Introduction to the cubic ellipsoid nuclear model

An interpretation of the nuclear and atomic structures

Summary

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Abstract

This study suggests that the nuclear structure determines the atomic properties and proposes a geometric nuclear model to confirm this claim.
Our main goal is not to obtain more accurate results than existing models, but to establish a different point of view for the interpretation of nuclear and atomic physics.

According to the model, the nucleus, in general, has an ellipsoidal shape built from a three-dimensional lattice of proton-neutron bonds (treated here as a cubic system) and nuclear shells populated with protons similar to the atomic shells of the periodic table.

The model was first tested and confirmed on various nuclear phenomena and then its link to atomic physics was demonstrated and analyzed.
Its main results are:

- a nuclear geometry from which the periodic system is derived.
- its agreement with various nuclear phenomena.
- demonstrating the link between the nuclear structure and the atomic properties through the correlation between the nuclear geometry and the atomic covalent radius.
- the interpretation of atomic phenomena in the light of the model.

This article summarizes the main stages of the research. A detailed analysis and description of each research phase is published in separate articles.

Content

Introduction

The nucleus and the atom are governed by different forces, have a size difference of about five orders of magnitude and, according to current physics, the nucleus is seen as a point charge and its shape is not related to the structure of the atom or its properties. In addition, due to the size of the nucleons, which is in the range of their de Broglie wavelength, it is believed that the nucleus cannot be considered as a group of spherical or located particles. Yet in this study we discuss two hypotheses:

- it is possible to create a tangible geometric nuclear model.
- the nuclear structure determines the atomic properties.

The study was developed in stages; each step is related to at least one article, which describes the technical aspects of a specific subject in detail, so that in order to remain clear and focused, instead of a detailed description, only a brief reference is given, to describe the main points of the topic.
The process is based on an "if-then" argument, that is, if the assumption is true, what requirements must the nuclear structure fulfill.
After the model is built, its feasibility is tested with respect to various nuclear phenomena; then the link between the model and the atomic structure is presented and atomic phenomena are discussed in the light of the model.
The model development process includes two stages according to the research questions.
The first stage deals with the development of the model and its testing and consists of the following stages:

- requirements for the nucleus, under which the hypotheses hold.
- the development of a geometric nuclear model.
- the creation of a mass formula that matches the model.
- a comparison of the mass formula calculations with experimental data.
- testing the model on various nuclear phenomena, to ensure there are no contradictions with the common theory.

In the second phase, evidence is sought to link between the nuclear model and the atomic properties, and additional conclusions are drawn regarding atomic phenomena:

- demonstrating that the nuclear structure determines the atomic properties by showing the relationship between the nuclear geometry and the atomic covalent radius.
- interpreting atomic phenomena according to the model.

In the appendix the main subjects are shown, on which the model was tested or further developed.

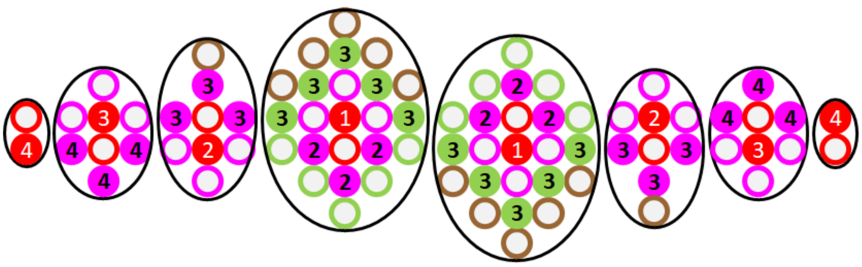
Part 1: the model and its mass formula

The model at a glance

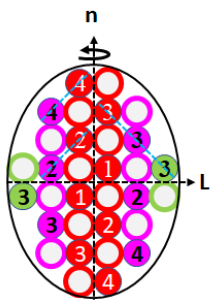
The model suggests the following shape and properties of the nucleus:

