Из истории конференции

Воспоминания участника

ELBRUS 2021, March 1-5

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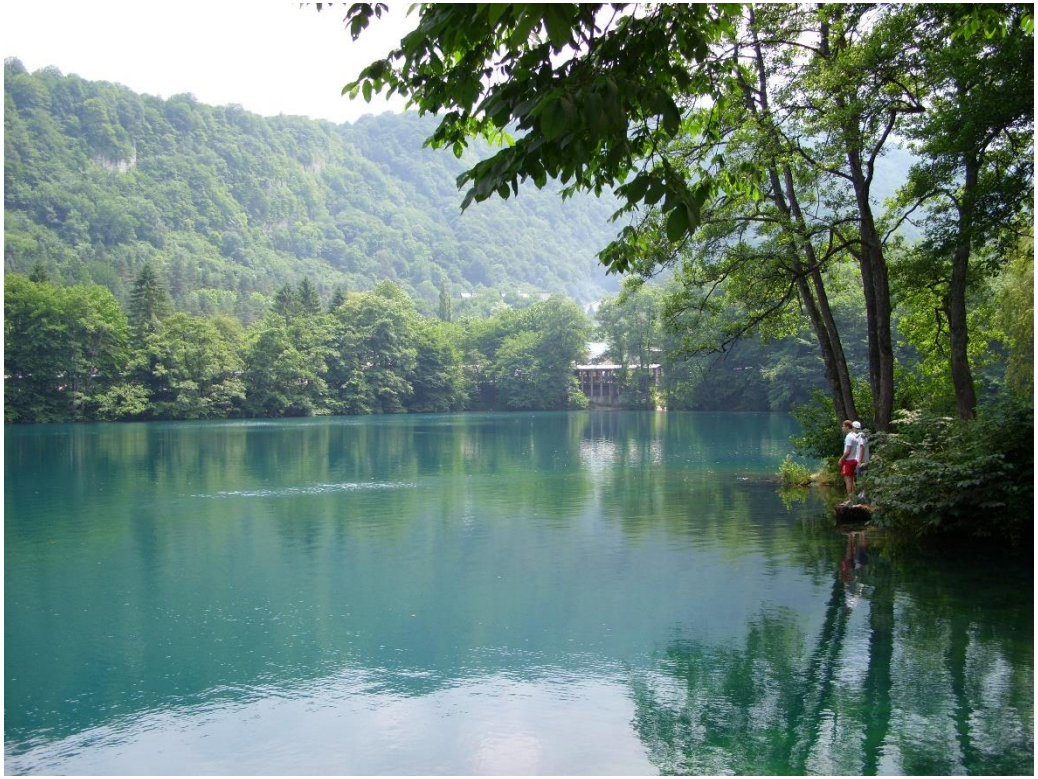

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ELBRUS 2021, March 1-5

Atomic number similarity law in individual electronic shells of all natural elements

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ELBRUS 2021, March 1-5

Outline

1. **Basis of the method used**
2. **Algorithm of the method application**
3. **Experimental data in atomic *K*, *L*, *M* shells**
4. **Experimental and RLDA data in atomic *N*, *O*, *P* shells**
5. **Reconstructed data**
6. **Conclusion**

1.1 Basis of the method used

- The quantization condition:

$$S_{n0}(E) = \int \sqrt{2(E - U(r)}\, dr = \pi n, \text{ if } l = 0;$$

$$S_{nl}(E) = \int \sqrt{2(E - U(r) - \lambda^2/r^2}\, dr = \pi(n - \lambda)$$

$$E_{nl}(Z) - E_{n0}(Z) \sim \lambda^2, \quad \lambda = l + 1/2$$

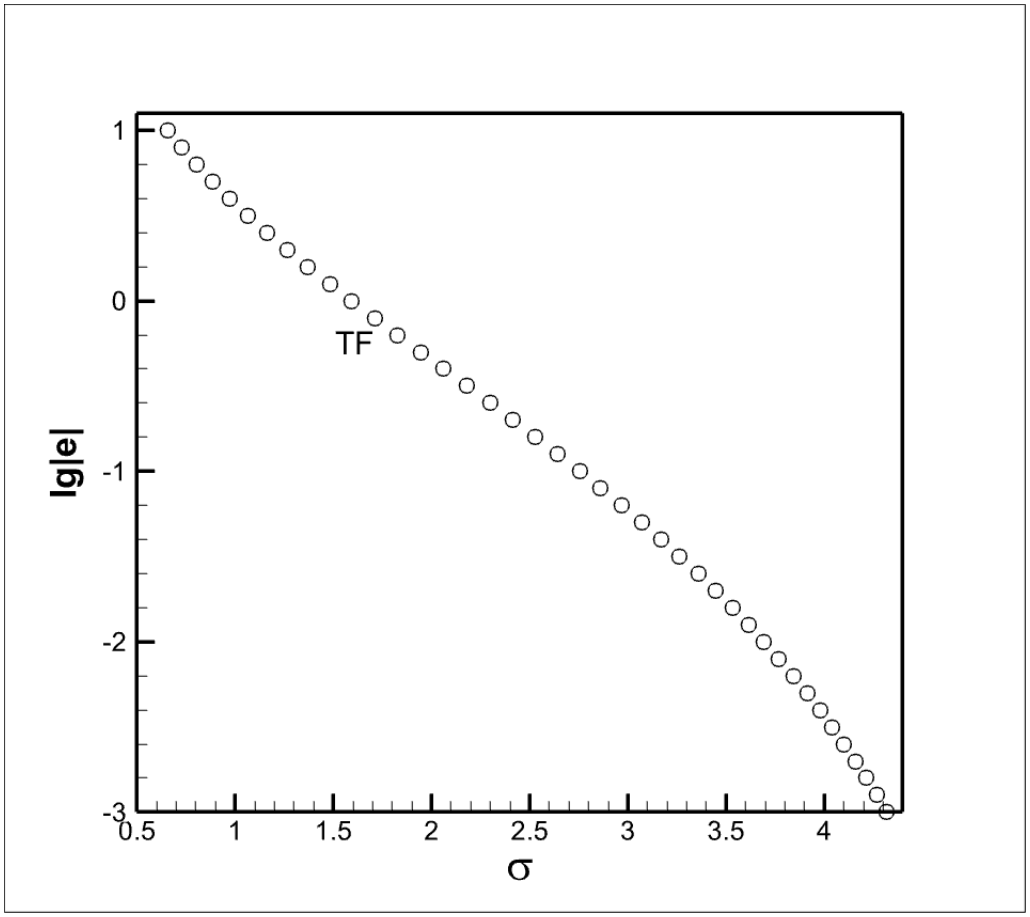
- Then electron energy levels **in TF atom** are

