THE HENRYK NIEWODNICZAŃSKI
INSTITUTE OF NUCLEAR PHYSICS
POLISH ACADEMY OF SCIENCES

Approximate atomic models for fast computation of suprathermal electron collisions with high-Z impurities in tokamak plasmas

Garching 05.05.2022

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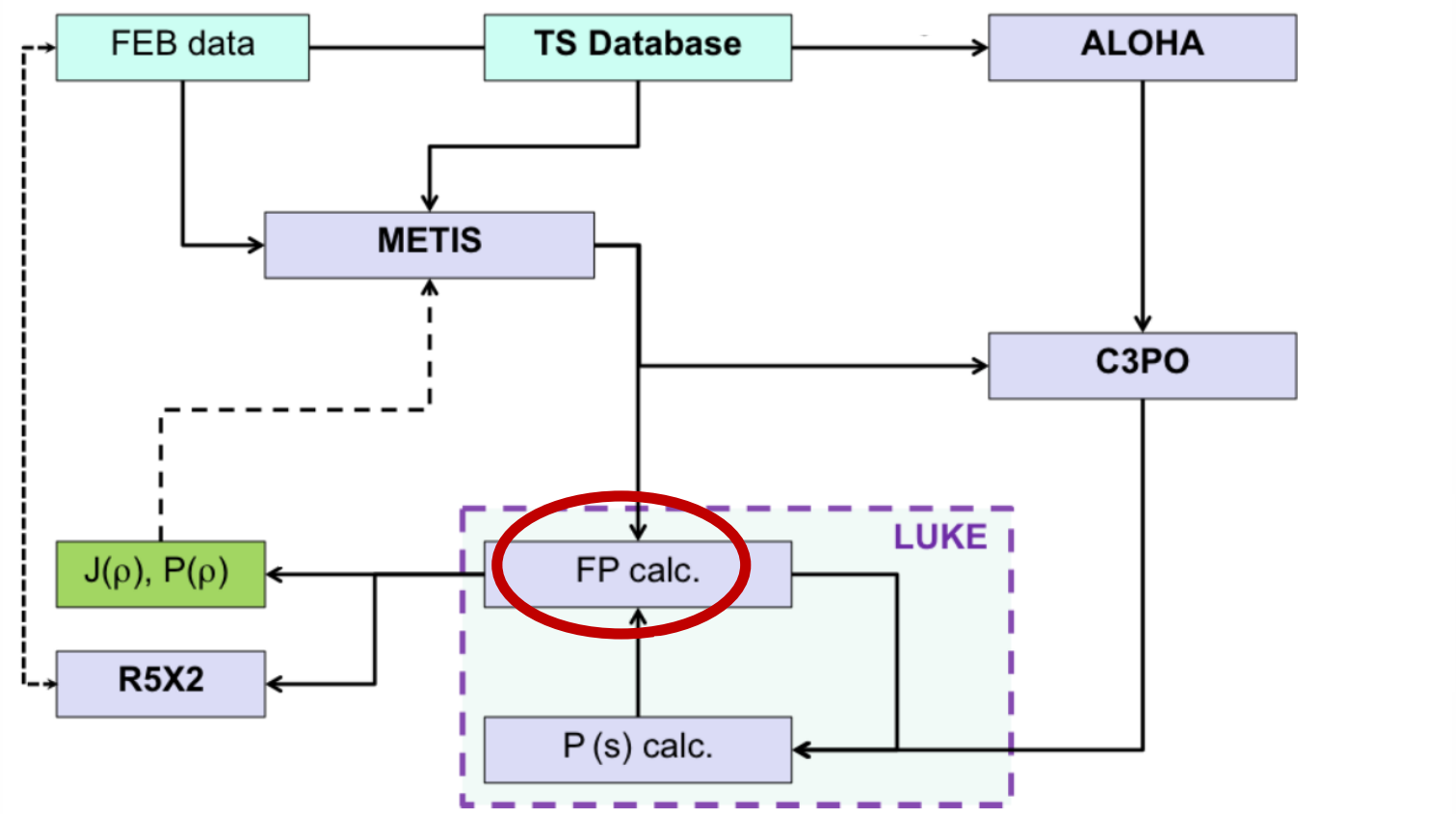
Chain of codes to simulate LHCD on WEST tokamak



Source: E. Nilsson *et al*, 2013 *Nucl. Fusion* **53** 083018.

Fokker-Planck equation solving

$$C^{ab} = \nu_D^{ab}\mathcal{L}(f_a) + \frac{1}{\boldsymbol{p}^2}\frac{\partial}{\partial \boldsymbol{p}}\left[\boldsymbol{p}^3\,\nu_s^{ab} f_a + \frac{1}{2}\,\nu_{||}^{ab}\frac{\partial f_a}{\partial \boldsymbol{p}}\right]$$

C^{ab}- collision operator for collisions between particle species *a* and *b,*
$\mathcal{L}(f_a)$ – Lorentz scattering operator,
$\boldsymbol{p} = \gamma \boldsymbol{v}/c$ - normalized momentum,
f_a - velocity distribution function of species *a.*

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Deflection frequency
(elastic collisions)

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Slowing-down frequency (inelastic collisions)

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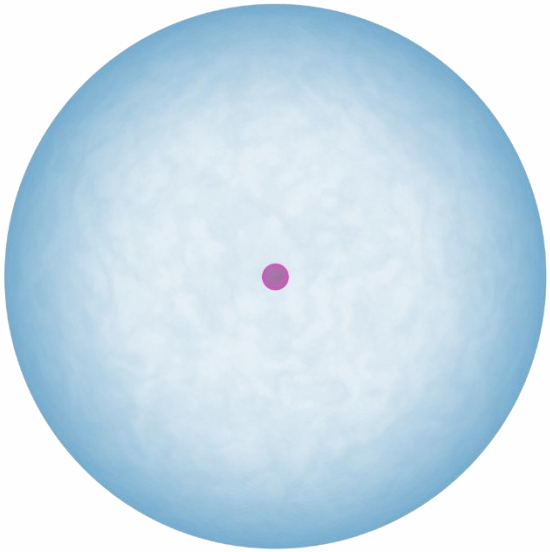
Physical background