- the nucleus has an ellipsoid shape.
- the lattice of bonds between the nucleons forms a cubic system.
- protons are connected only to neutrons (**p**-**n** bonds).
- neutrons are connected mainly to protons.
- the population of the nuclear shells with protons are equal to the population of the atomic shells with electrons.
- the nuclear principal quantum number, **n**, grows with the distance from the origin (the center of the nuclear ellipsoid).
- the perpendicular distance from the **z**-axis in the **x**-**y**-plane represents the angular momentum (**L** - the sub-orbitals).
- the precise spin distribution is assumed to be symmetrically divided between the upper and lower parts of the ellipsoid.
- the nucleus possibly rotates around its **z**-axis and vibrates in the x-y plane.

As an example we observe the Krypton nucleus Kr_{36}^{84}.
Following illustrations show the nuclear cross sections of its x-y planes along the z-axis and its cross section in the x-z plane.



__x-y__ planes along the __z__ axis

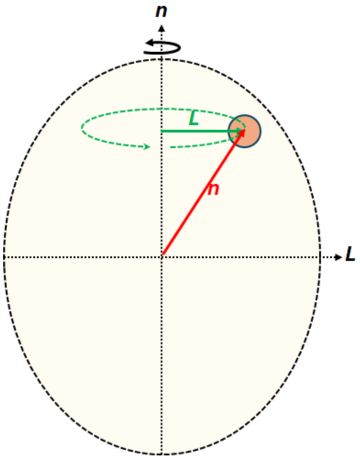


__x-z__ plane

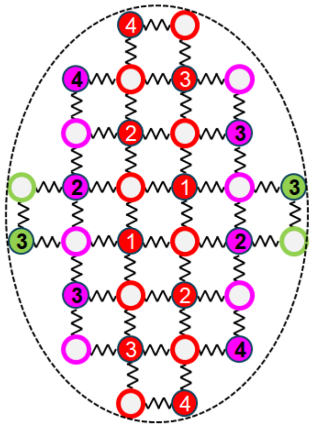
Legend: protons*: full circles according to the orbitals* ***S***, ***P***, ***D***, ***F***.
numbers*: principal quantum number.*
neutrons*: hollow circles with colors according to their orbital.*
excess neutrons*, beyond the number equal to the protons (unpaired neutrons).*

Explanation via illustrations

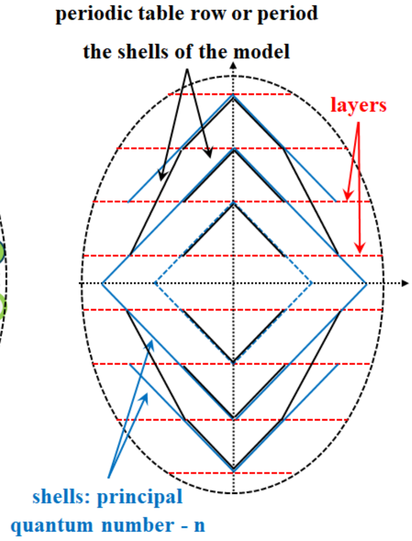
Following drawings describe the model via cross sections in the **x-z**-plane of the nucleus.



1*: a nucleon*
in the nucleus



2*: the bonds between*
the nucleons



3*: layers, shells, rows/periods*

1. a nucleon (**circle**) is observed inside the ellipsoid (dashed line) that encloses the nucleons and schematically defines the nuclear surface:
   - the distance from the origin refers to its principal quantum number **n**.
   - the distance from the **z**-axis refers to its angular momentum **L**.

2. the bonds between the nucleons are shown for visibility as springs.
   - **protons**: full circles of the **s**, **p** and **d** sub-orbitals.
   - **numbers**: principal quantum number.
   - **neutrons**: hollow circles.

3. the difference between the nuclear layers and shells.
   - **layers**: are developed in the x-y planes.
   - **shells**: share the same principal quantum number between all their nucleons.
   - **rows/periods**: (according to the periodic table) these are the real shells of the model.