$$E_{n0}(Z) = Z^{4/3} e(\sigma_n), \quad \sigma_n = \pi n Z^{-1/3}, \quad \text{if } l = 0;$$

$$E_{nl}(Z) = E_{n0}(Z) + Z^{2/3} d(\sigma_n)\lambda^2$$

Where $e(\sigma)$ and $d(\sigma)$ are **universal** functions

1.2 Functions $e(\sigma)$ in TF model for atoms Z = 10 - 92

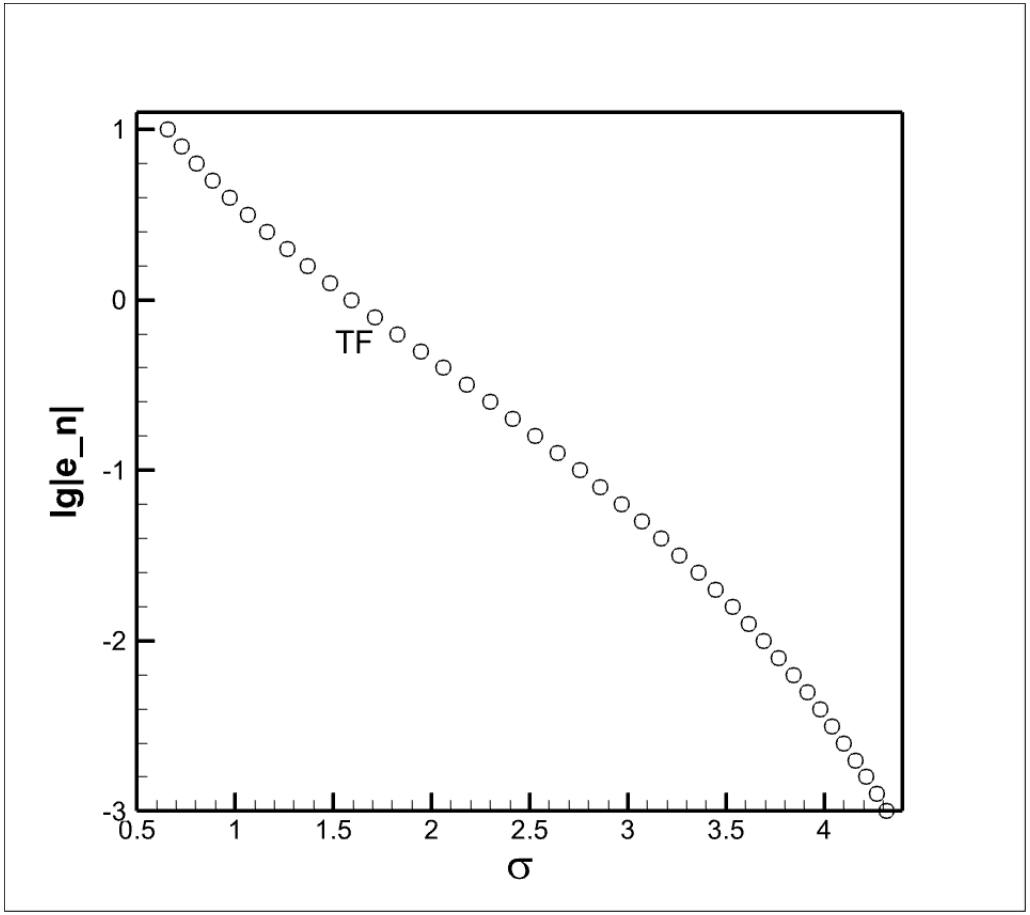


2.1 Algorithm for representing experimental electron binding energies (EBE) in atoms

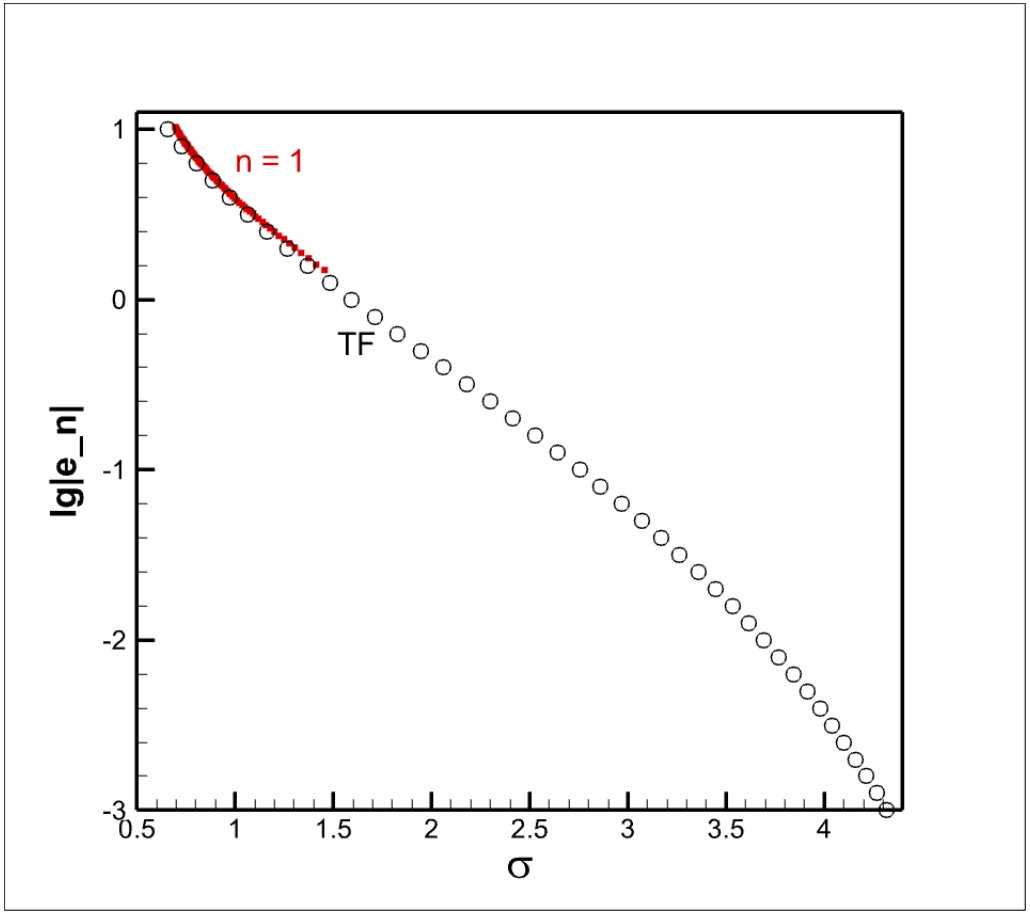
$$e_n(\sigma_n) = \frac{E_{no}}{Z^{4/3}}, \qquad \sigma = \frac{\pi n}{Z^{1/3}},$$