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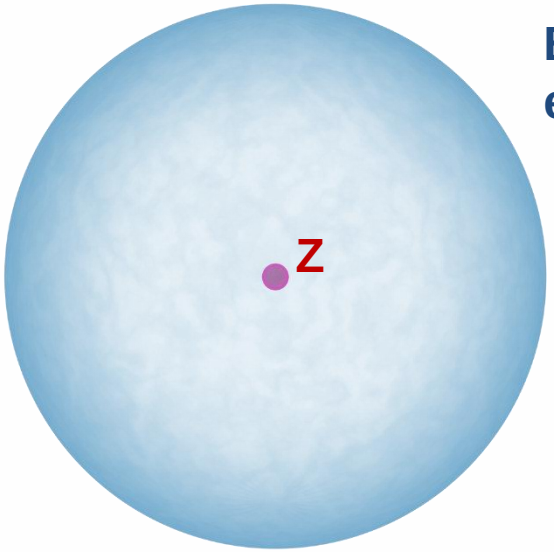
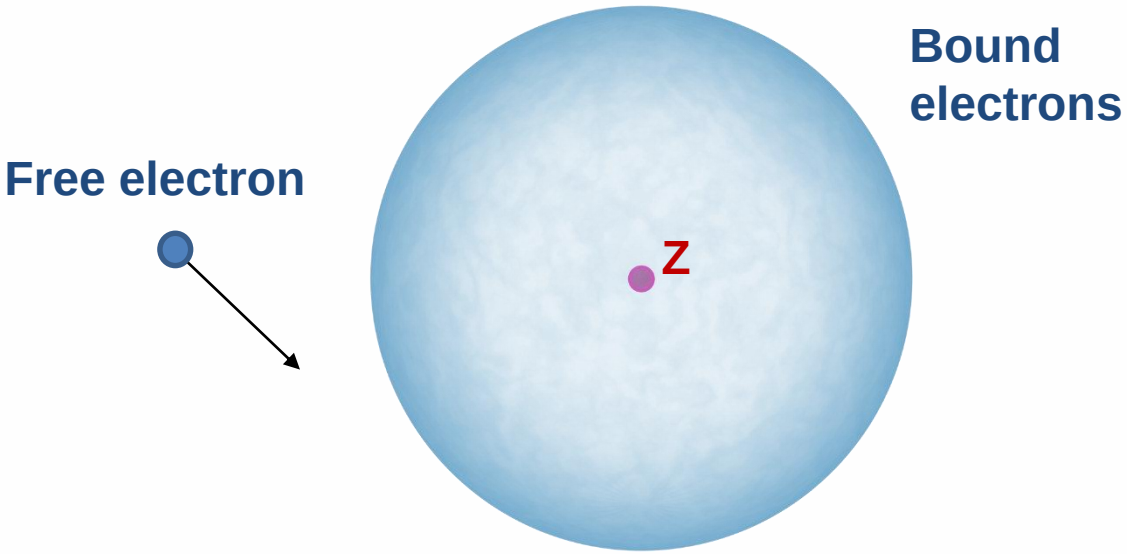
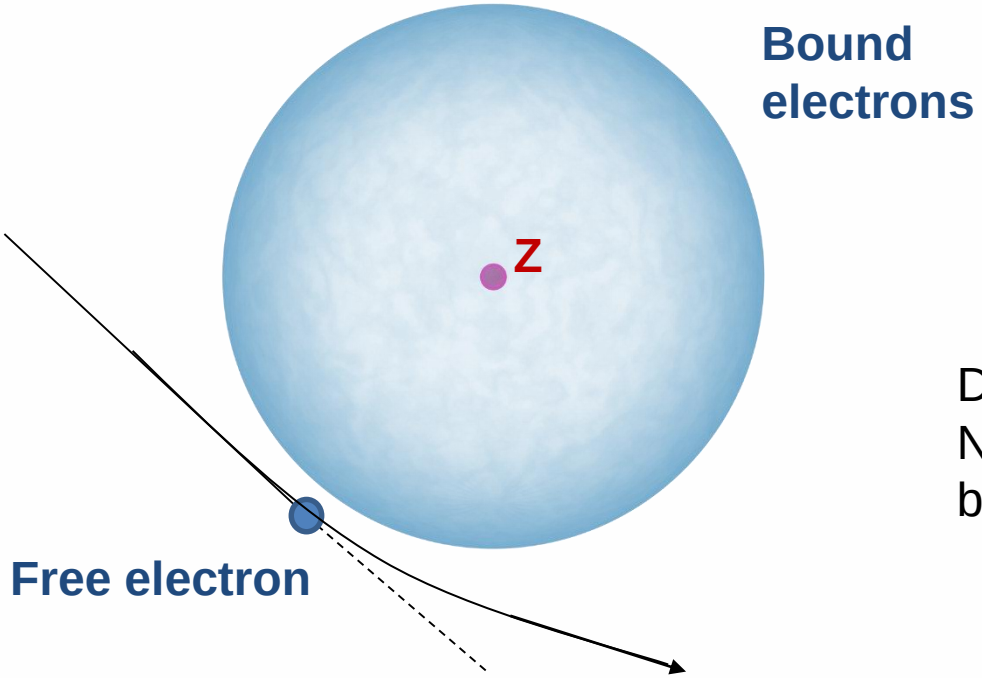