Remark: in this study the term shell is sometimes used instead of row of the periodic table.

The requirements

Assuming that the model holds, the requirements are derived from the experimental data, the structure of the periodic table and the "physical common sense".
The requirements are rough and simple, to enable an initial development of a simplified nuclear model.

The nuclear properties

- The nuclear shape should make sense from a physical point of view.
- The system of bonds between the nucleons is assumed to be homogeneous and periodic; this means that the nuclear density (the distance between two neighboring nucleons) is assumed to be (at least nearly) constant in all three dimensions and for all nuclei.
- In a stable nucleus a proton is connected only to neutrons (**p-n** bond) because it is assumed that the **p-p** bond has a too strong electric repulsion; otherwise we could expect to observe a stable He_2^2 atom for instance (diproton).
- In a stable nucleus a neutron is preferably connected with protons (**p-n** bond) because it is assumed that the proton stabilizes the neutron and that the **n-n** bond alone (with no protons involved) is unstable; otherwise we could expect to observe a stable **n-n** nucleus (neutronium).
- The spin of the nucleons shall be equally and symmetrically divided in the nucleus.
- The nuclei of all isotopes shall have the correct total nuclear spin.

Nuclear shells

- the nuclear shells shall be populated with protons similarly to the atomic shells (here referred to the rows of the periodic table).
- the same holds for the orbitals and sub-orbitals and their population sequence.
- the nuclear proton distribution shall be equal for all isotopes of the same element.
- Pauli's exclusion principle must hold.

A comparison with experimental data

A theoretical mass formula suitable for the model (unlike the common semi-empirical one) shall be constructed to test the matching between the theoretical and experimental data.

The model

We get the following model:

- The nuclear structure:
  - the shape of the nucleus is in general an ellipsoid.
  - its core consists of a cubic system of proton-neutron bonds.
  - the excess neutrons, beyond those that are paired with protons, are in the envelope of the ellipsoid.
- Properties:
  - the shells of the nucleons grow with their distance from the origin (the center of the ellipsoid). This refers to the principal quantum number n.
  - the perpendicular distance of the nucleons from the z-axis (in the x-y-plane) depicts the angular momentum (and so the sub-orbitals).
  - the nucleons are evenly distributed with protons and neutrons with spin-up or spin-down, except for one proton and/or one neutron if their number is odd.
  - the nucleus possibly rotates around its main axis (the **z**-axis).
- The model attempts to assert the following:
  - a justification of the periodic table.
  - the correct nuclear population of protons and neutrons.
  - reasoning why different isotopes of the same element have equal electronic properties.
  - the correct nuclear spin.
  - it agrees with Pauli's exclusion principle.
- Examining the model:
  - the ellipsoid shape is reasonable from a physical point of view.
  - a theoretical mass formula that matches the model was created and delivered good results.

The Mass formula

The mass formula was built in accordance with the theory of the model (unlike the semi-empirical one [7], [8], [9]: $m_{calc_x} = Z_x \cdot m_p + N_x \cdot m_n - \frac{(E_{b_x} - E_{c_x})}{c^2}$

- A_x: the atomic mass (number of nucleons) of the nucleus x.
- m_{calc_x}: the calculated mass of the nucleus x.
- Z_x: the atomic number (number of protons) of the nucleus x.
- m_p: the mass of the proton.
- N_x: the number of neutrons ($N_x = A_x - Z_x$) in the nucleus x.
- m_n: the mass of the neutron.
- E_{b_x}: the total energy of the bonds between nucleons in the nucleus x.
- E_{c_x}: the total electric energy (between all protons) in the nucleus x.
- c: the speed of light.