$$d_{nlj}(\sigma_n) = \frac{E_{nlj} - E_{no}}{(l+1/2)^2 Z^{2/3}}, \quad j = l \mp 1/2$$

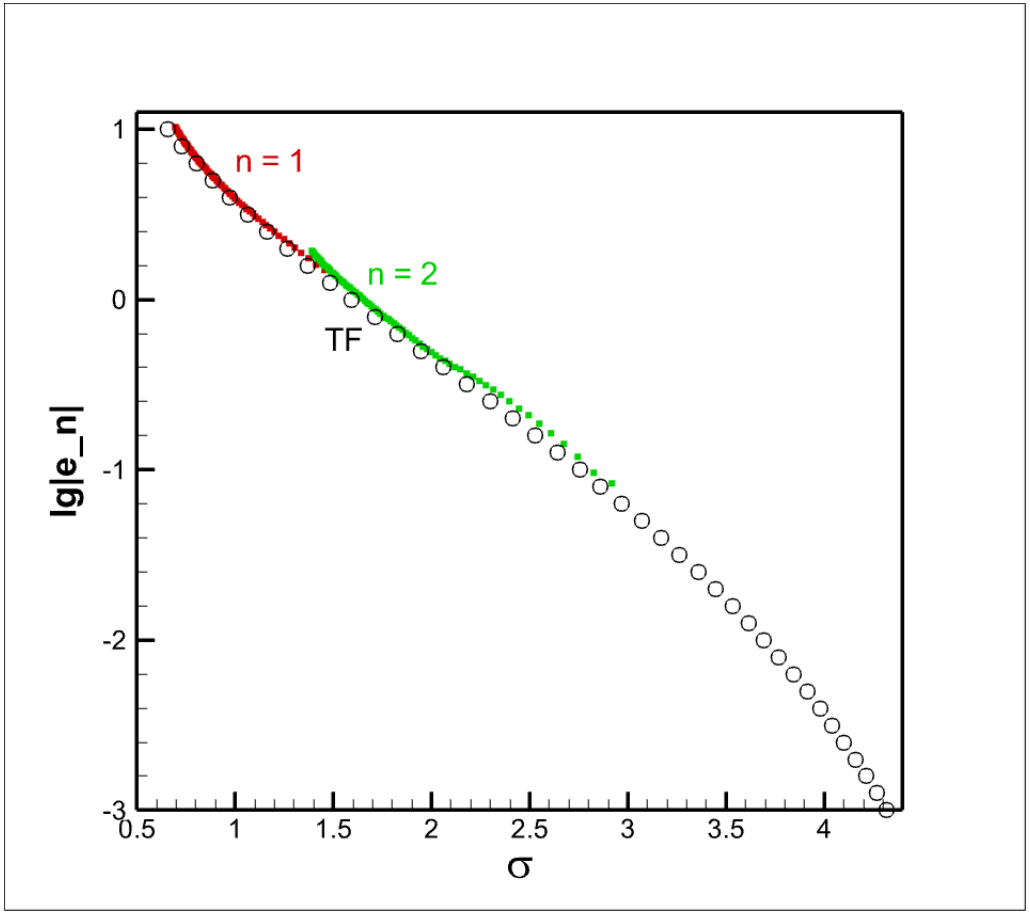
2.2 Functions $e(\sigma)$, TF and reconstructed from all the experimental s-levels E_{n0} for atoms Z = 10 - 92



