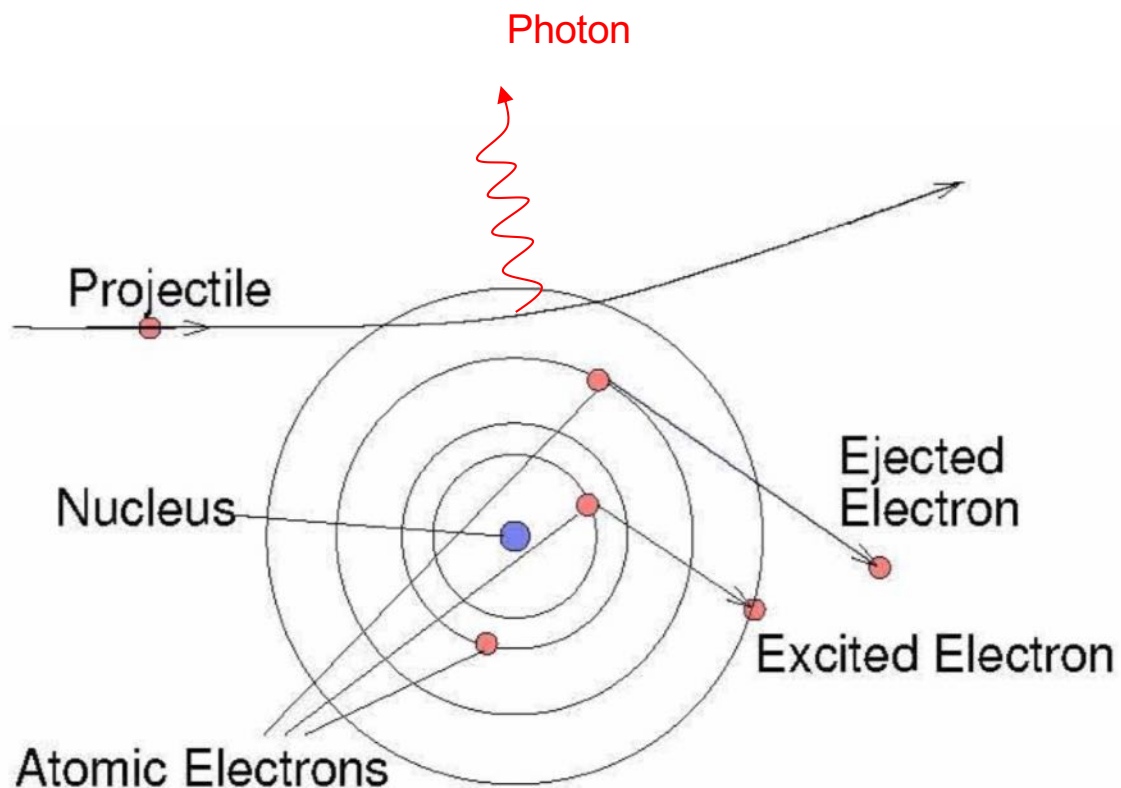




**Elastic scattering**

*Ionization*

**Inelastic scattering**

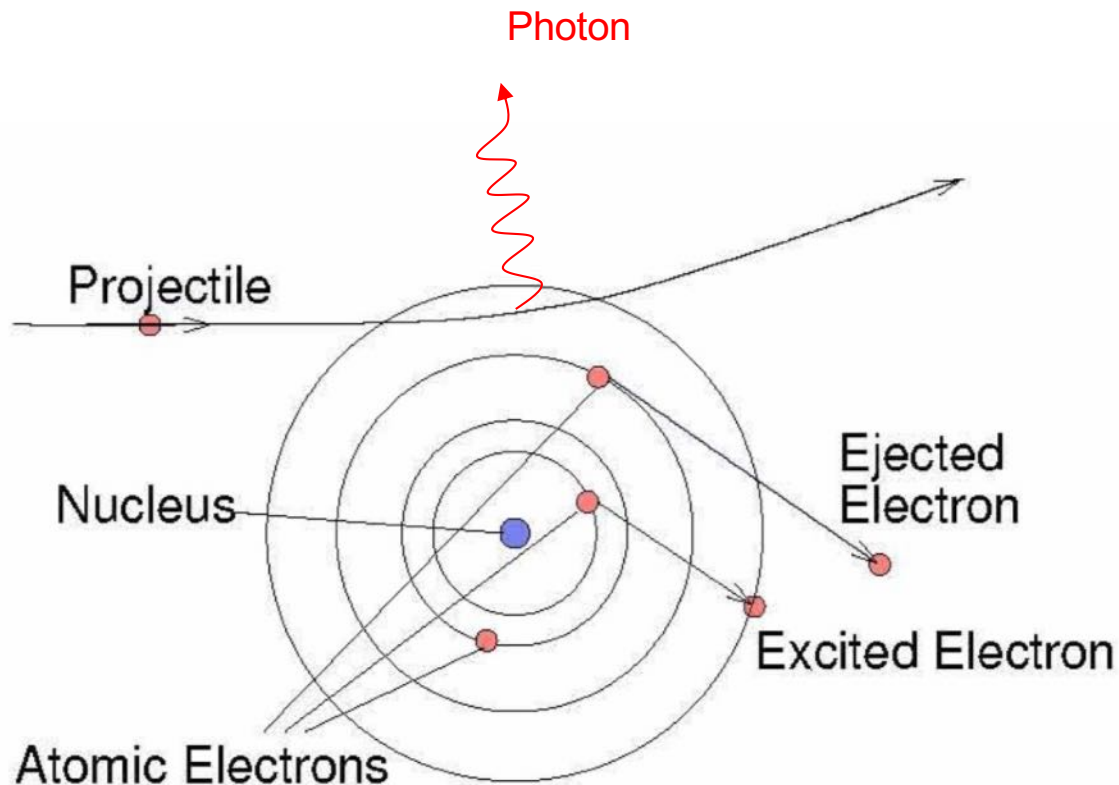


*Bremsstrahlung*

**Elastic scattering**

*Ionization*

**Inelastic scattering**



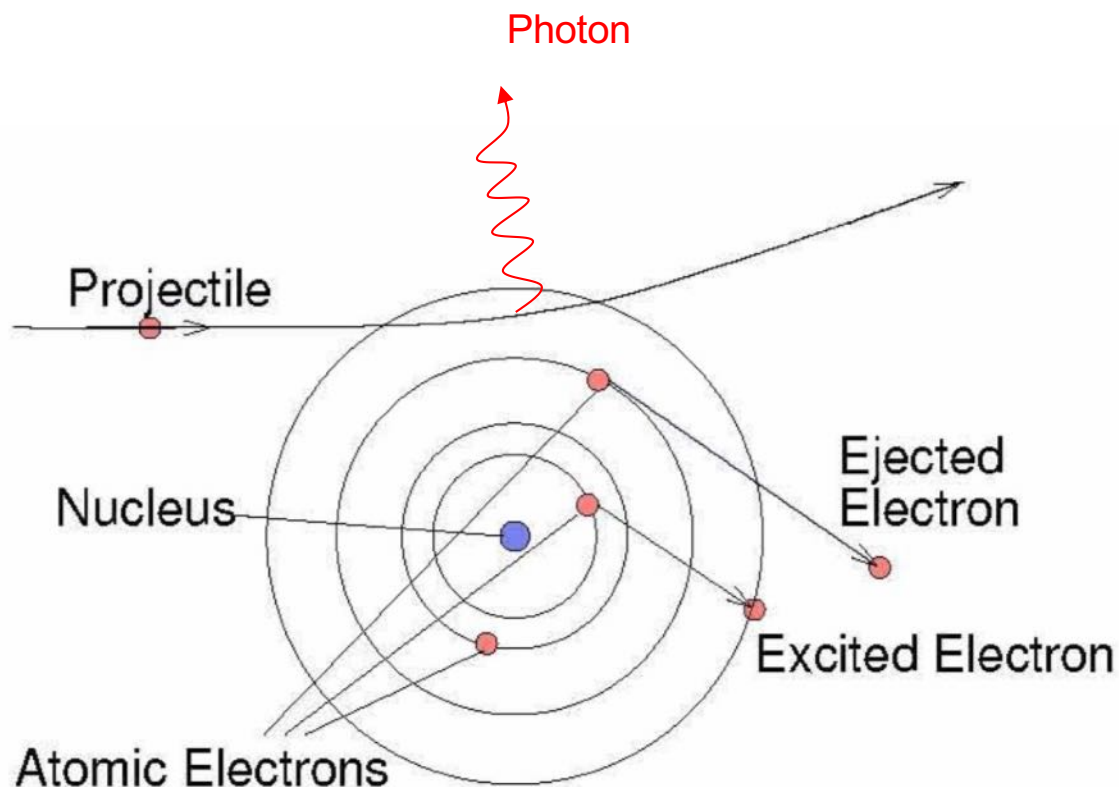
*Bremsstrahlung*

**Elastic scattering**

*Ionization*

**Inelastic scattering**

*Line emission*



*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 :  $\nu_{coll} \times \tau_{lifetime} \ll 1$