Bound electrons

Physical background

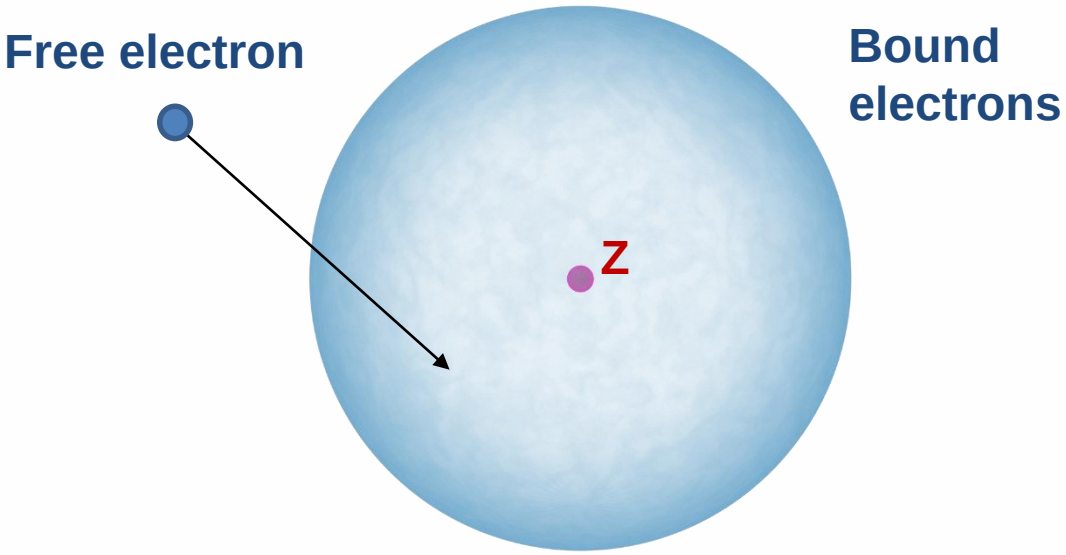


Physical background



Deflection is small
Nucleus is screened by
bound electrons

Physical background



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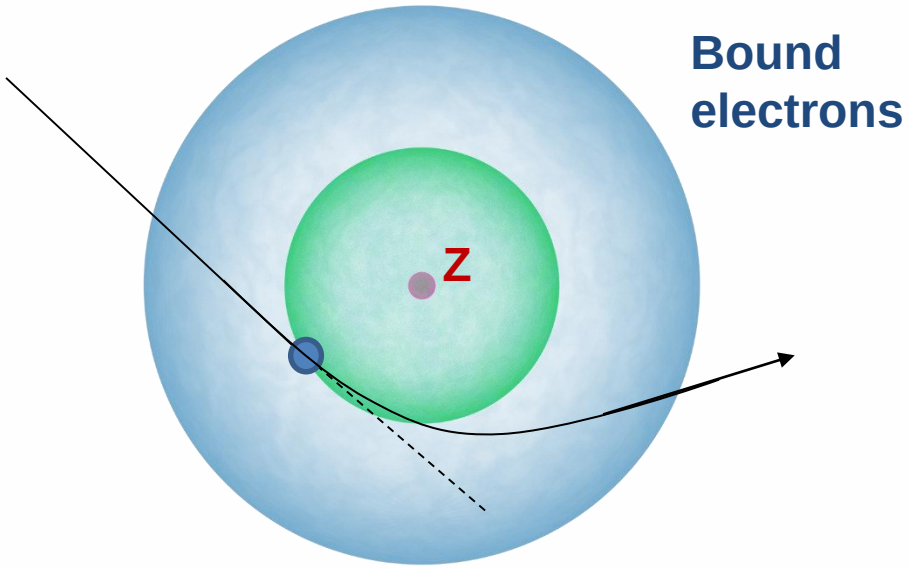
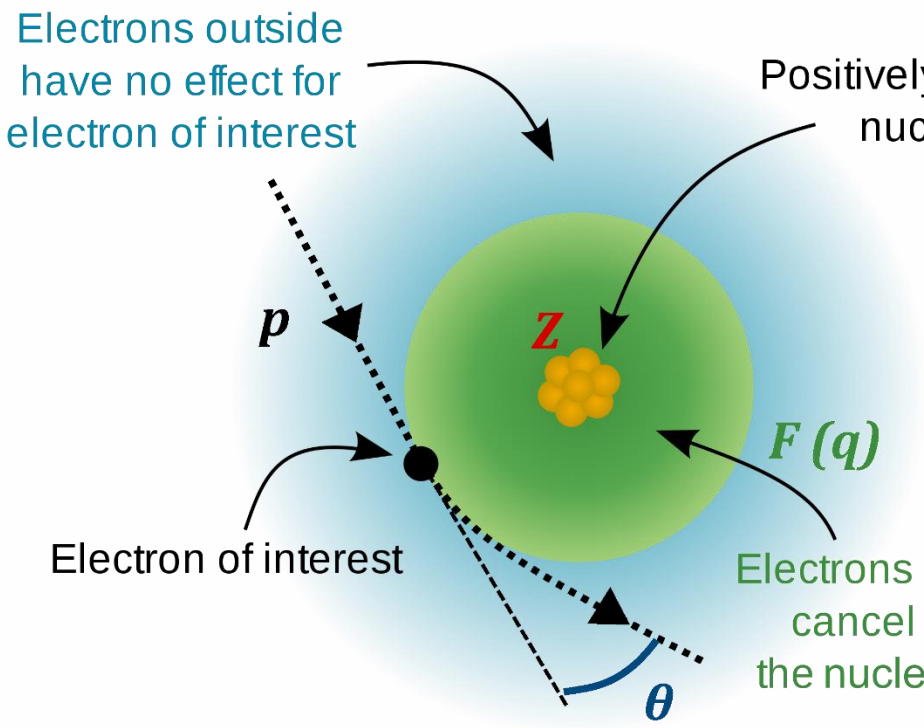


Physical background

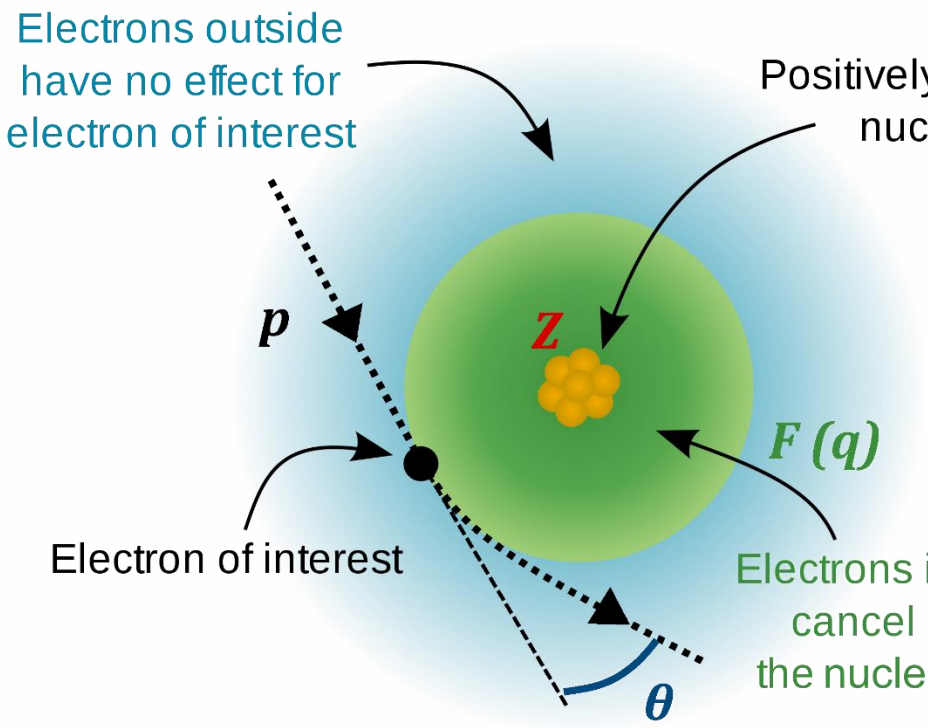


$$\boldsymbol{p}_{initial} - \boldsymbol{p}_{final} = \boldsymbol{q}$$

$$F(\boldsymbol{q}) = \int \rho(\boldsymbol{r}) e^{-i\mathbf{qr}/a_0}\, d^3r$$

Source: A. Jardin *et al*, 2020 IFJ PAN REPORT NO 2105/AP.
https://www.ifj.edu.pl/badania/publikacje/raporty/2020/2105.pdf

Physical background



F(q) = 0 **No screening**

0 < F(q) < N **Partial screening**

F(q) = N **Full screening**

N – number of bound electrons

Source: A. Jardin *et al*, 2020 IFJ PAN REPORT NO 2105/AP.
https://www.ifj.edu.pl/badania/publikacje/raporty/2020/2105.pdf

Elastic collision frequency

$$\frac{d\sigma_e^{coll}}{d\Omega} = \frac{{r_0}^2}{4\boldsymbol{p}^4}\left(\frac{cos^2(\theta/2)\boldsymbol{p}^2+1}{sin^4(\theta/2)}\right)[Z-F(\boldsymbol{q})]^2$$

r_0 – the classical electron radius,
θ - deflection angle,
$\boldsymbol{p} = \gamma\boldsymbol{v}/c$ - normalized electron momentum,
$\boldsymbol{v}$ – impacting electron velocity,
c – the speed of light in vacuum,
γ – Lorentz factor,
Z – atomic number.

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$$F(\boldsymbol{q}) = \int \rho(\boldsymbol{r}) e^{-i\mathbf{qr}/a_0}\, d^3r$$

→ Depends on electron density

r_0 – the classical electron radius,
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$\boldsymbol{p} = \gamma\boldsymbol{v}/c$ - normalized electron momentum,
$\boldsymbol{v}$ – impacting electron velocity,
c – the speed of light in vacuum,
γ – Lorentz factor,
Z – atomic number.