$E_{b_x} = e_b \cdot n_{b_x}$:

- e_b: the energy of a single nucleon-nucleon bond in the nucleus (assuming they are equal for all bond types and bonds in all nuclei).
- n_{b_x}: the number of nucleon-nucleon bonds in the nucleus x.

$$E_{c_x} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{d_0}\left\{\frac{1}{2}\sum_i^{Z_x}\sum_{j\neq i}^{Z_x}\frac{1}{d_{i,j}}\right\} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{d_0}e_{c_x} \quad \text{where} \quad e_{c_x} := \frac{1}{2}\sum_i^{Z_x}\sum_{j\neq i}^{Z_x}\frac{1}{d_{i,j}}$$

- d_0: the minimum distance between two neighboring nucleons (assuming all nuclei have the same cubic structure and distance between their nucleons).
- $d_{i,j}$: the unitless distance between the protons of the indices *i* and *j* measured in multiples of d_0: $d_{i,j} = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2 + (z_j - z_i)^2}$
- e_{c_x}: the unitless total electric energy of the nucleus (sum of the reciprocal distances).

The absolute relative error of the calculation for the nucleus x is:

$$rel\_err_x = \left| \frac{m_{calc_x} - m_{meas_x}}{Z_x \cdot m_p + N_x \cdot m_n - m_{meas_x}} \right| = \left| \frac{m_{calc_x} - m_{meas_x}}{mass\_defect_x} \right|$$

- m_{meas_x}: the measured mass of the nucleus x.
- $mass\_defect_x$: $Z_x \cdot m_p + N_x \cdot m_n - m_{meas_x}$ is the mass defect of the nucleus x. Remark: rel_err_x is represented here in percentage.

The mass formula depends thus only on the two variables:

- e_b: the energy of a single nucleon-nucleon bond.
- d_0: the minimum distance between two neighboring nucleons.

The implementation requires two preliminary calculation steps for all nuclei:

- drawing the nucleus x and counting the number of nucleon-nucleon bonds n_{b_x}.
- calculating the relative total electric energy of the nucleus e_{c_x}.

The mass formula calculation results

The mass formula calculation was performed on isotopes of elements with larger abundant from Lithium, Li_3^7 to Plutonium, Pu_{94}^{244} (for several elements more than one isotope was taken). Experimental data were taken from [1].
Nuclei till approximately Argon, Ar_{18}^{40} show larger relative errors than those of heavier nuclei; this phenomenon is known also for the common mass formula [7], [8], [9]. We assume here that this occurs in small nuclei either due to a variation in the distance d_0 between the nucleons or due to a shift from the cubic form.

The results (after an improvement process) for 327 nuclei from Ar_{18}^{40} to Pu_{94}^{244} were:

maximum	average	st. dev.	≤ 2%	≤ 1%	≤ 0.5%
2.0%	0.4%	0.4%	100%	93%	68%

After expanding the range to 358 nuclei from N_7^{14} to Pu_{94}^{244} the results were:

maximum	average	st. dev.	≤ 2%	≤ 1%	≤ 0.5%
3.6%	0.5%	0.5%	98%	89%	64%

This is within reasonable range [7], [10].

The calculation parameters were found as:

- $d_0 = 1.62 \pm 0.03\, fm\ (fm = 10^{-15}\, m)$
- $e_b = 5.72 \pm 0.03\, MeV$

this seems to be within range as well [5].

We get through $d_0 \approx (r_n + r_p)$ a rough estimation for the sum of the radii of the proton and neutron and estimate the relative error:

- $r_n \approx 0.80\, fm$ [3] *(Neutron radius)*, $r_p \approx 0.84\, fm$ [4] *(Proton radius)*
- $r_n + r_p \approx 1.64\, fm$
- relative deviation for d_0: $\left|\frac{d_0 - (r_n + r_p)}{(r_n + r_p)}\right| = \left|\frac{1.62 - 1.64}{1.64}\right| = \left|\frac{0.02}{1.64}\right| \approx 1.3\%$

This strengthens the hypothesis of the model.