## ▪ Elastic scattering and screening effect

- e-i collisions dominated by small angle deflections → 1<sup>st</sup> 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*  $\rho(r)$

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

## ▪ 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*  $\rho(r)$

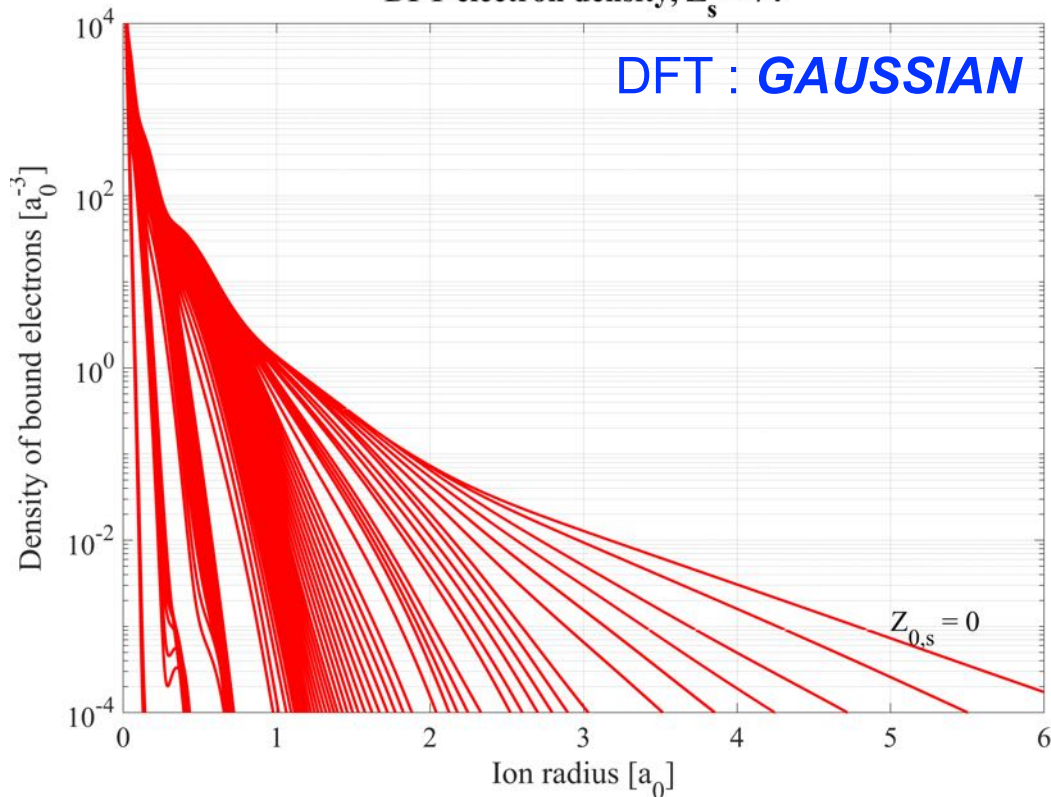
$$\langle \hbar\omega_{Z_{0,s}} \rangle = (1/Z_{0,s}) \sum_{ik} f_{ik} \ln(\hbar\omega_{ik})$$

- 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,  $T_e \in \{10-10^4\}$  eV and  $E_c \in \{10^{-2}-10^3\}$  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.**

**DFT** : Density functional theory

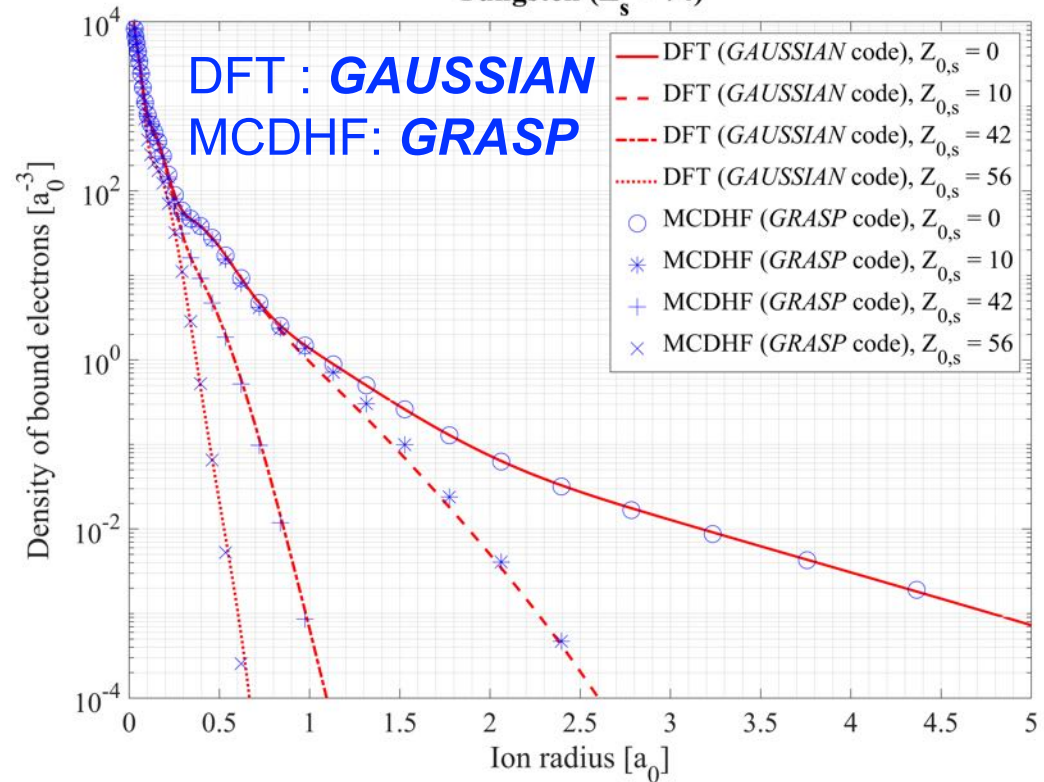
**MCDHF** : Multi-Configuration Dirac-Hartree-Fock model

DFT electron density,  $Z_s = 74$



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

Tungsten ( $Z_s = 74$ )