$\boldsymbol{q} = 2\boldsymbol{p}\sin(\theta/2)/\alpha$ is the momentum transfer,
$\alpha \approx 1/137$ – the fine structure constant,
$\boldsymbol{r}$ - atomic radius as a spatial coordinate measured from the centre of the atom,
a_0 – the Bohr radius,
N – the number of bound electrons.

Elastic collision frequency

$$\frac{d\sigma_e^{coll}}{d\Omega} = \frac{{r_0}^2}{4\boldsymbol{p}^4}\left(\frac{cos^2(\theta/2)\boldsymbol{p}^2+1}{sin^4(\theta/2)}\right)[Z-F(\boldsymbol{q})]^2$$

$$F(q) = 4\pi\int_0^\infty \rho(r)\frac{ra_0}{q}sin(qr/a_0)dr$$

Depends on electron density

r_0 – the classical electron radius,
θ - deflection angle,
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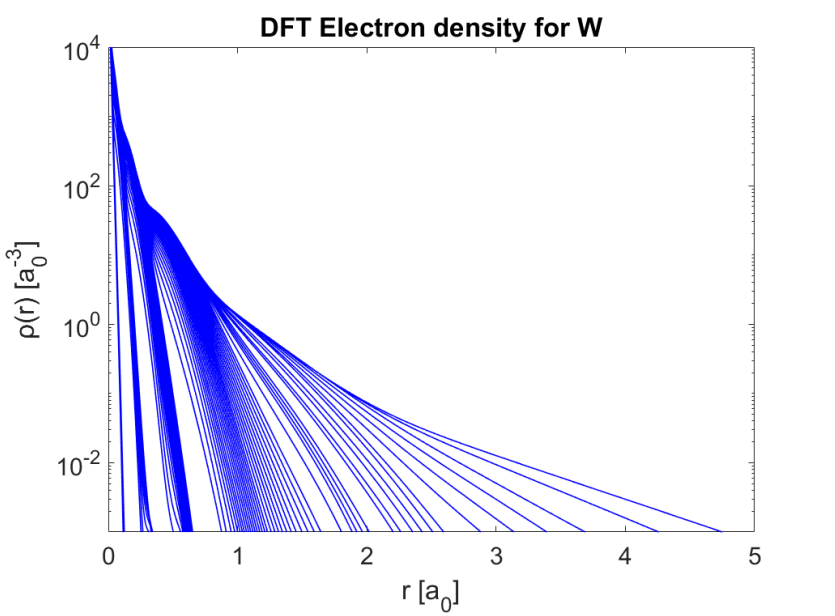
$r = |\boldsymbol{r}|$,
a_0– the Bohr radius,
N – the number of bound electrons.

Atomic models

Quantum mechanical model

- Density functional theory (**DFT**)



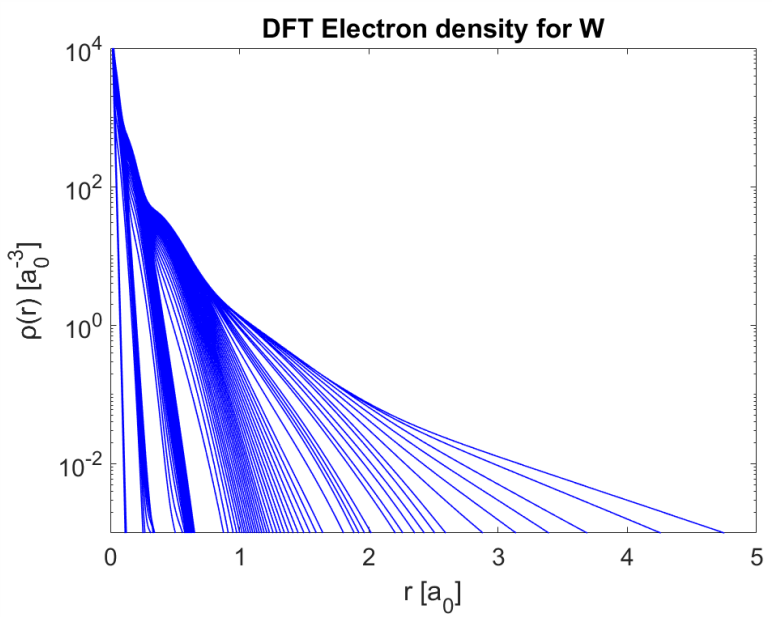
Atomic models

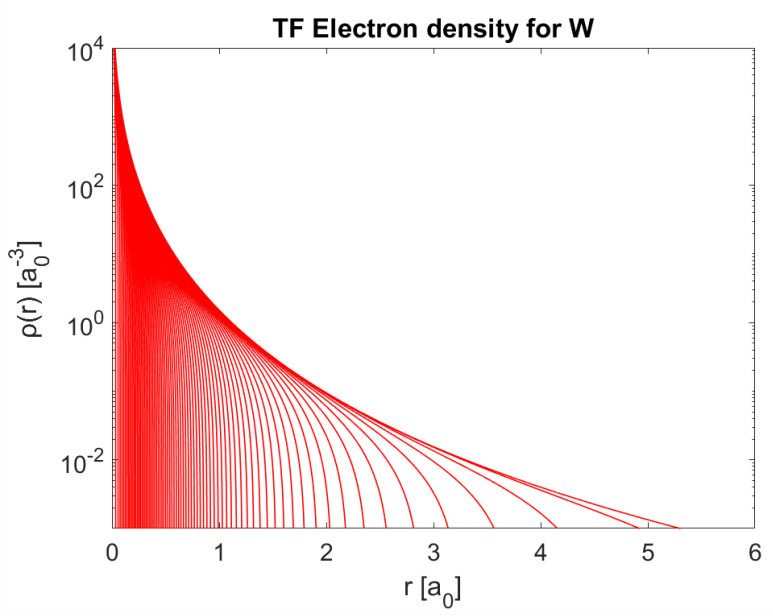
Quantum mechanical model

- Density functional theory (**DFT**)

Semi-empirical approximations:

- Thomas-Fermi (**TF**)
- Pratt-Tseng (**PT**):





Form factor calculation

$$F(q) = 4\pi \int_0^\infty \rho(r) \frac{r a_0}{q} sin(qr/a_0) dr$$

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Numerical integration:

- Density functional theory (DFT)
- Thomas-Fermi (TF)
- Thomas-Fermi-Dirac (TFD)

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Numerical integration:

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- Thomas-Fermi (TF)
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Numerically calculated integral can only be used to solve equations for collision frequencies in numerical way, which is time consuming!