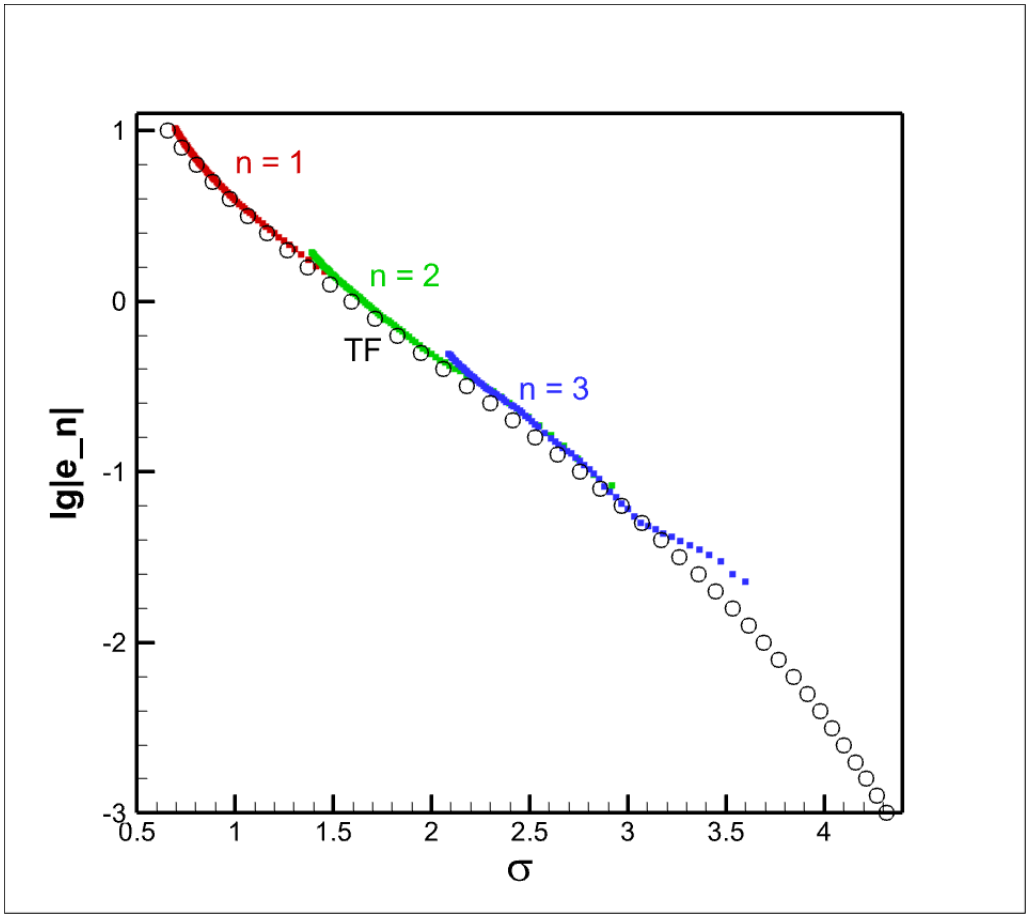
2.3 Functions $e(\sigma)$, TF and reconstructed from all the experimental s-levels E_{n0} for atoms Z = 10 - 92



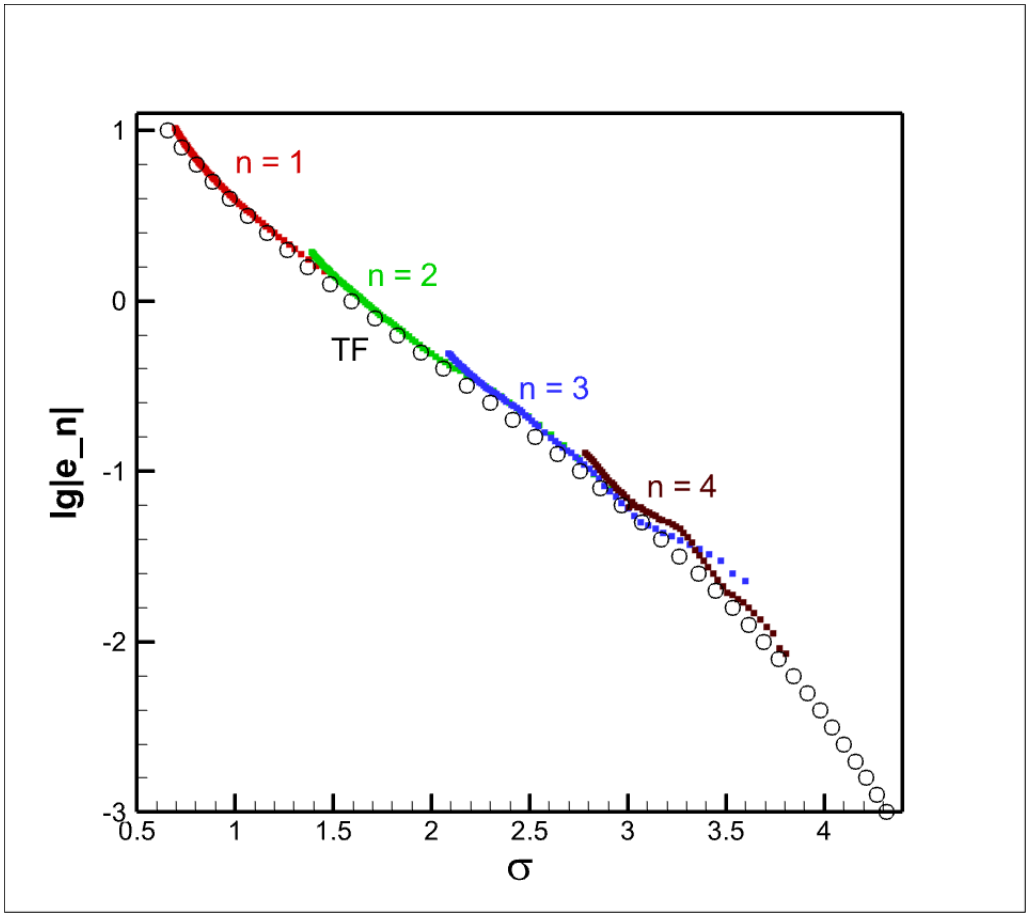
2.4 Functions $e(\sigma)$, TF and reconstructed from all the experimental electron s-levels E_{n0} for atoms Z = 10 - 92