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

Weakly ionized atoms



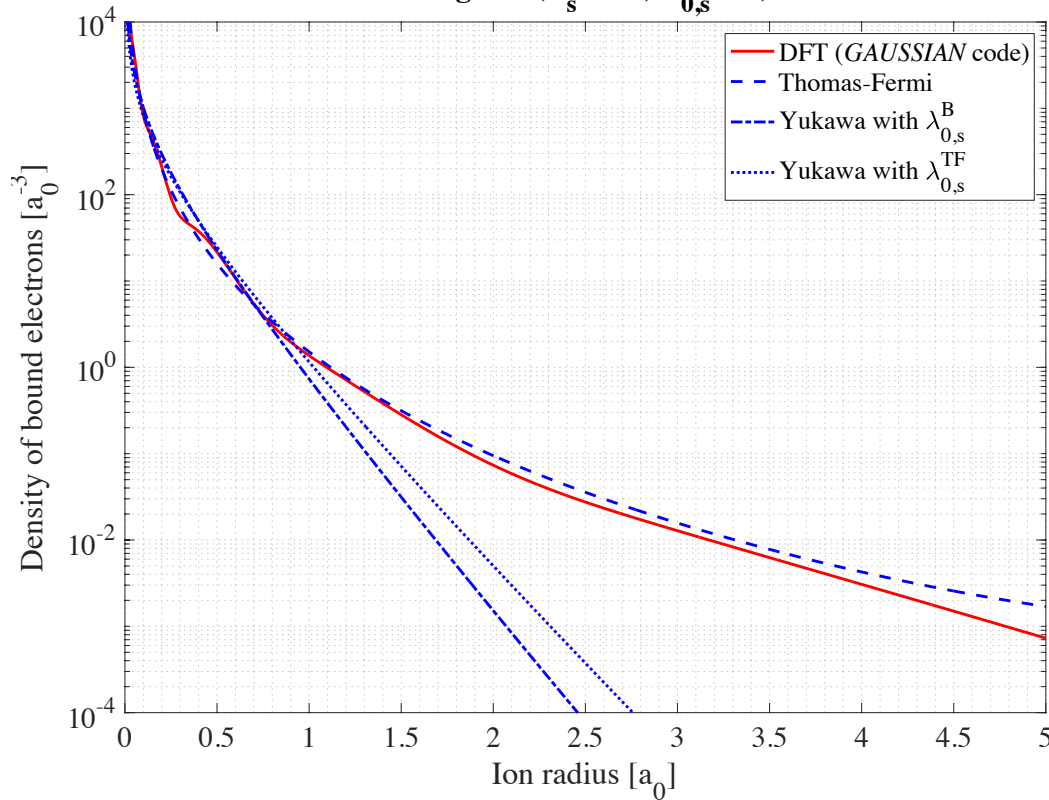
Thomas-Fermi model

Strongly ionized atoms

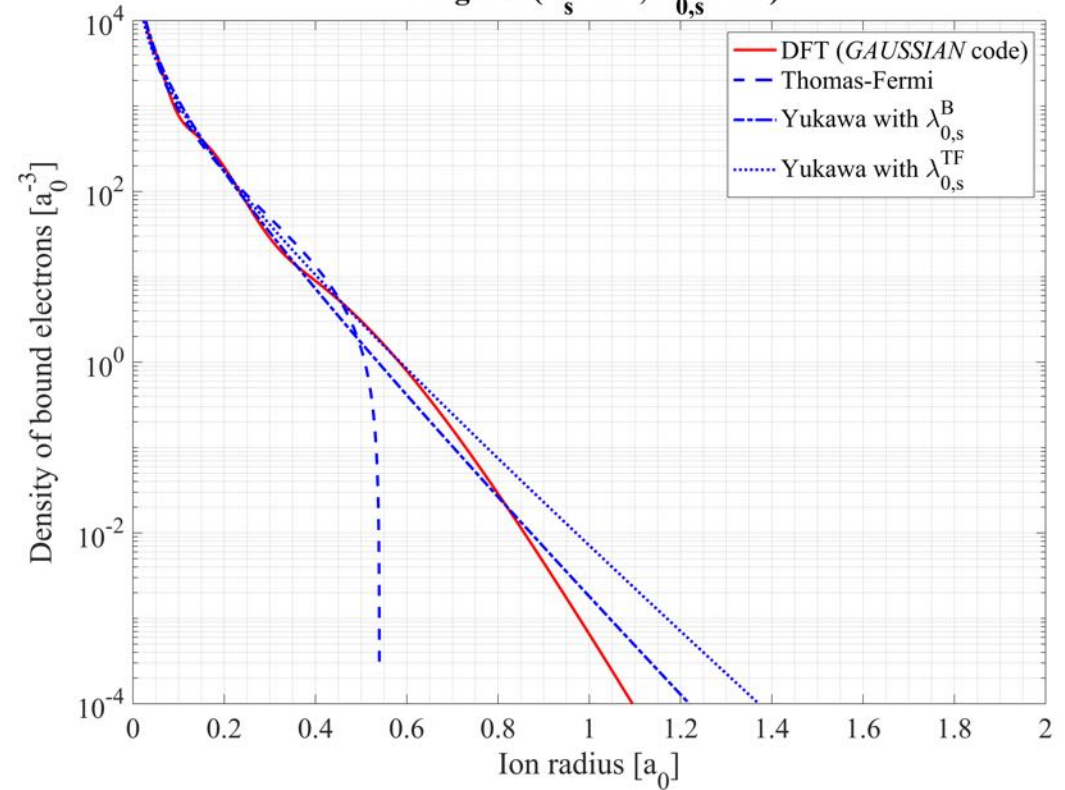


Yukawa model

Tungsten ( $Z_s = 74, Z_{0,s} = 0$ )



Tungsten ( $Z_s = 74, Z_{0,s} = 42$ )





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

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

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

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

- **Analytic atomic form factor** :

$$F_{Z_{0,s}}(\bar{q}) = (Z_s - Z_{0,s}) \sum_i \frac{\bar{A}_{Z_{0,s,i}}}{1 + (\bar{q} \bar{a}_{Z_{0,s,i}}/2)^2} \quad \bar{q} = q/(m_e c) \quad \bar{a}_{Z_{0,s,i}} \equiv 2\bar{\lambda}_{Z_{0,s,i}}^{-1}/\alpha$$

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

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

- **Determination of  $(\bar{A}_{Z_{0,s,i}}, \bar{\lambda}_{Z_{0,s,i}})$  is an ill-posed problem.** Standard non-linear regression techniques are useless.
- **Method of moments :**  $\langle \bar{r}^l \rangle = \langle \bar{r}^l \rangle^{num}$  where  $\langle \bar{r}^l \rangle^{num}$  is determined from ab initio quantum numerical calculations (DFT or MCDHF) → Uniqueness of the solution if it exists.
- Defining  $\mathcal{R}_l \equiv \langle \bar{r}^l \rangle / (l + 1)!$  where

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

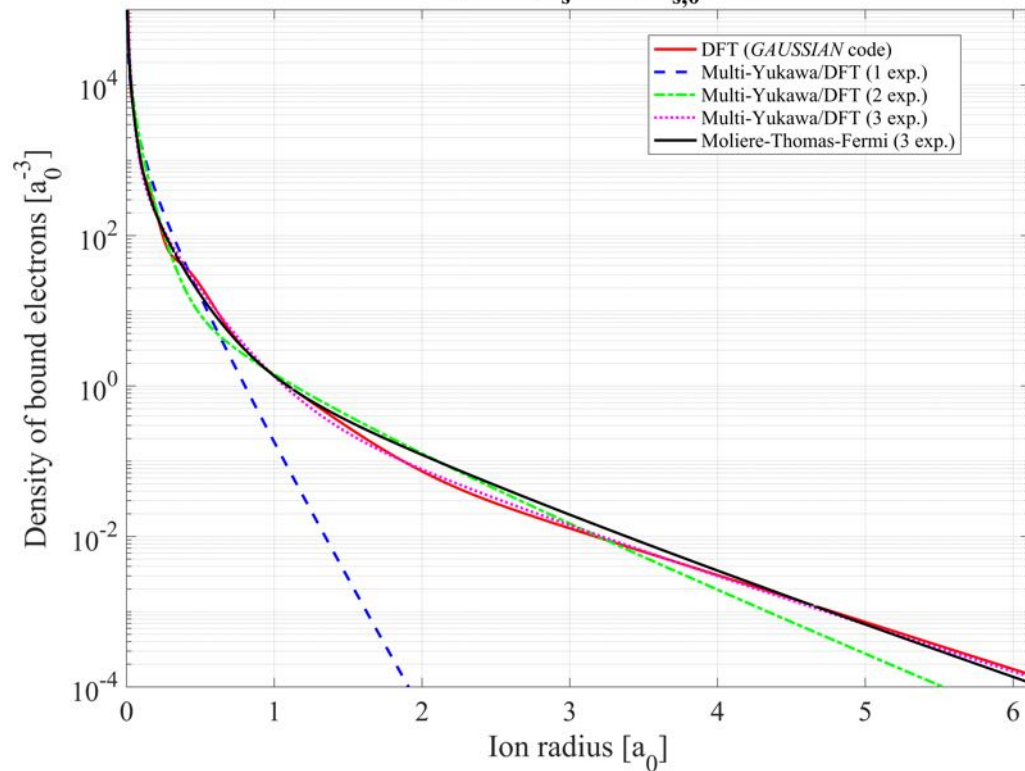
$$\mathcal{R}_l^{num} = \frac{1}{(l + 1)!} \frac{4\pi}{(Z_s - Z_{0,s})} \int_0^\infty \bar{r}^{l+2} \bar{\rho}_{Z_{0,s}}^N(\bar{r}) d\bar{r}$$

- 2/ equations to be solved, where  $l$  is the number of exponentials
- If no solution found  $l \rightarrow l - 1$

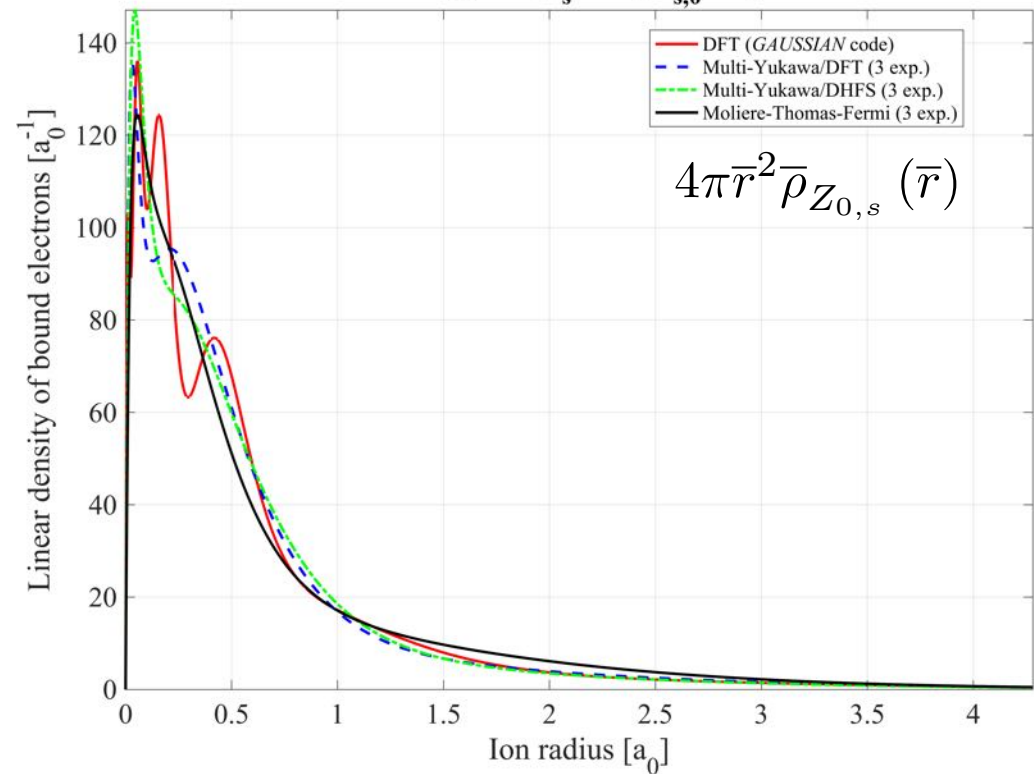
F. Salvat, et al., Phys. Rev. A, 36(2) (1987) 467–474