Form factor calculation

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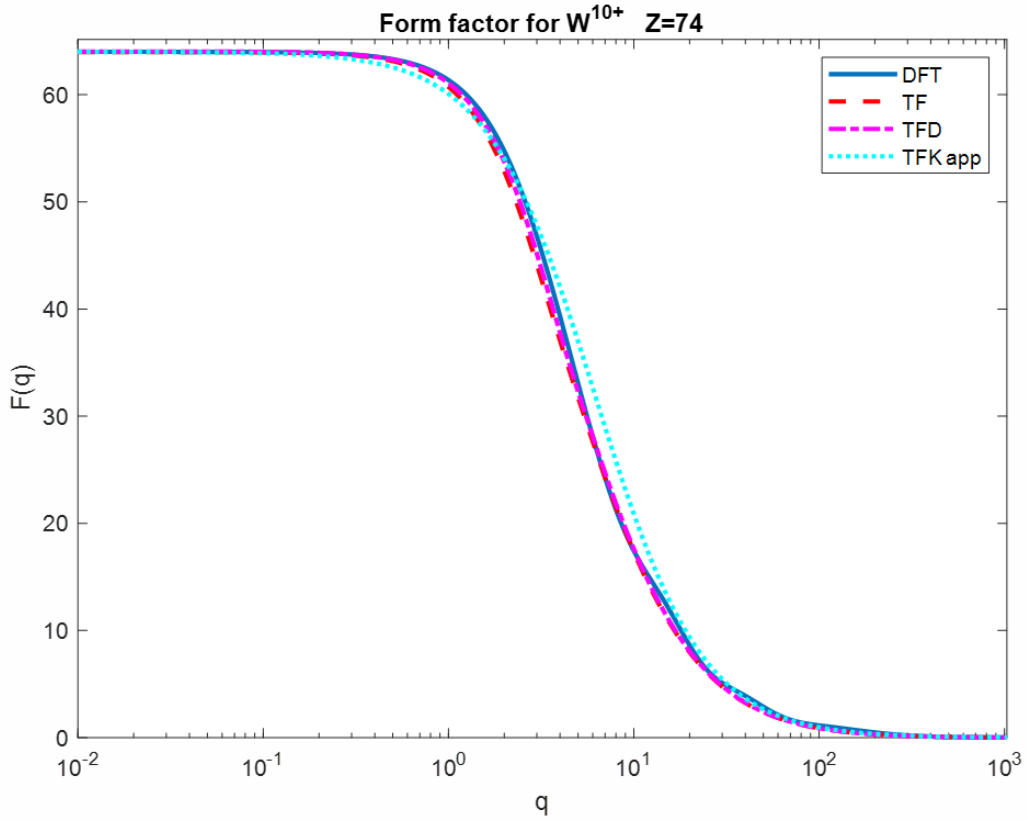
Numerical integration:

- Density functional theory (DFT)
- Thomas-Fermi (TF)
- Thomas-Fermi-Dirac (TFD)

Analytic integration:

- Thomas-Fermi Kirillov approximation (TFK)
- Pratt-Tseng (PT)

Results: DFT vs TF models



DESCRIPTION

- Form factor for tungsten ion W^{+10} calculated with different models
- Results from DFT, TF and TFD models are calculated with the numerical integration
- TFK approximation is calculated with an analytic integral

Figure of merit

$$RMS = \sqrt{\frac{1}{N^2} * \frac{1}{n} * \sum_{i=1}^{n} (F_{DFT}(q_i) - F_2(q_i))^2}$$

F_{DFT} – form factor calculated with DFT approach
F_2 – compared form factor
N – number of electrons in ion
n – number of q values

Figure of merit

$$RMS = \sqrt{\frac{1}{N^2} * \frac{1}{n} * \sum_{i=1}^{n} (F_{DFT}(q_i) - F_2(q_i))^2}$$

Root Mean Squared

Figure of merit

$$RMS = \sqrt{\frac{1}{N^2} * \frac{1}{n} * \sum_{i=1}^{n} (F_{DFT}(q_i) - F_2(q_i))^2}$$

Absolute difference

Root Mean Squared

Figure of merit

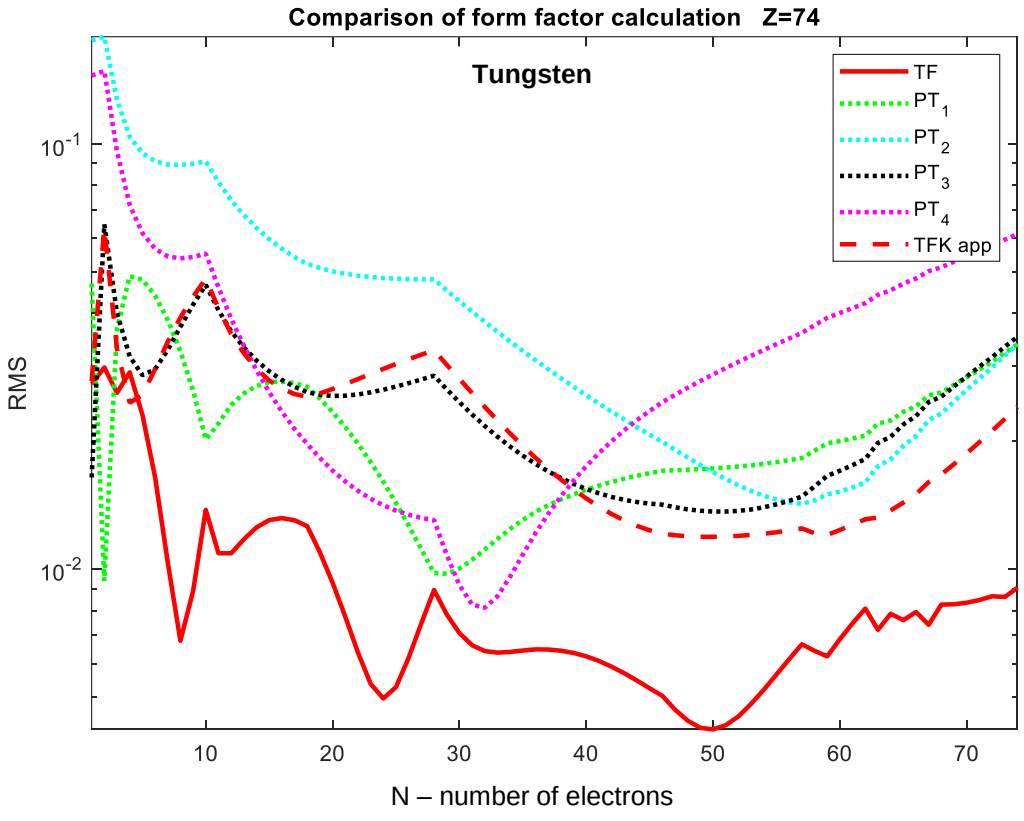
$$RMS = \sqrt{\frac{1}{N^2} * \frac{1}{n} * \sum_{i=1}^{n} (F_{DFT}(q_i) - F_2(q_i))^2}$$

Normalization

Root Mean Squared

Absolute difference

Results comparison



DESCRIPTION

- RMS of the **absolute** difference between form factors calculated with DFT and TF/TP electron density models:

$$\mathrm{RMS} = \frac{1}{N}\sqrt{\frac{1}{n}\sum_{i=1}^{n}(F_{DFT}(q_i) - F_2(q_i))^2}$$

Can we make it better?