Discussion of the results and conclusions - part 1

The cubic ellipsoid nuclear model offers a perspective on nuclear and atomic physics, that is different than the common one and tries to justify this idea via calculations. It does not seem to contradict these theories, but rather to expand their understanding and open new research directions of the nuclear theory and possibly also to other fields of physics.

The model aims to obtain the following:

- a tangible nuclear model.
- shells and orbitals in accordance with those of the periodic table.
- presence of the excess neutrons in the nuclear envelope.
- total nuclear spin that matches the experimental data.
- maintaining Pauli's exclusion principle.

The mass formula:

- is based on parameters that relate directly to the theory of the model (as opposed to the common semi-empirical mass formula) and therefore offers advantages from a physics perspective.
- has only two parameters (as opposed to the common one with five parameters).
- calculations are in good agreement with the experimental data. The results are in a range that is not far from the results of the common mass formula [7], [10], yet again, here the results are directly linked to the model.
- the distance d_0 between two neighboring nucleons agrees with the sum of the neutron and proton radii; this strengthens the model assumption and the concept of this mass formula.

Part 2: the link between the nuclear geometry and the atomic properties

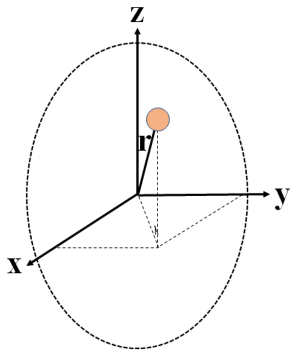
This study is based on two main parts. The first is the creation of the model, and testing it to ensure that it makes sense, as discussed in the section above.
Yet to confirm the model hypothesis, a direct link between the nuclear structure and the atomic properties must be shown; we claim to achieve this in this section.

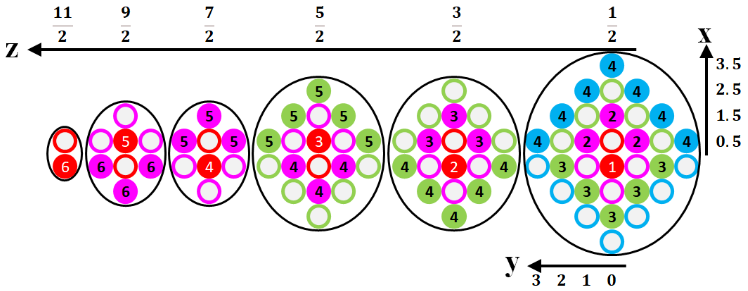
Relative nuclear distance - definition and calculation

As a preparation step, we make two definitions:

- a valance proton: the proton, that was last added to the current, in-filling process, sub-orbital of the nucleus.
- the relative nuclear distance: the relative geometric distances of the valance proton from the nuclear center.

The following illustrations demonstrate the way the relative nuclear distance of the valance proton is calculated from the nuclear geometry via $r_{x,y,z} = \sqrt{x^2 + y^2 + z^2}$.





a proton in the nucleus

*the **x-y** planes along the nuclear **z** axis (upper half only)*
***protons**: full circles according to the orbitals **S**, **P**, **D**, **F**.*
***numbers**: principal quantum number. **neutrons**: hollow circles.*

Note: the variables x, y, z, refer to the distances of the protons from the nuclear center; due to the nuclear geometry, there is an apparent shift so that for instance the position of the central proton is $(x, y, z) = (0.5, 0, 0.5)$ and not $(x, y, z) = (0, 0, 0)$ as we might intuitively expect.