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

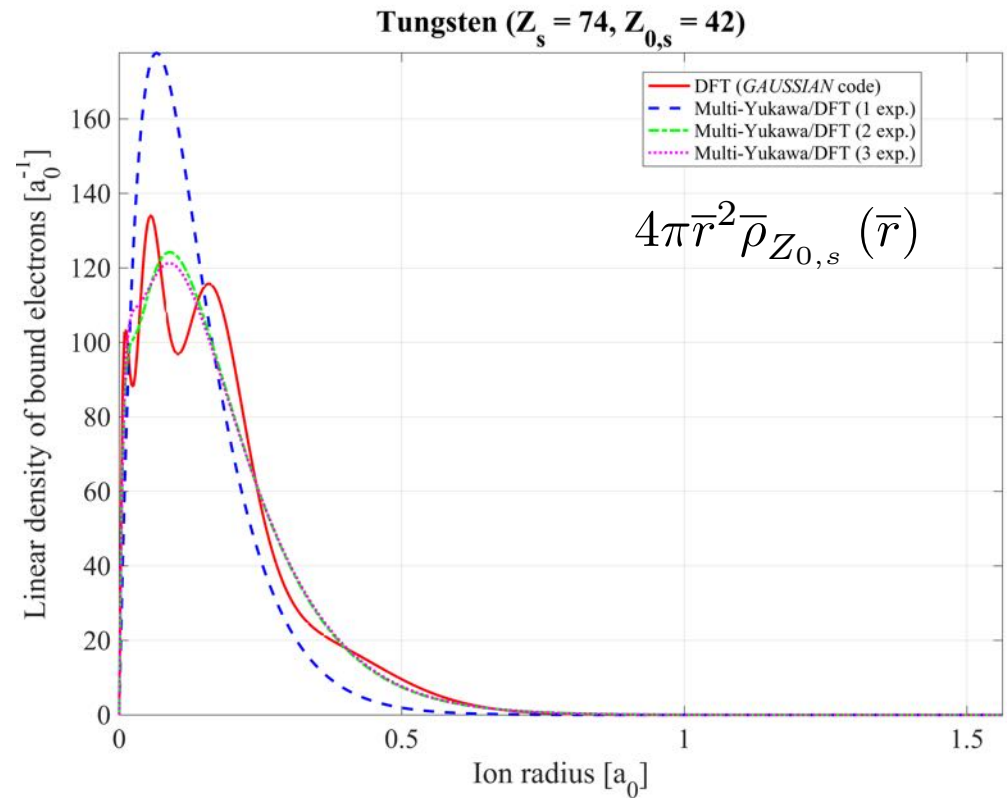
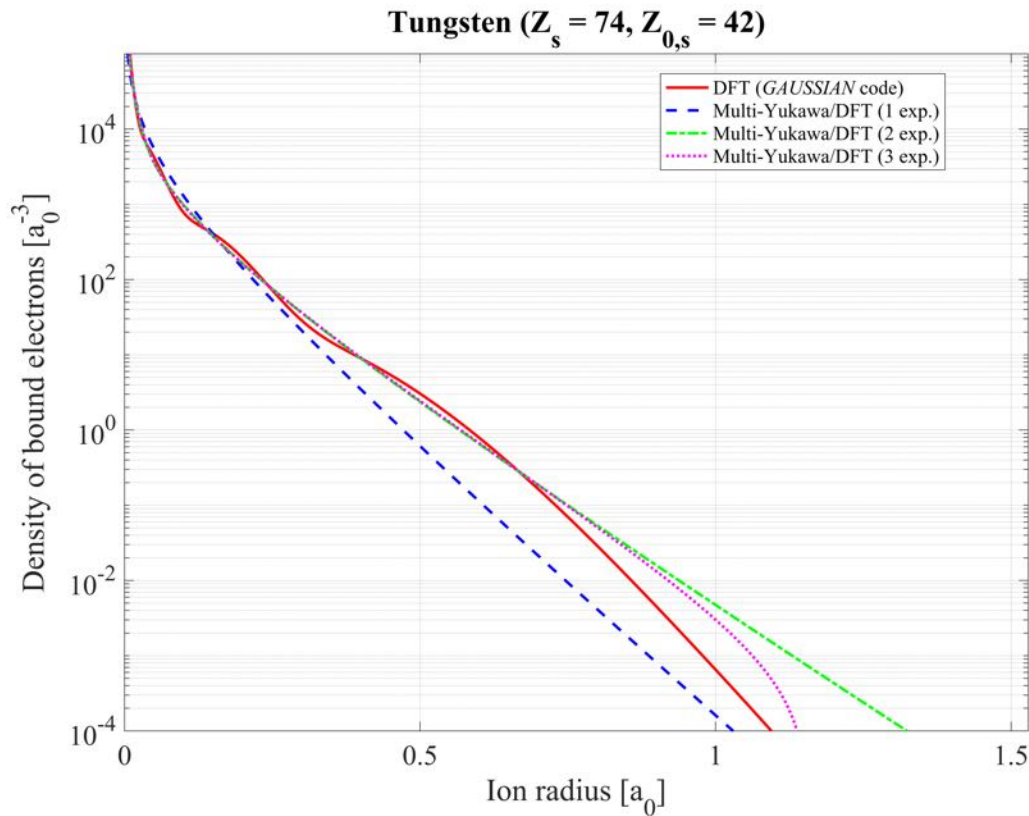
Tungsten ( $Z_s = 74, Z_{s,0} = 0$ )



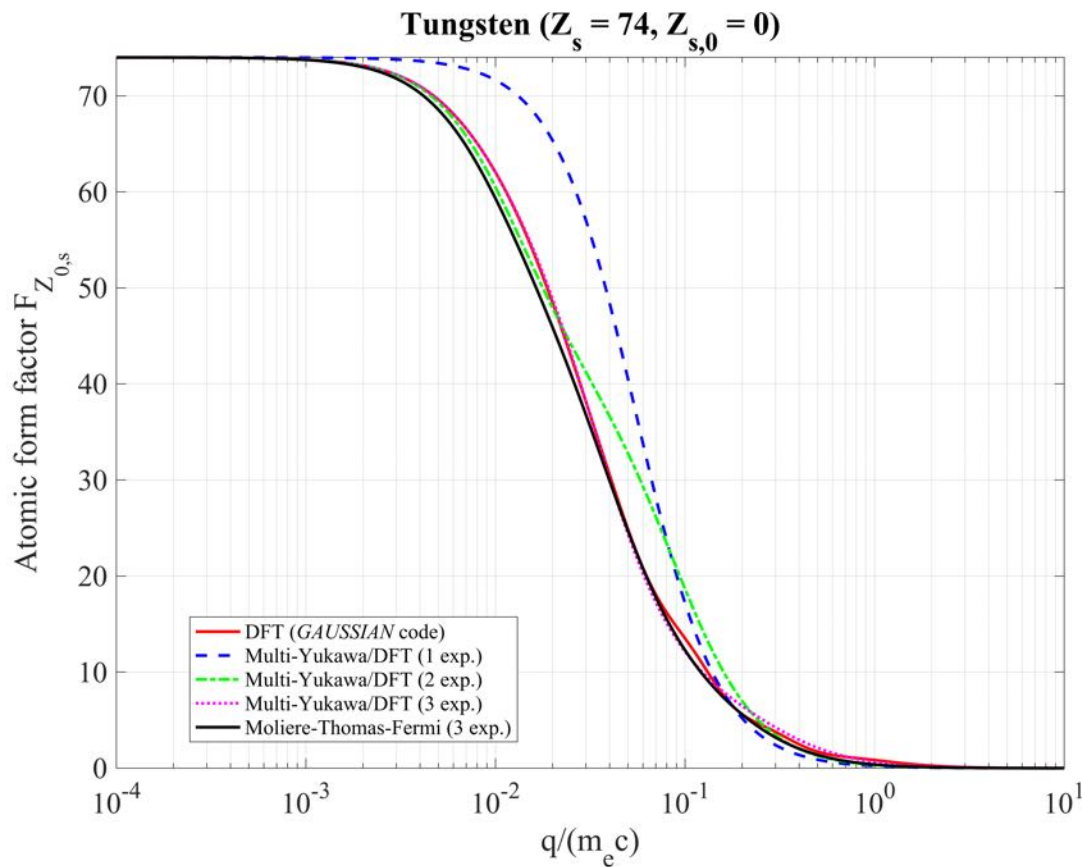
Tungsten ( $Z_s = 74, Z_{s,0} = 0$ )