Multi-exponential PT model - PT_{opt}

Electron density:

$$\rho_{PT}(r) = \frac{N}{4\pi r a^2} exp\left(-\frac{r}{a}\right)$$

Atomic form factor:

$$F_{PT}(q) = \frac{N}{1 + (qa)^2}$$

Multi-exponential PT model - PT_{opt}

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Atomic form factor:

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$$\rho_{PT_{opt}}(r) = \frac{1}{4\pi r}\left[\sum_{i=1}^{5} \frac{N_i}{a_i^2} \exp\left(-\frac{r}{a_i}\right)\right]$$

$$F_{PT_{opt}}(q) = \sum_{i=1}^{5} \frac{N_i}{1+(q a_i)^2}$$

Multi-exponential PT model - PT_{opt}

Grouping of the electrons in the PT_{opt} model					
Electron group	N_1	N_2	N_3	N_4	N_5
Max. number of bound electrons in each group	2	8	18	28	rest
Total bound electrons when group fully occupied	2	10	28	54	rest

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$$a_i(Z,N) = 1/\sqrt{{\lambda_i}^2 * \frac{(1-x^{n_{s,i}+1})}{1-x}}, \text{ where } x = \frac{Z-N}{Z}$$

$$\lambda_i(Z) = c_{1,i} * Z^{c_{2,i}}$$

$$n_{s,i}(Z) = c_{3,i} * Z^{c_{4,i}}$$

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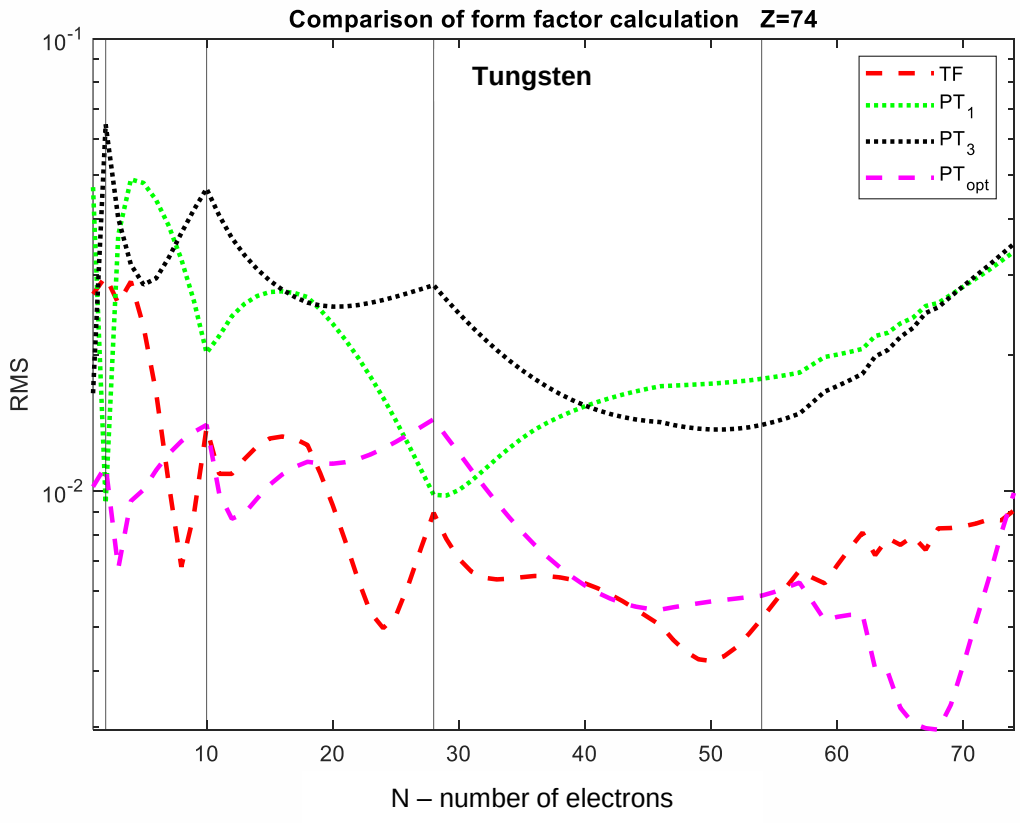
Optimized parameters for PT_{opt} model

		i = 1	i = 2	i = 3	i = 4	i = 5
$\lambda_i(Z)$	$c_{1,i}$	1.1831	0.1738	0.0913	0.0182	0.7702
	$c_{2,i}$	0.8368	1.0987	0.9642	1.2535	0.2618
$n_{s,i}(Z)$	$c_{3,i}$	0.3841	0.6170	1.0000	1.0000	1.0000
	$c_{4,i}$	0.5883	0.0461	1.0000	1.0000	1.0000

Results: PT_{opt}



DESCRIPTION

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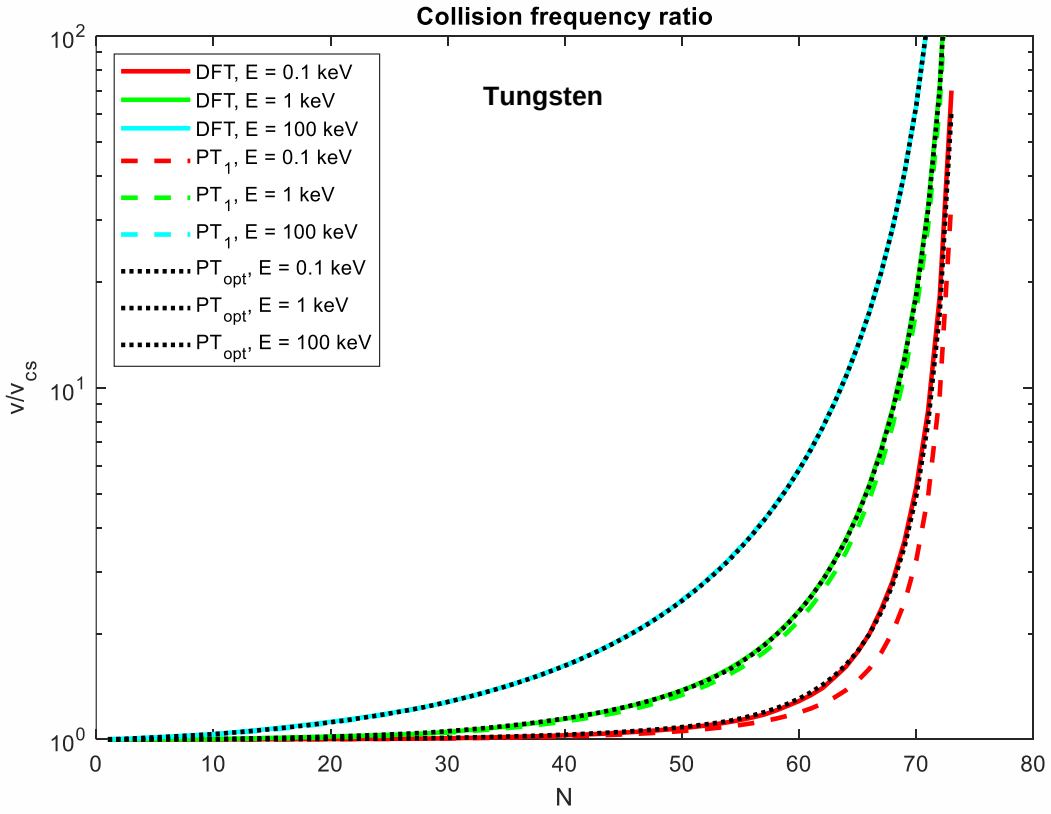
$$\mathrm{RMS} = \frac{1}{N}\sqrt{\frac{1}{n}\sum_{i=1}^{n}(F_{DFT}(q_i) - F_2(q_i))^2}$$