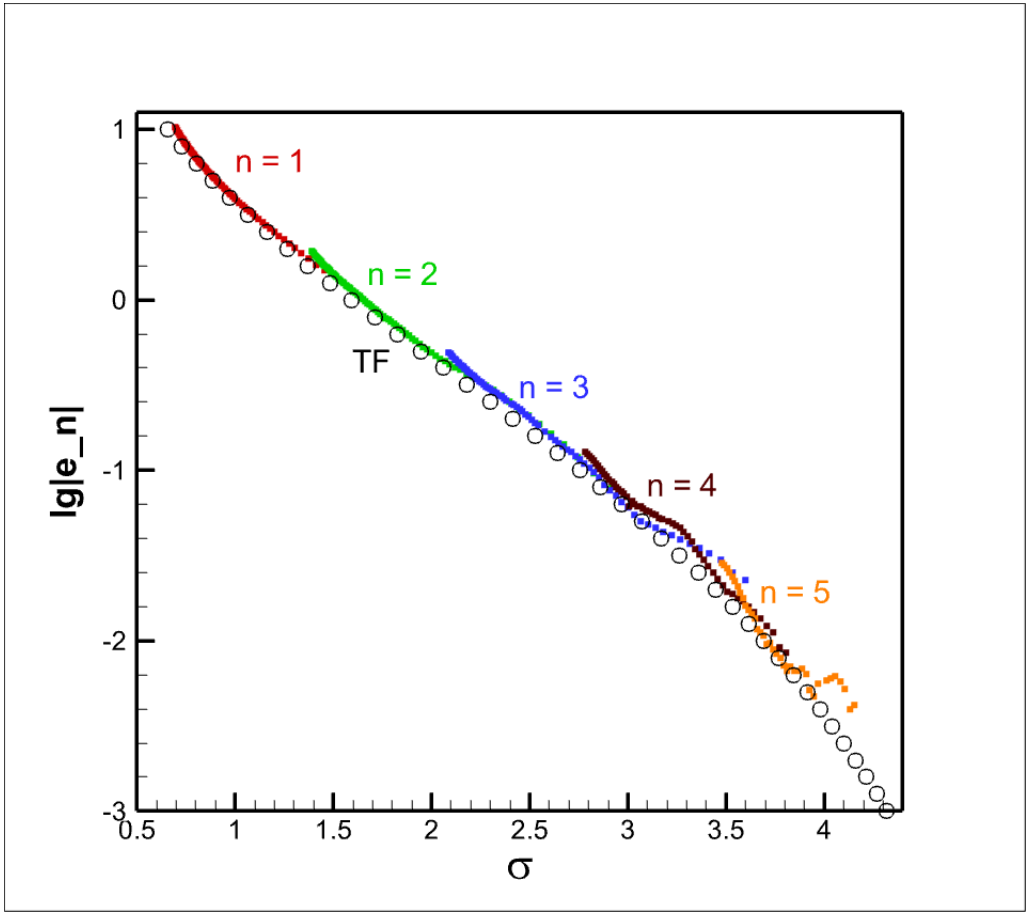
2.5 Functions $e(\sigma)$, TF and reconstructed from all the experimental s-levels E_{n0} for atoms Z = 10 - 92



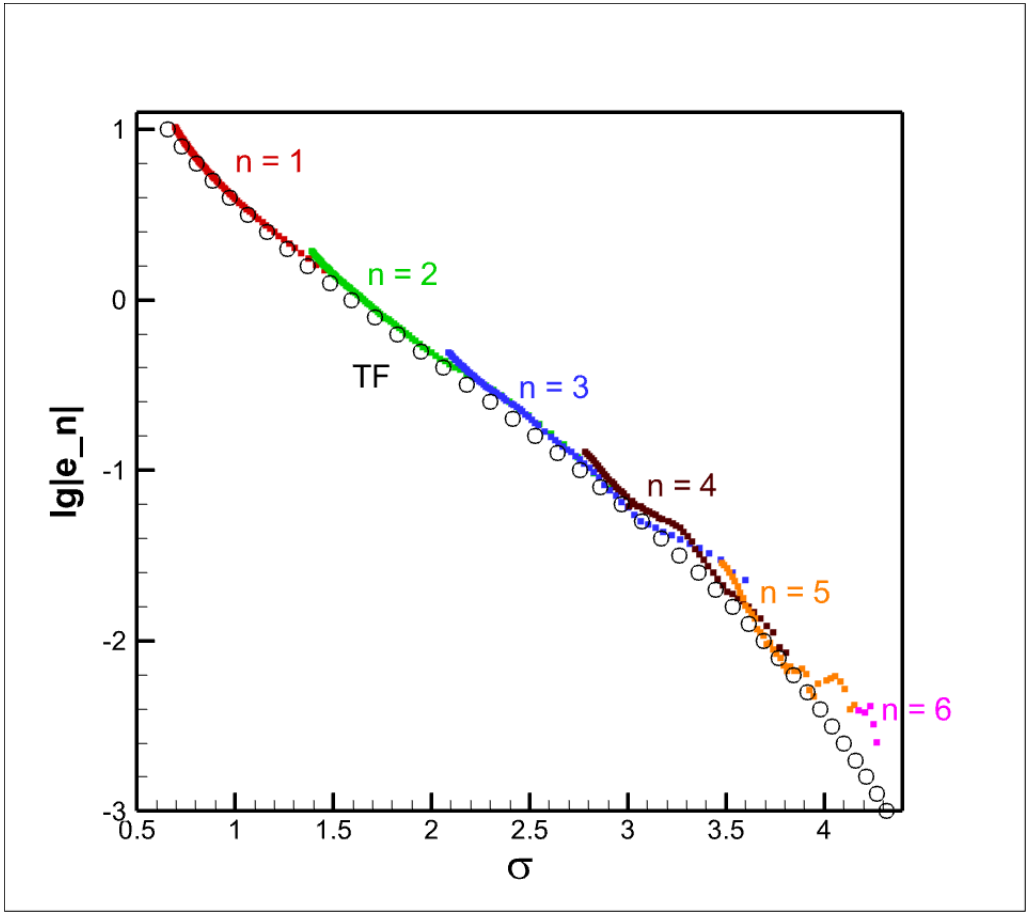
2.6 Functions $e(\sigma)$, TF and reconstructed from all the experimental ns-levels E_{n0} for atoms Z = 10 - 92