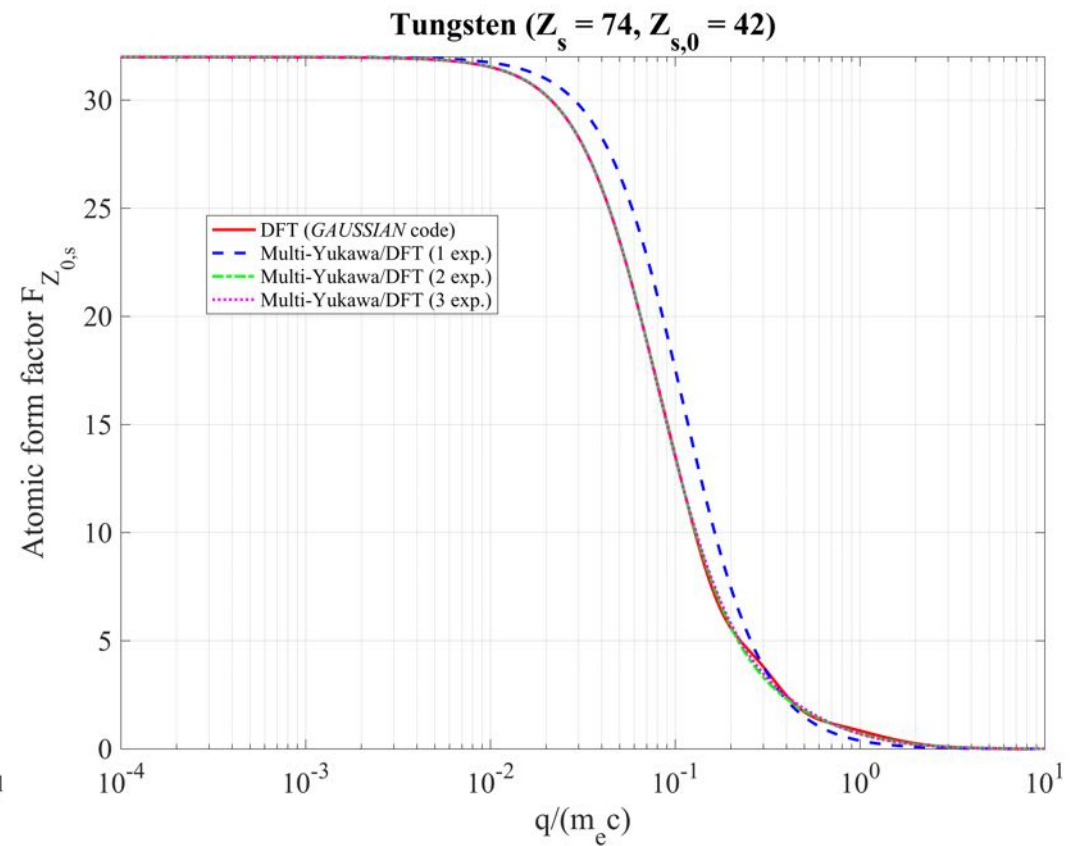
## Partially ionized tungsten $Z_{0,s} = 42$



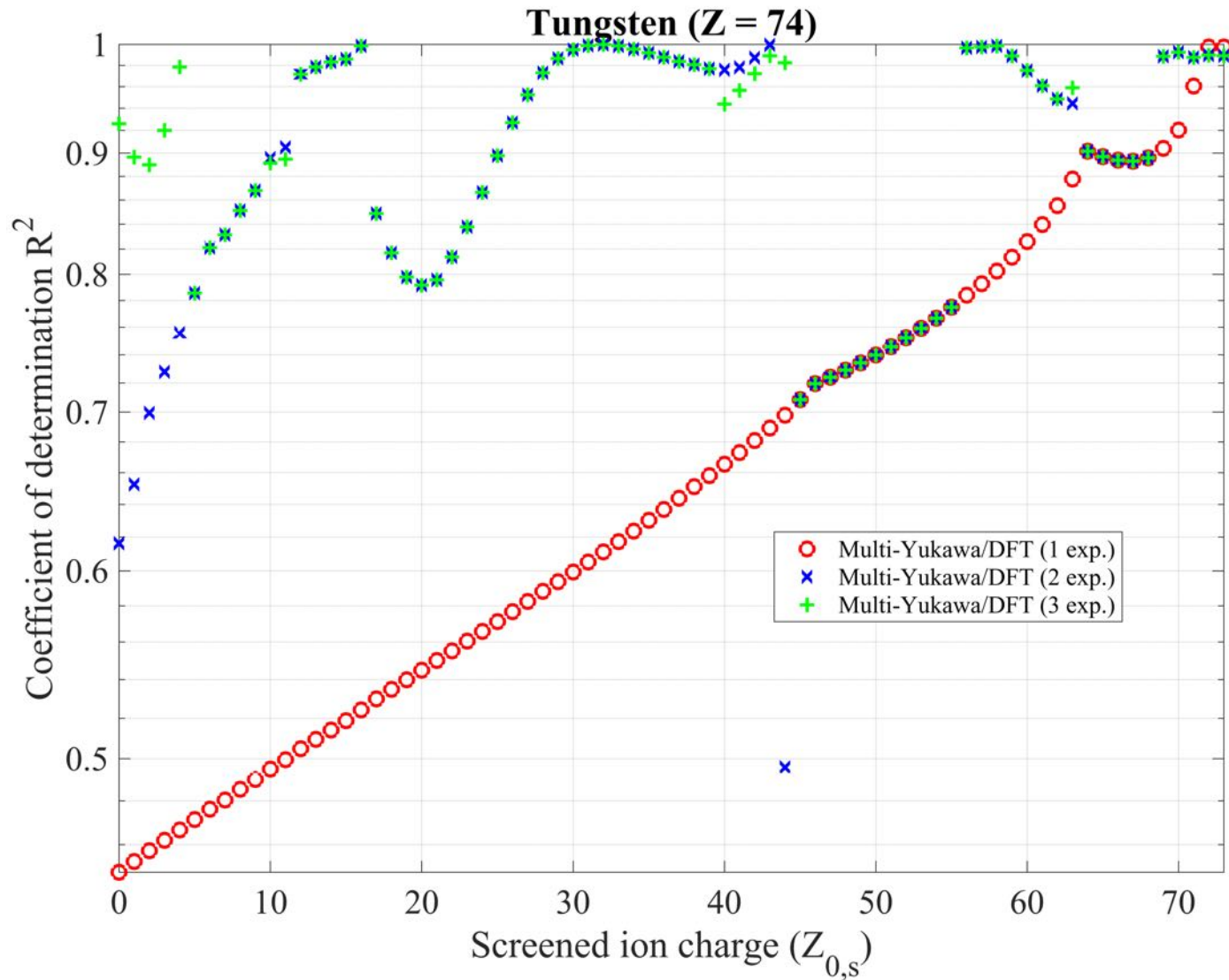
Neutral tungsten  $Z_{0,s} = 0$



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



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



Electron-ion Fokker-Planck collision operator :

$$\mathbf{C}_{e,Z_0,s} (f_e, f_{Z_0,s}) \simeq -\nabla_p (\mathbf{A}_{Z_0,s} f_e (t, \mathbf{x}, \mathbf{p})) + \nabla_p \nabla_p (\mathbb{D}_{Z_0,s} f_e (t, \mathbf{x}, \mathbf{p}))$$

**Friction vector :**  $\mathbf{A}_{Z_0,s} = \int d^3 \mathbf{p}_s f_{Z_0,s} (t, \mathbf{x}, \mathbf{p}_s) \int d\Omega \frac{d\sigma_{e,Z_0,s}}{d\Omega} u_s \Delta \mathbf{p}$

Mott-Rutherford cross-section

**Diffusion tensor :**  $\mathbb{D}_{Z_0,s} = \frac{1}{2} \int d^3 \mathbf{p}_s f_{Z_0,s} (t, \mathbf{x}, \mathbf{p}_s) \int d\Omega \frac{d\sigma_{e,Z_0,s}}{d\Omega} u_s \Delta \mathbf{p} \Delta \mathbf{p}^T$