Results: collision frequency



DESCRIPTION

DFT – high accuracy, low speed

PT1 – high speed, not so accurate

PT opt – high accuracy, high speed

- Collision frequency ratio
  $\frac{\nu}{\nu_{cs}} = \frac{partial\ screening\ case}{complete\ screening\ case}$
- Plasma parameters:
  - electron density
    $n_e = 5 \cdot 10^{19}\ m^{-3}$
  - electron temperature
    $T_e = 3\ keV$

Fokker-Planck equation solving - reminder

$$C^{ab} = \nu_D^{ab}\mathcal{L}(f_a) + \frac{1}{p^2}\frac{\partial}{\partial p}\left[p^3\,\nu_s^{ab}\,f_a + \frac{1}{2}\,\nu_{||}^{ab}\,\frac{\partial f_a}{\partial p}\right]$$

Deflection frequency (elastic collisions)

Slowing-down frequency (inelastic collisions)

Parallel-diffusion frequency (parallel-diffusion)

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Inelastic collisions - Stopping power

Formal definition:

$$S(v) = -\frac{1}{n}\frac{dE(v)}{dx}$$

S(v) – stopping power
E(v) – particle kinetic energy
v – particle velocity
n – scatterer density
x – length of the particle trajectory

Inelastic collisions - Stopping power

Formal definition:

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Bethe-Bloch theory (with further corrections) [ICRU Report 1984]:

$$S(v) = \frac{4\pi e^4}{mv^2} N \left[ln\frac{2mv^2}{I} - \beta^2 - \frac{\delta}{2} - \frac{U}{2} \right]$$

S(v) – stopping power
E(v) – particle kinetic energy
v – particle velocity
n – scatterer density
x – length of the particle trajectory

N – number of bound electrons in target atoms
β = v/c - relativistic correction
δ – density-effect correction factor
U – shell-effect correction factor

Source: ICRU Report 49, Stopping Powers and Ranges for Protons and Alph Particles (1984).

Inelastic collisions - Stopping power

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Mean excitation energy

Source: ICRU Report 49, Stopping Powers and Ranges for Protons and Alph Particles (1984).

Mean excitation energy

Formal definition:

$$lnI = \frac{\sum_{n\neq 0} f_{n0} lnE_{n0}}{\sum_{n\neq 0} f_{n0}}$$

lnI – mean excitation energy
E_{n0} - energy of transition 0 -> n
f_{n0} – oscillator strength of transition 0 -> n

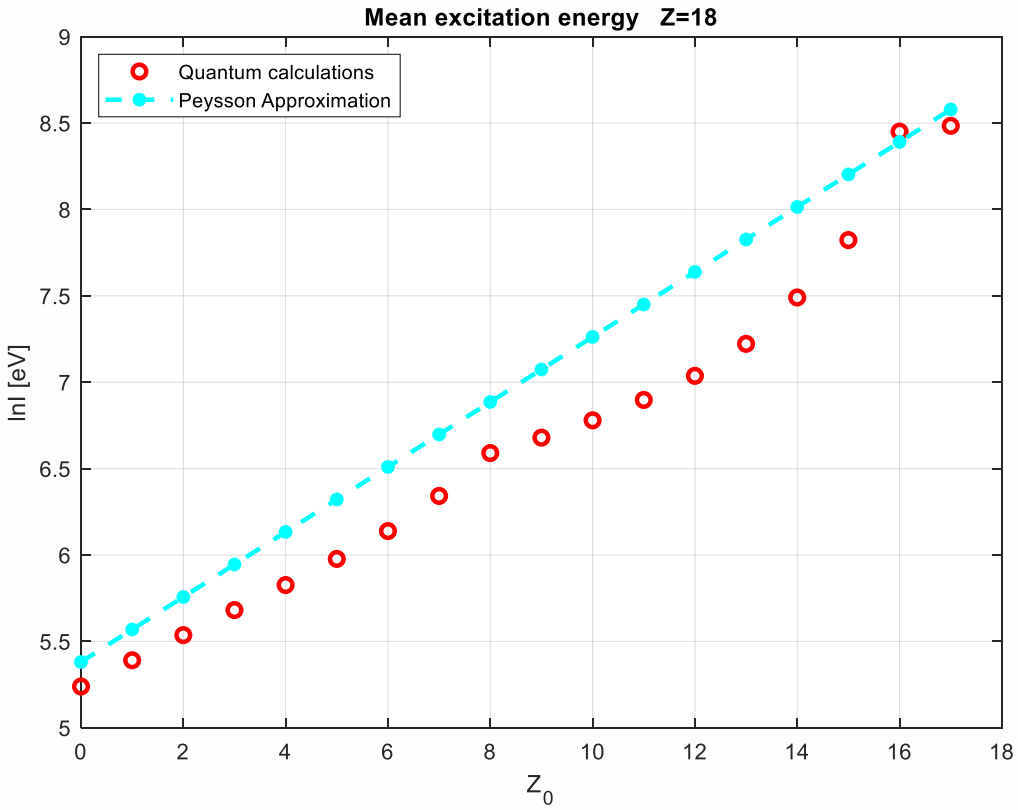
Mean excitation energy – Current approach

- Interpolation between
  - Neutral atom: $I_Z = 10\ Z\ eV$
  - Hydrogen like atom: $I_{1,Z} = I_{1,H}\ Z^2 = 13.6\ Z^2\ eV$
- With exponential function

$$I_N = exp\left(a\frac{Z-N}{Z-1} + b\right)$$

- Where $b = \ln(10\ Z)$, $a = \ln\left(13.6\ Z^2\right) - b$

Results – Mean excitation energy



DESCRIPTION

- Interpolation used in LUKE compared to quantum calculations by Sauer at.al

Source: S. P. Sauer et al, Advances in Quantum Chemistry Vol. 71 (Academic Press, New York, 2015), p. 29.

Mean excitation energy

Formal definition:

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Local plasma approximation [Lindhard 1953] (LPA):

$$lnI = \frac{1}{N}\int d^3r 4\pi r^2 \rho(r) ln(\gamma \hbar \omega_0)$$

$$\omega_o = \sqrt{4\pi e^2 \rho(r)/m}$$

lnI - mean excitation energy
E_{n0} - energy of transition 0 -> n
f_{n0} - oscillator strength of transition 0 -> n

ω_0 - local plasma frequency
r - atomic radius
$\hbar$ – reduced Planck constant

Source: J. Lindhard and M. Scharff, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 27 (1953) no. 15.