A comparison between the atomic covalent radius and the relative nuclear distance

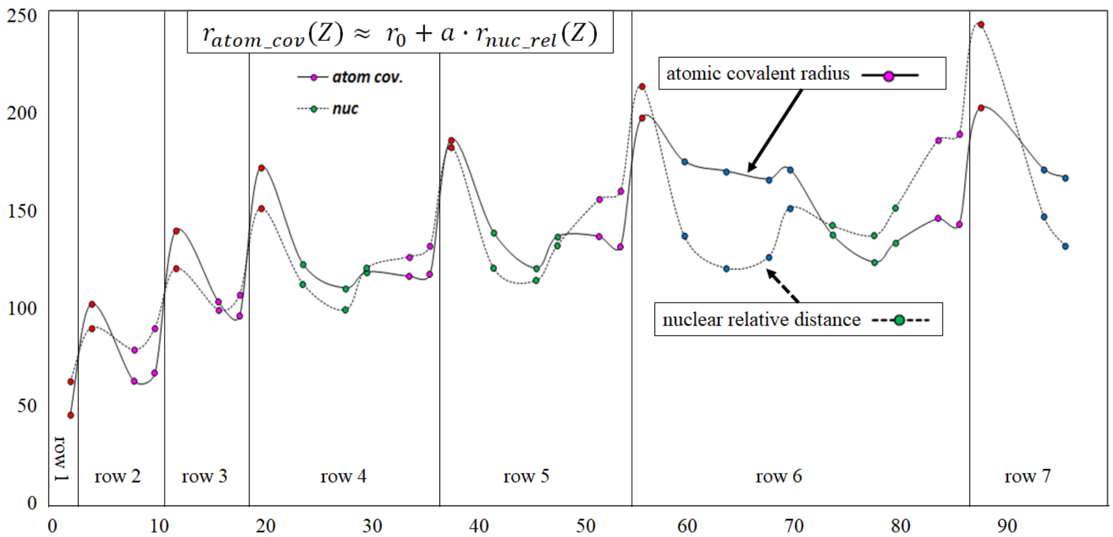
The cubic ellipsoid nuclear model was first built in the search for a connection between the nuclear structure and the atomic properties. We now look for the pattern of the atomic covalent radius and compare it with the "relative nuclear distance" (as described above) of the corresponding nuclear suborbital.
Each atomic covalent radius must be associated with the correct "valance proton" (as described above), therefore we only refer to nuclei with symmetric shape of the sub-orbitals (s, p, d, f) in the atomic number of the range $Z \in [1, 96]$:

- $s = \{He_2;\ Ca_{12};\ He_2; Ca_{20};\ Sr_{38};\ Ba_{56};\ Ra_{88}\}$
- $p = \{O_8, Ne_{10};\ S_{16}, Ar_{18};\ Se_{34}, Kr_{36};\ Te_{52}, Xe_{54};\ Po_{84}, Rn_{86}\}$
- $d = \{Cr_{24}, Ni_{28}, Zn_{30};\ Mo_{42}, Pd_{46}, Pd_{48};\ W_{74}, Pt_{78}, Hg_{80}\}$
- $f = \{Nd_{62}, Gd_{64}, Er_{68}, Yb_{70};\ U_{92}, Cm_{96}\}$

two curves are observed and compared:

- The atomic covalent radius, taken from [11].
- The "relative nuclear distance" (calculated according to the illustrations above).

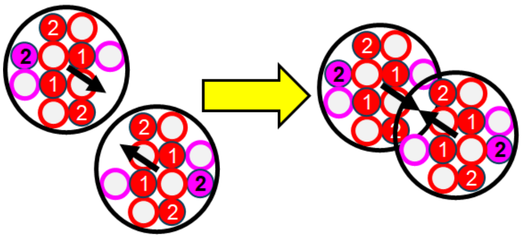
The comparison between the two curves is implemented in relative values, since the two curves refer to different sizes and units; the atomic covalent radius is given in $[pm]$: $10^{-12}m$, whereas the nuclear distance in relative values (the adjustment parameters have the values $r_0 \approx 40,\ a \approx 30$).