Coulomb collision (1<sup>st</sup> Born approximation) :

$$\frac{d\sigma_{e,Z_{0,s}}}{d\Omega} = Z_{0,s}^2 \frac{r_e^2}{4} \frac{(1-x^2) \bar{p}^2 + 1}{\bar{p}^4 x^4}$$

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

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

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

Coulomb logarithm    Screening function

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



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

$$df_e/dt|_{coll} \equiv \sum_s \sum_{Z_{0,s}} \mathbf{C}_{e,Z_{0,s}}(f_e, f_{Z_{0,s}}) + \mathbf{C}_{e,e}(f_e, f_e) \equiv \nabla_{\mathbf{p}} \cdot \mathbf{S}_{\mathbf{p}}^{coll}(f_e)$$

Coordinate system  $(p, \xi, \varphi)$   $\rightarrow$

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

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

### 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

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

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

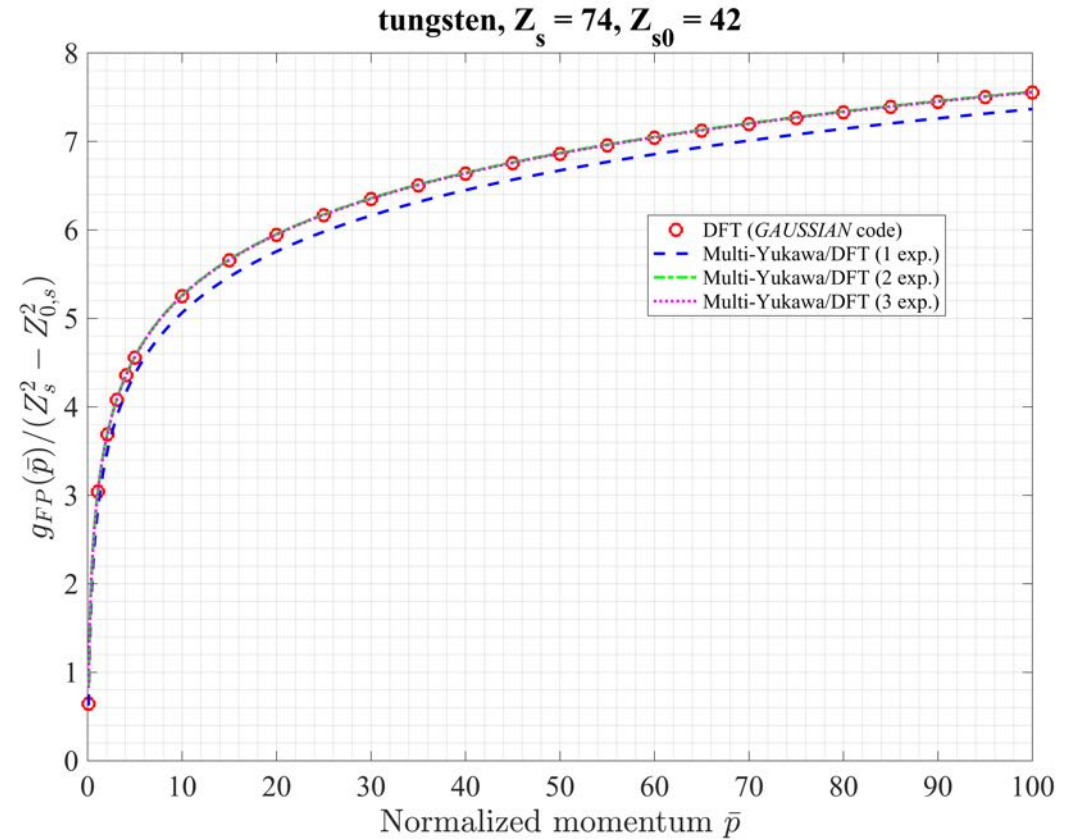
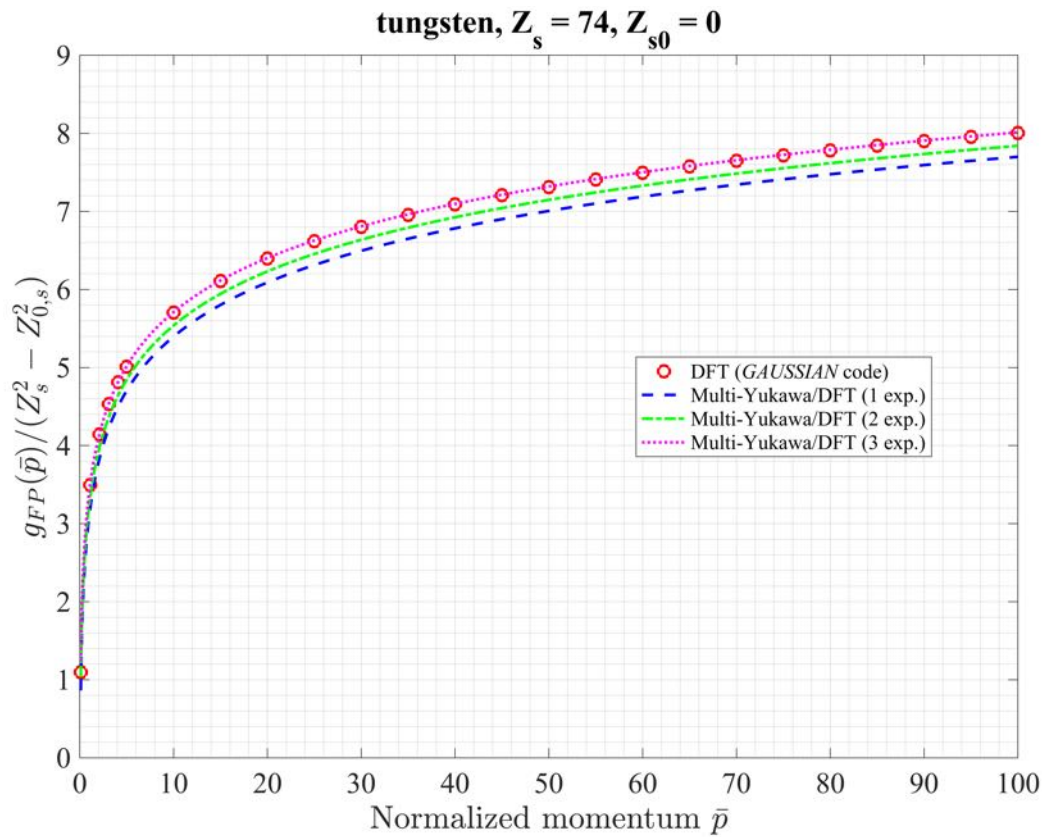
$$\begin{aligned}
 g_{Z_{0,s}}(\bar{p}) &= Z_s (Z_s - Z_{0,s}) \sum_i \bar{A}_{0,s,i} \ln \left( 1 + (\bar{p} \bar{a}_{Z_{0,s,i}})^2 \right) \\
 &\quad - \frac{(Z_s - Z_{0,s})^2}{2} \sum_i \bar{A}_{0,s,i}^2 \left( \frac{(\bar{p} \bar{a}_{Z_{0,s,i}})^2}{1 + (\bar{p} \bar{a}_{Z_{0,s,i}})^2} + \ln \left( 1 + (\bar{p} \bar{a}_{Z_{0,s,i}})^2 \right) \right) \\
 &\quad + 2 (Z_s - Z_{0,s})^2 \sum_i \sum_{j>i} \bar{A}_{0,s,i} \bar{A}_{0,s,j} \tilde{g}_{Z_{0,s},2,i,j}(\bar{p})
 \end{aligned}$$

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

- Fully analytic expression
- Arbitrary number of exponentials

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

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



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

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

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

Atomic physics is described by the mean excitation energy

- Since the energy loss over a distance  $\Delta x$  is equivalent of the work of an effective drag force,

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

- Incorporation in LUKE Fokker-Planck code :  $F_p^{coll} = F_p^{e-i} + F_p^{e-e} + F_p^{excitation} + F_p^{ALD}$

Dominant terms

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

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

▪ *Mean excitation energy* →  $\langle \hbar\omega_{Z_{0,s}} \rangle = (1/Z_{0,s}) \sum_{ik} f_{ik} \ln(\hbar\omega_{ik})$

- $f_{ik}$  : dipole oscillator strength of the transition
- $\omega_{ik}$  : dipole frequency for the transition between  $|i\rangle$  and  $|k\rangle$  quantum states

Hydrogenoid mean excitation energy :  $14.99 \times Z_s^2$  eV

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

Bloch relation

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

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

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)