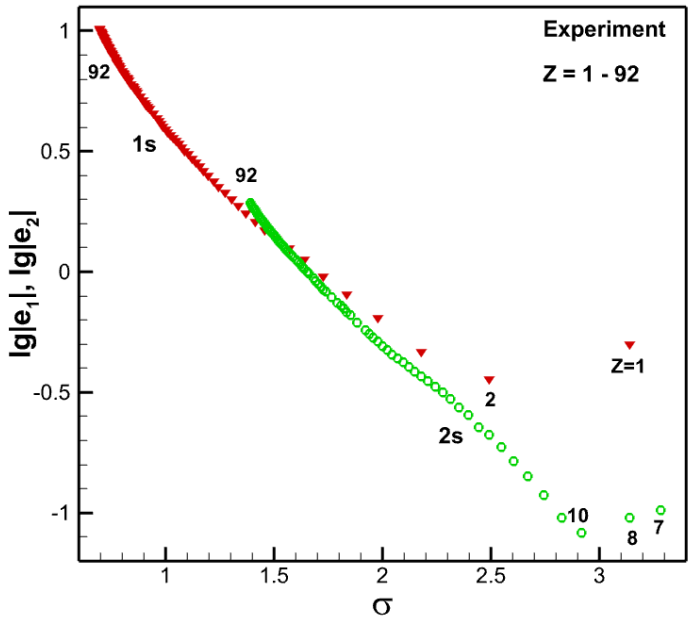
2.6 Functions $e(\sigma)$, TF and reconstructed from all the experimental s-levels E_{n0} for atoms Z = 10 - 92

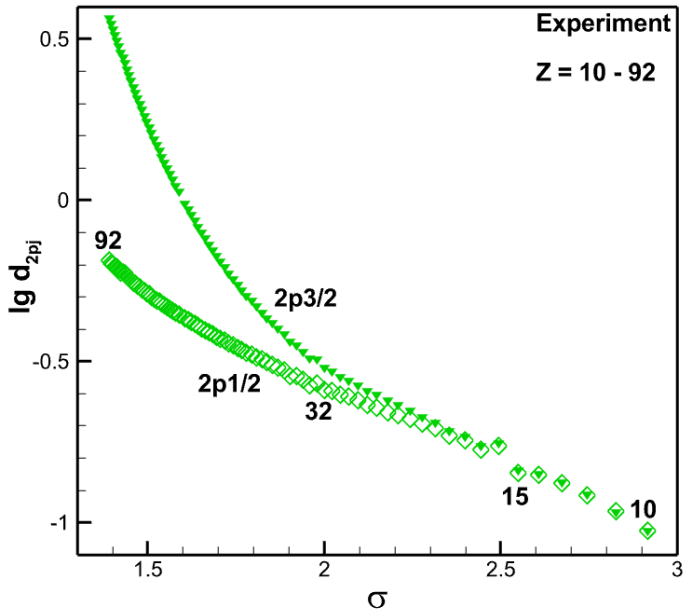


2.7 Functions $e(\sigma)$: TF and reconstructed from all the experimental s-levels E_{n0} for atoms Z = 10 - 92

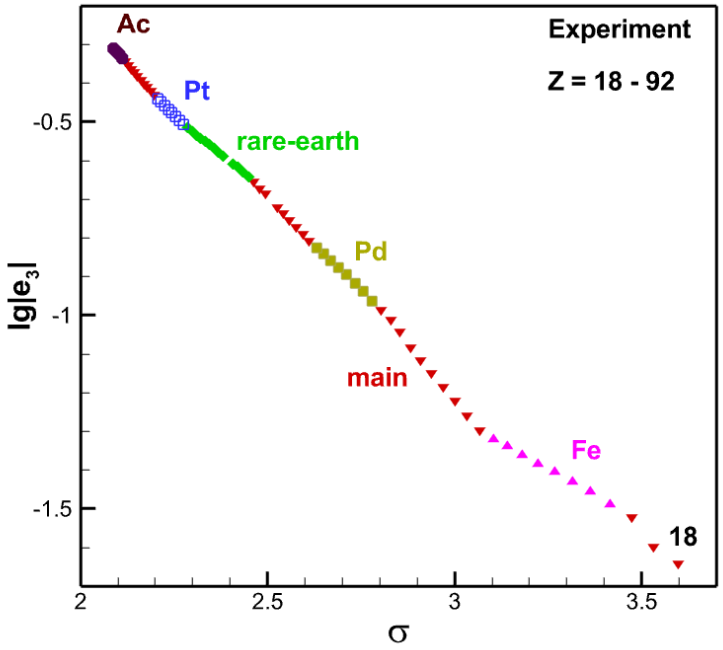


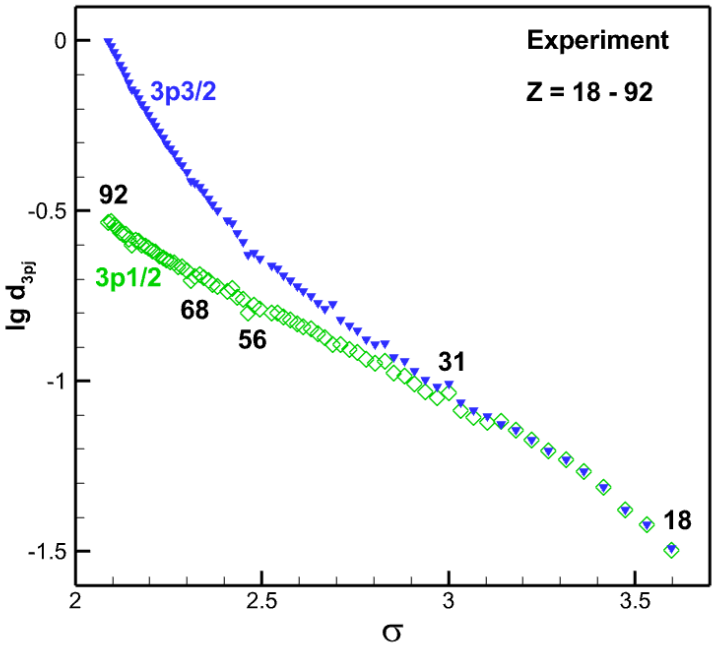
3.1 *K* and *L* shells. Electron binding energies (EBE) in all natural atoms Z = 1 - 92 from experimental data.