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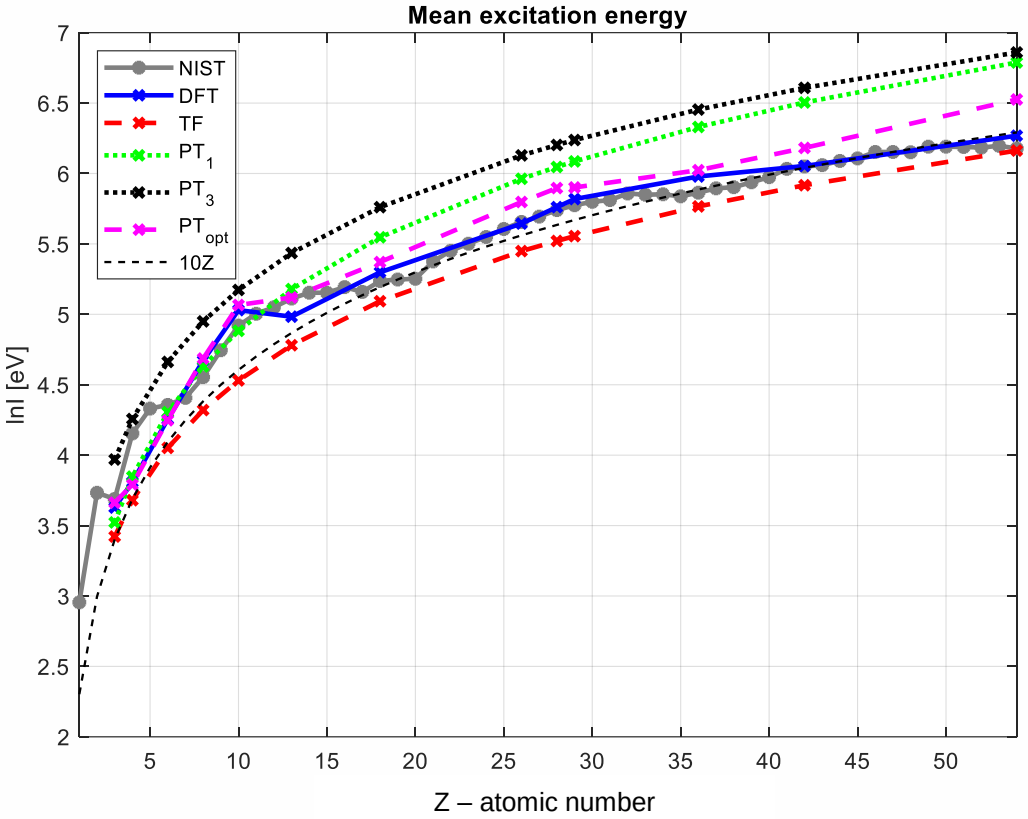
Depends on electron density (atomic model)

Source: J. Lindhard and M. Scharff, K. Dan. Vidensk. Selsk. Mat. Fys. Medd. 27 (1953) no. 15.

Results – neutral atoms

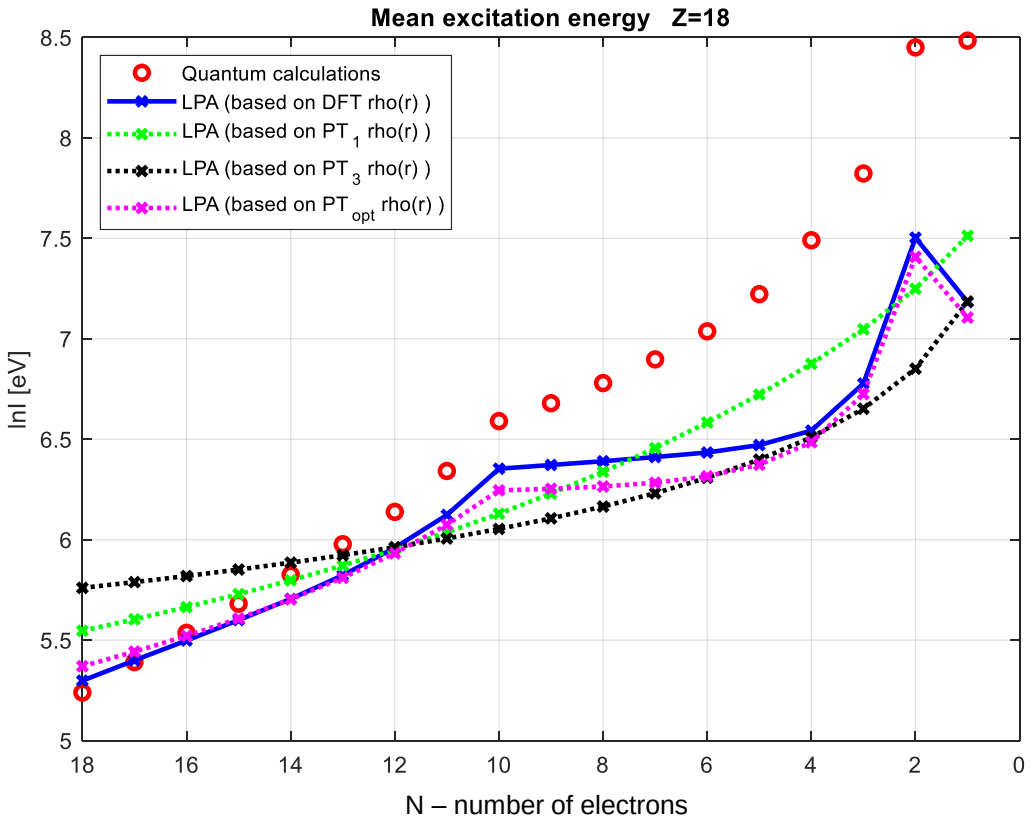


DESCRIPTION

- Mean excitation energy of neutral atoms
- Comparison of results from NIST Database and data calculated with LPA based on different electron density models
- LPA calculations cover only limited number of data points

Source: *NIST X-Ray Mass Attenuation Coefficient* https://physics.nist.gov/PhysRefData/XrayMassCoef/tab1.html

Results – Argon ions



DESCRIPTION

- Mean excitation energy of argon ions
- Comparison of results from multi-configurational self-consistent field calculations by Sauer et al. and LPA based on different electron density models

Source: S. P. Sauer et al, Advances in Quantum Chemistry Vol. 71 (Academic Press, New York, 2015), p. 29.

Alternative solution

- Calculate **all significant transition energies and oscillator strength for every ion** of interest and use the definition of mean excitation energy:

$$lnI = \frac{\sum_{n\neq 0} f_{n0} lnE_{n0}}{\sum_{n\neq 0} f_{n0}}$$

Reference

J. Walkowiak, A. Jardin, J. Bielecki, Y. Peysson, D. Mazon, D.Dworak, K. Król, and M. Scholz, *Approximate atomic models for fast computation of the Fokker–Planck equation in fusion plasmas with high-Z impurities and suprathermal electrons*, Physics of Plasmas **29**, 022501 (2022);

https://doi.org/10.1063/5.0075859

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