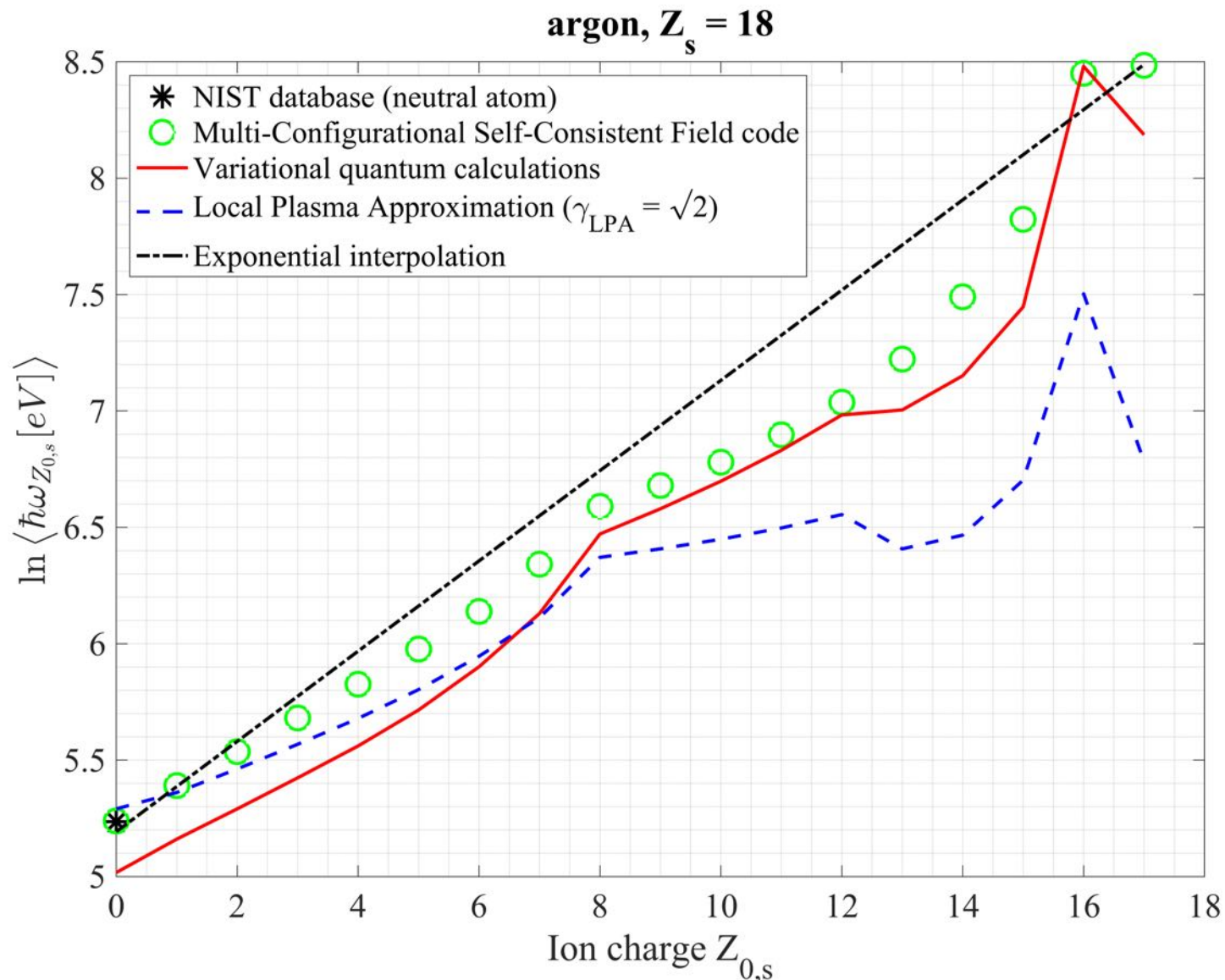
W.K. Chu and D. Powers. Phys. Letters, 40A(1) (1972) 23–24, 1972

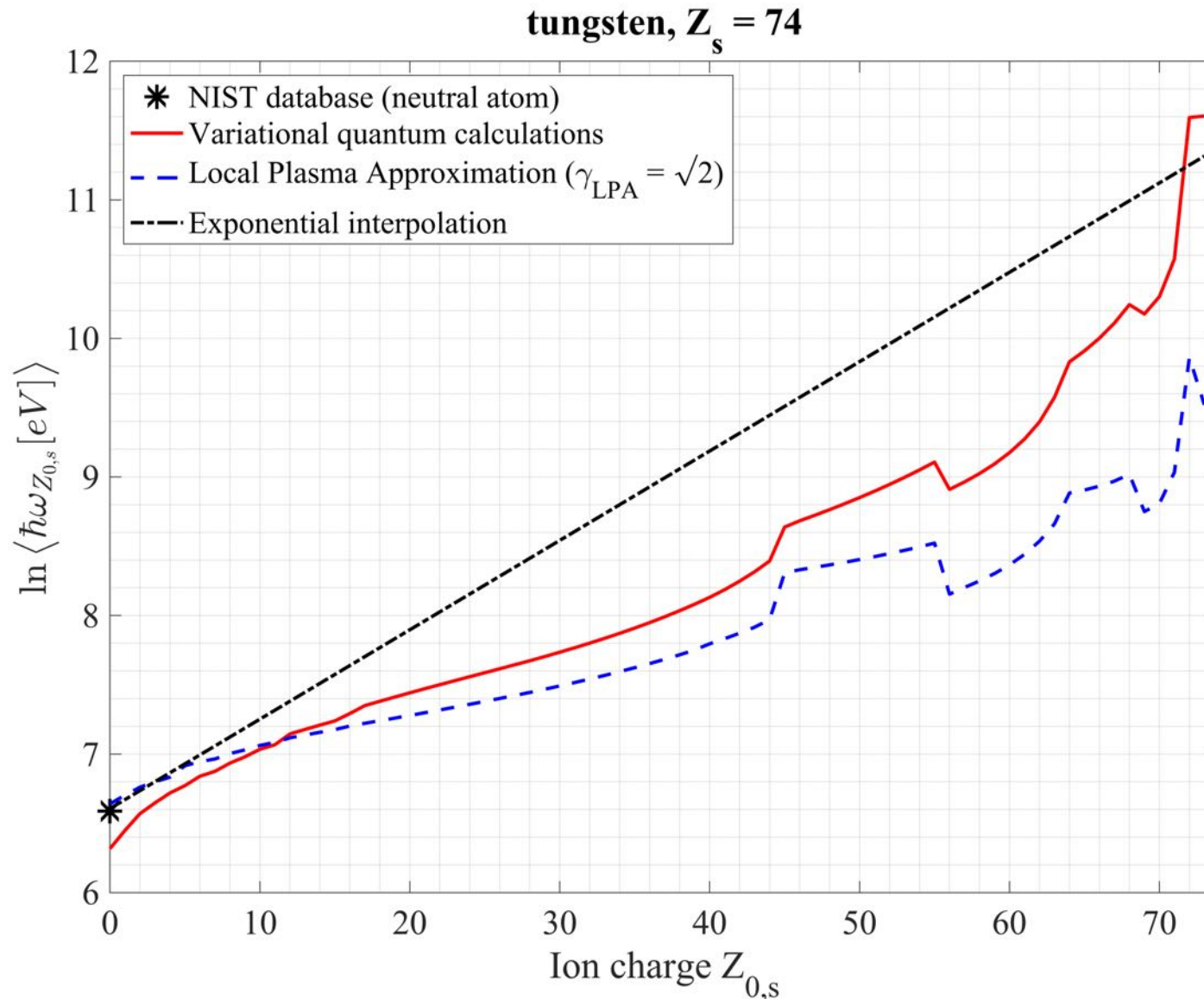
- **Variational quantum description :**  $\langle \hbar\omega_{Z_0,s} \rangle^2 = 2 \frac{K_0}{\langle \bar{r}^2 \rangle} \alpha^2 m_e c^2$

The *averaged kinetic energy of the cloud of bound electrons*  $K_0$  is determined using the virial theorem (non-relativistic limit) :  $2K_0 \simeq \langle U_{Z_0,s} \rangle / N_s$

$$\langle \hbar\omega_{Z_0,s} \rangle = \frac{\alpha^2 m_e c^2 \sqrt{N_s}}{\sqrt{6 \sum_i \bar{\lambda}_{Z_0,s,i}^{-2} \bar{A}_{Z_0,s,i}}} \times \sqrt{\sum_i \bar{A}_{Z_0,s,i}^2 \frac{\bar{\lambda}_{Z_0,s,i}}{2} + \sum_i \sum_{j \neq i} \bar{A}_{Z_0,s,i} \bar{A}_{Z_0,s,j} \frac{\bar{\lambda}_{Z_0,s,i}^2}{\bar{\lambda}_{Z_0,s,i} + \bar{\lambda}_{Z_0,s,j}}}$$

- Single exponential limit :  $\langle \hbar\omega_{Z_0,s} \rangle = \alpha^2 m_e c^2 \sqrt{\bar{\lambda}_{Z_0,s,1}^3 N_s / 12}$
- Thomas-Fermi model for neutral atoms :  $\bar{\lambda}_{Z_0,s,1} = 1.13 Z_s^{1/3}$   
 $\langle \hbar\omega_{Z_0,s} \rangle = 9.44 Z_s \text{ eV} \longrightarrow \text{Bloch relation } \sim 10 Z_s \text{ eV is well retrieved}$







- 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.