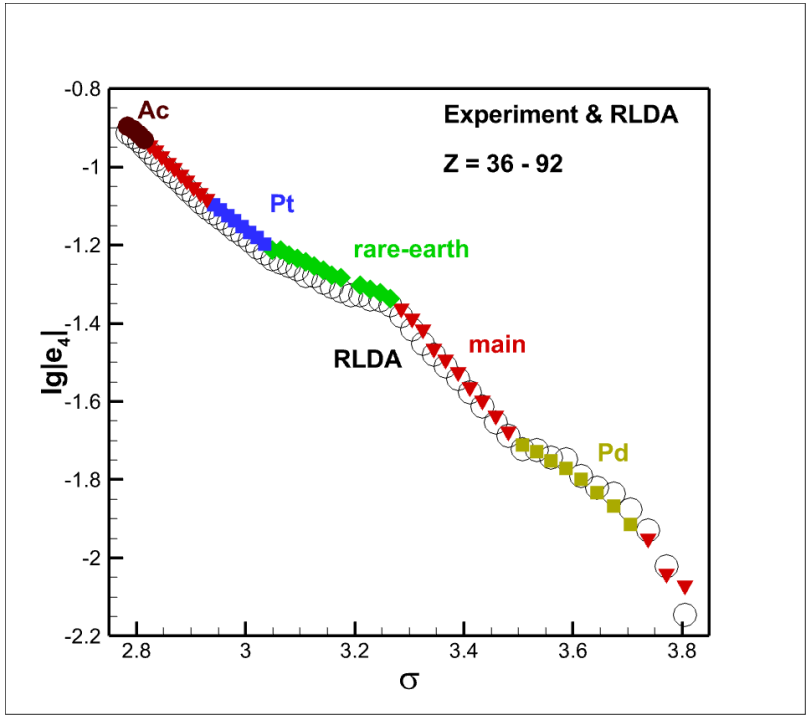


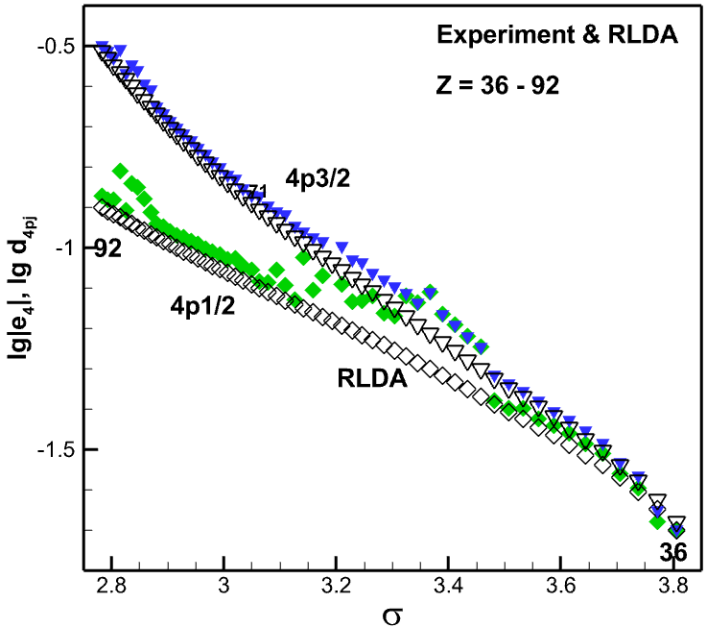
3.2 *M* shell. **Experimental EBE** in the atomic groups (different color symbols)