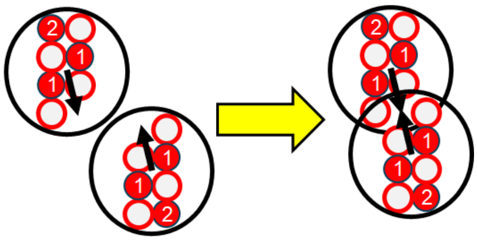


We observe a seemingly correlation between the two curves, although the atomic curve is taken from the experimental data and the relative nuclear distance is a geometric property, measured according to the ellipsoid model; therefore, we conclude that this implies a basic connection between these two entities, that is, a connection between the nuclear and atomic structure.
This strengthens the hypothesis of the model.

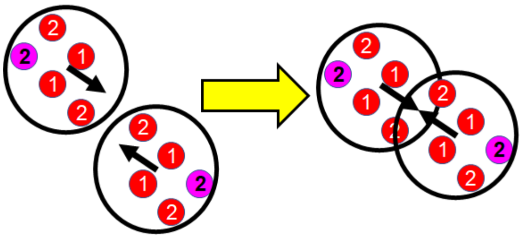
The atomic covalent radius - geometric interpretation

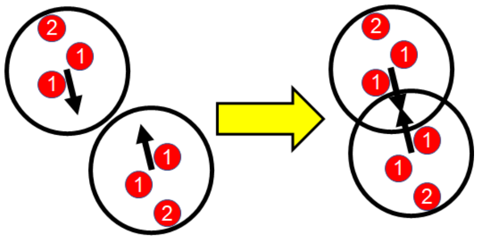
We now want to visually explain the link between the "valance proton" and the atomic covalent radius (in the x-z plane). We observe pairs of atoms, first before their combination to molecules (left from each row) and then (right from the rows) as molecules; the black arrows depict the covalent radius, that is generally smaller than the most distant position on the nuclear surface. The covalent bond is assumed to occur so that the molecule strives to complete symmetry.
First we show it, as if the bond is between the nuclei, to be clear what position we are talking about:





Then we use the same illustrations for the atom and treat it as if the atomic shape is similar to the nuclear one (we leave electrons in the positions of the protons and remove the neutrons).





the source of attraction are the protons of the suborbital that is being filled (see also appendix: ionization energy); electrons from the corresponding suborbital partially move towards the bonding position due to the greater positive attraction there.

The mechanism raised here could mean also, that the angles of the chemical bonds between atoms are influenced by the nuclear structure. We thus obtain an additional hypothesis, that the atomic shape may correlate with the nuclear shape.

Discussion of the results and conclusions - part 2

We found a correlation between the nuclear geometric structure and the atomic covalent radius.
If we accept the model assumption, we can expect the atomic and nuclear shape to correlate with each other; this correlation is therefore expected between the valence electron and the "valance proton".
We emphasize that the covalent atomic radius is not necessarily the “furthest point” on the "atomic surface", but rather the point that matches the "valence proton". This is a strong hint for a correlation between the nuclear and atomic geometries and their properties.
The van der Waals radius, for example, probably corresponds better to the "furthest position" on the surface of the atom.

We summarize our conclusions:

- The nuclear structure determines the atomic properties.
- The nuclear geometry determines the atomic covalent radius.
- The nuclear geometry may also determine the atomic shape and molecular geometry.

This unexpected correlation between the nuclear geometry and the atomic covalent radius might be the proof to the cubic ellipsoid nuclear model.

Moreover, it may imply a different interpretation of the bound electron; when analyzing the ionization energy (see appendix), we concluded that the source of attraction of the valence electron includes only the protons of the corresponding nuclear suborbital and not those of the entire nucleus. This may mean that there are differences in nuclear-atom interactions compared to what we currently believe.

Appendix - testing the model on various phenomena

The next research stages

The purpose of the research is to look at nuclear and atomic physics from a different perspective rather than improving the mass formula or obtaining more accurate results.
The main goal is to explore the hypothesis, that the nuclear structure determines the atomic properties, so various nuclear and atomic phenomena shall be dealt considering the model, to ensure that the model can address them with no contradictions.
Here we briefly present the various studies in which we aim to validate the model. The topics are divided according to their fields.