- Case of three exponentials expandable to any number of exponentials :
  - $\bar{\lambda}$  should be **a real and positive solution** of the polynomial equation :

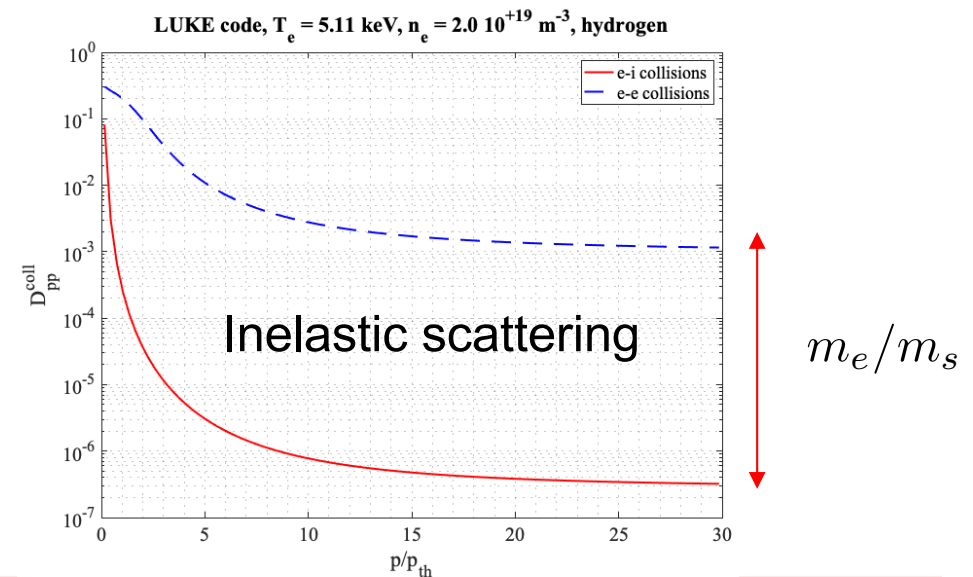
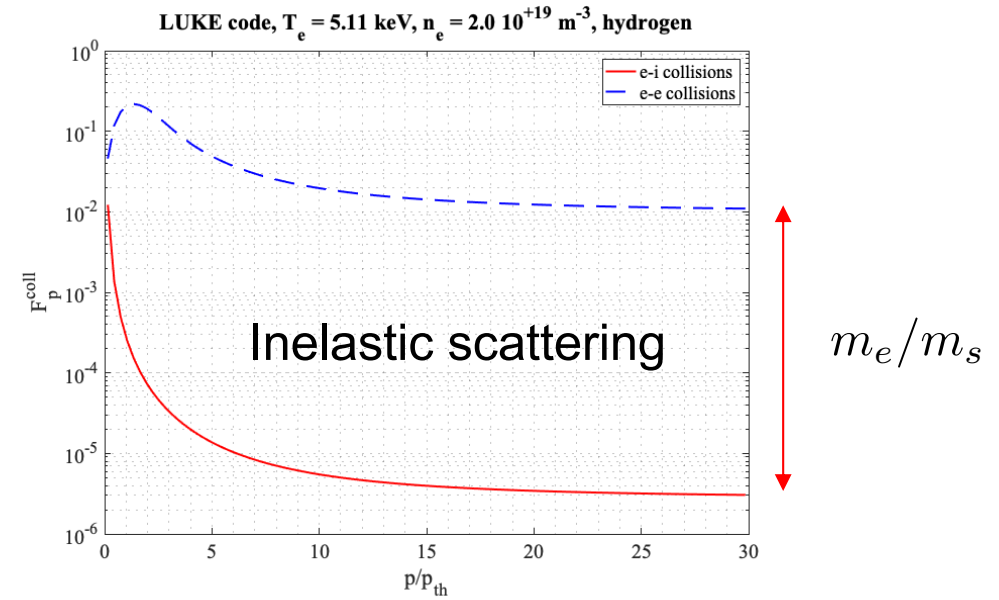
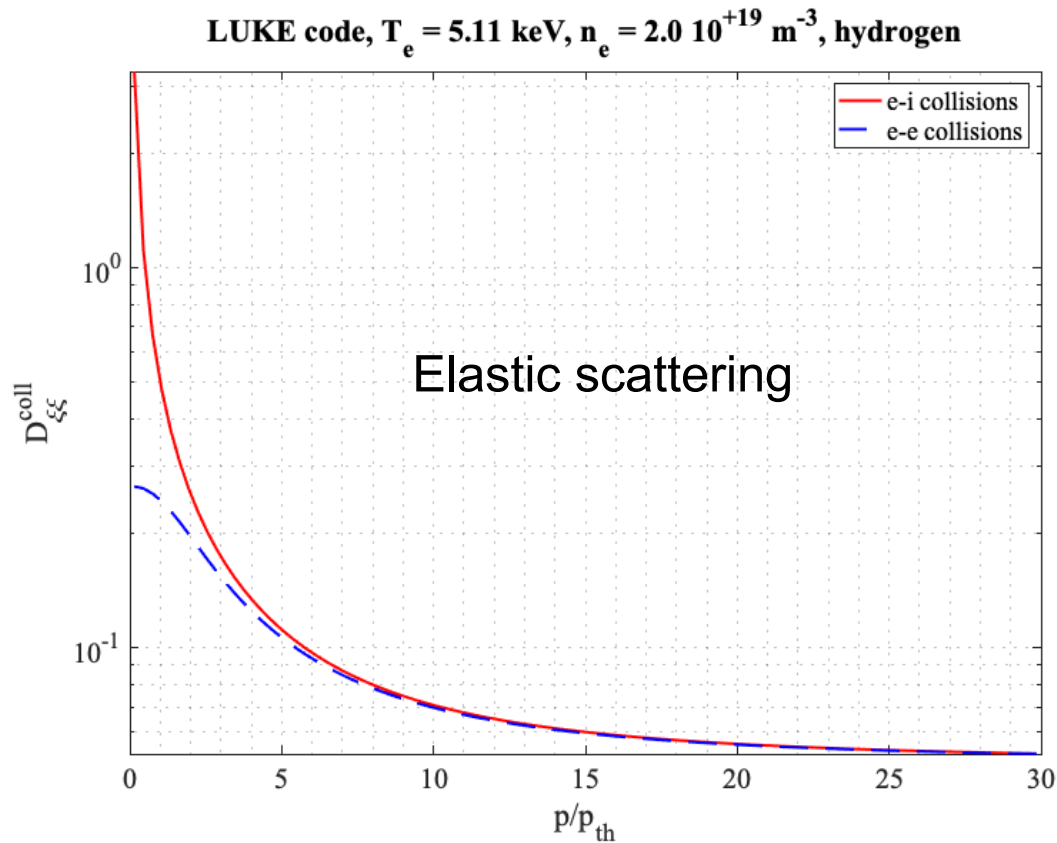
$$\bar{\lambda}^3 - X_1 \bar{\lambda}^2 + X_2 \bar{\lambda} - X_3 = 0$$

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

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

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

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



$$g_{Z_0,s}^{num}(\bar{p}) = (Z_s^2 - Z_{0,s}^2) (\ln(2\bar{p}/\alpha) + \gamma_{EM} - 1) + 2Z_s N_s \hat{I}_{1,Z_0,s} + N_s^2 \left( \frac{1}{2} - \hat{I}_{2,Z_0,s} \right)$$

$$\hat{I}_{1,Z_0,s} \equiv \frac{4\pi}{N_s} \int_0^\infty \bar{\rho}_{Z_0,s}^{num}(\bar{r}_1) \bar{r}_1^2 \ln \bar{r}_1 d\bar{r}_1$$

$$\hat{I}_{2,Z_0,s} = \frac{4\pi^2}{N_s^2} \int_0^\infty \bar{\rho}_{Z_0,s}^{num}(\bar{r}_1) \hat{J}_{2,Z_0,s}(\bar{r}_1) \bar{r}_1 d\bar{r}_1$$

$$\hat{J}_{2,Z_0,s}(\bar{r}_1) = \int_0^\infty \bar{\rho}_{Z_0,s}^{num}(\bar{r}_2) \bar{r}_2 d\bar{r}_2 \left( (\bar{r}_1 + \bar{r}_2)^2 \ln(\bar{r}_1 + \bar{r}_2) - (\bar{r}_1 - \bar{r}_2)^2 \ln|\bar{r}_1 - \bar{r}_2| \right)$$

DFT

where  $\gamma_{EM}$  is the Euler-Mascheroni constant.

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