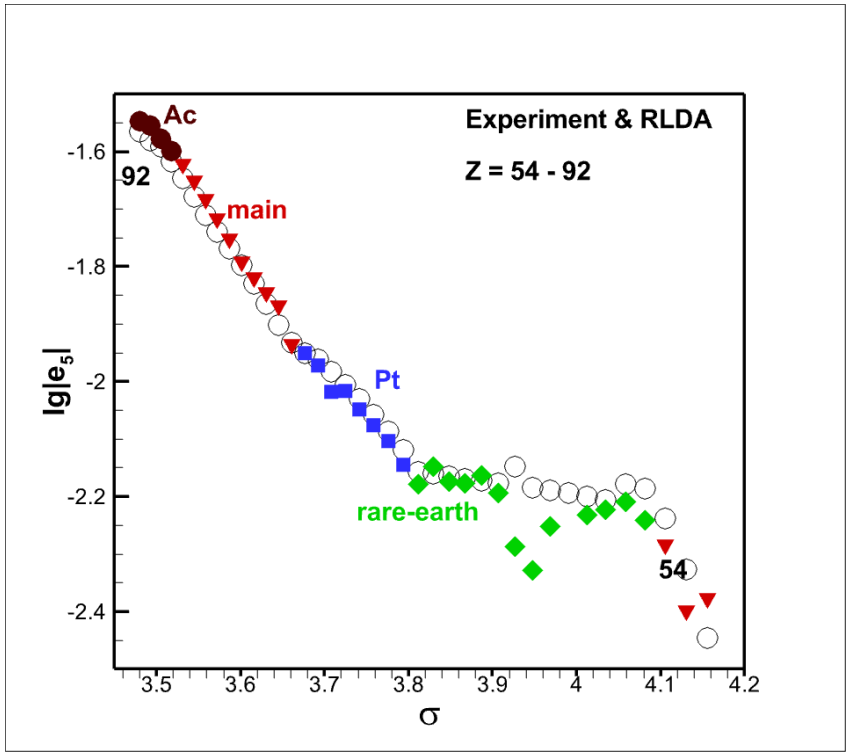


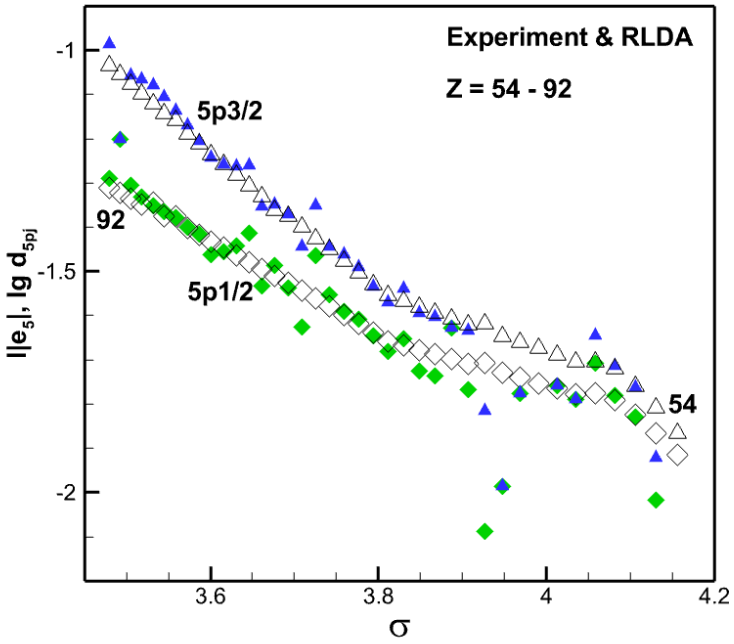
4.1 *N* shell. **Experimental** (color symbols) and **RLDA** (black open symbols) **EBE**



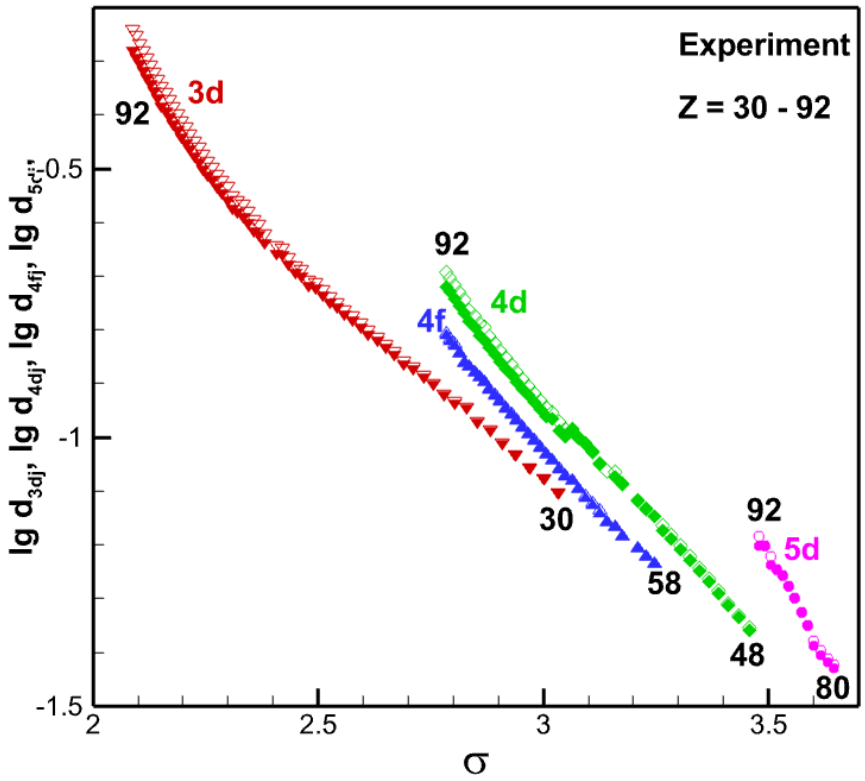


4.2 *O* shell. **Experimental** (color symbols) and **RLDA** (black open symbols) **EBE**





4.3 Function $d(\sigma)$ for experimental EBE in subshells: 3dj, 4dj, 5dj, 4fj



5.1 Analytic approximation of experimental curves

- $\lg|e_n(\sigma)| = \sum_{k=0}^{3} a_k^{(n)} \sigma^k$
- $\lg d_{nlj}(\sigma) = \sum_{k=0}^{3} b_k^{(nlj)} \sigma^k$

- $E_{n0}(Z) = Z^{4/3} e_n(\sigma_n), \quad \sigma_n = \pi n Z^{-1/3}, \quad \text{if } l = 0;$
- $E_{nlj}(Z) = Z^{4/3} e_n(\sigma_n) + Z^{2/3} d_{nlj}(\sigma_n) \lambda^2, \lambda = l + 1/2$

5.2 Analytic EBE estimates in comparison with data from other sources

Table 2. Orbital binding energies $|E_{nlj}|$ (eV) estimated by equation (5) in comparison with experimental data from [3–5].

Z	n	$l\,j$	equation (5)	[3]	[4]	[5]
2	1	s	24.52	24.6		24.59
5	1	s	186.8	188.0	186.4–187.3	192.2
9	1	s	703.2	696.7	684.0–694.0	692.4
9	2	s	33.24		23.70–33.64	37.21
15	2	s	186.3	189.0	187.7–188.0	191.4
		p 1/2	129.7	136.0	130.3	135.1[a]
		p 3/2	128.9	135.0	129.4–130.9	
16	2	s	228.3	231.0	229.2	232.1
		p 1/2	166.0	164.0	162.0–166.1	168.1[a]
		p 3/2	164.3	162.0	162.9–164.8	
31	3	s	160.1	159.5	161.0	161.0
		p 1/2	107.4	103.5	106.1–108.7	107.1[a]
		p 3/2	103.9	100.0	104.3–105.8	
48	4	s	109.4	109.8	109.8	112.4
83	4	s	939.5	939.0	939.0	940.8
76	5	s	87.84	84.0	94.6	87.1
85	5	s	193.2	195.0		194.7

[a] Excluding spin-orbit splitting.

Examples of the method application

- Analytic **description** of experimental ***K***, ***L*** X-ray **terms** in multi-electron atoms (***Z*** > **10**) and **control their reliability**
- **Analysis and correction** of experimental electron binding energies in **lanthanides**
- Discovering **patterns** in the measured **first ionization potentials** of **lanthanides and actinides**

6. Conclusions

1. The most **experimental EBE** in the reduced coordinates **e(σ), d(σ)** form **smooth dependences**, that is an **atomic number similarity law**.
2. The **deviation from the law** indicates a measurement error.
3. The found **atomic number similarity law** provide a way to **recover missing or erroneous data** with an accuracy **~1%**.
4. The available theoretical **RLDA model** does not satisfactorily describe the **EBE**.

Thank you for attention!