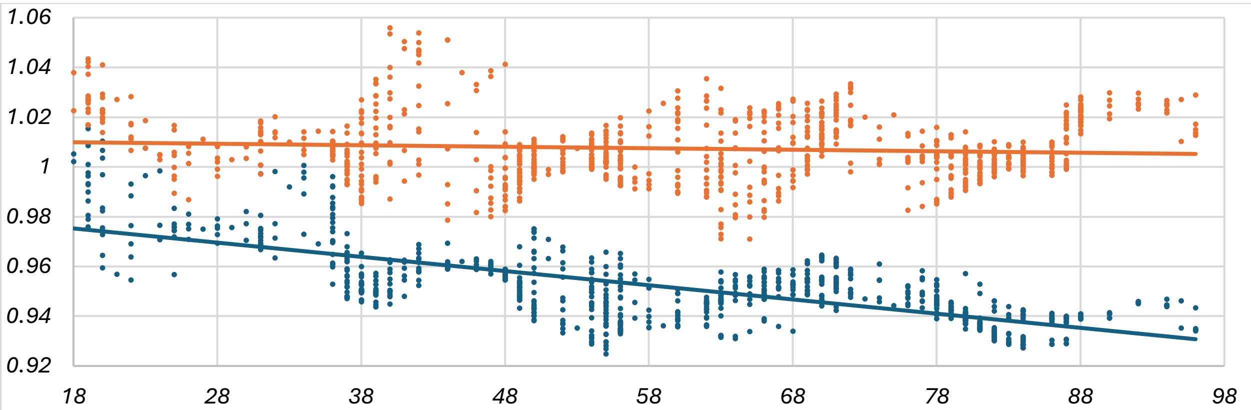
- Nuclear physics
  - the location of the excess neutrons in the nuclear envelope and the charge radius.
  - the radioactivity of heavy nuclei beyond lead.
  - the short half-life of superheavy nuclei (beyond $Z \approx 104$).
  - the nuclear fission mechanism and its most probable products.
- Astrophysics
  - white dwarfs and the minimum atomic size.
  - neutron stars
    - the TOV limit (transition from neutron star to black hole).
    - the maximum rotation frequency of pulsars.
- Atomic physics
  - the first ionization energy.
  - electronic transition rules as they arise from the nuclear structure.

As already mentioned, the goal is not to achieve better results, but to show that the new concept makes sense and thus opens up a different approach or interpretation of nuclear and atomic physics.

Nuclear phenomena

The charge radius and the location of the excess neutrons in the nuclear envelope

According to the liquid drop model an approximately constant value would be expected for the ratio between the nuclear charge radius $\boldsymbol{R_c}$ and the third root of $\boldsymbol{A}$, the atomic mass or the number of nucleons $\sqrt[3]{\boldsymbol{A}}$.
In this study, we assume that the nuclear core consists of p-n pairs and that the excess neutrons are located in the nuclear envelope. We therefore expect the nuclear charge radius $\boldsymbol{R_c}$ to be linear in $\sqrt[3]{\boldsymbol{2 \cdot Z}}$ rather than in $\sqrt[3]{\boldsymbol{A}}$ (with $\boldsymbol{Z}$ the atomic number; the constant **2** is added to express the dependence on the nuclear core); this is actually the case.
The following graph confirms this via comparison between $\frac{\boldsymbol{R_c}}{\sqrt[3]{\boldsymbol{A}}}$ and $\frac{\boldsymbol{R_c}}{\sqrt[3]{\boldsymbol{2 \cdot Z}}}$ for more than 800 nuclei from Ar_{18} to Cm_{96} vs. $\boldsymbol{Z}$ (for nuclei smaller than Ar_{18} the number of protons and neutrons is quite equal so there is no major difference between the two).



a comparison between $\frac{\boldsymbol{R_c}}{\sqrt[3]{\boldsymbol{A}}}$ *and* $\frac{\boldsymbol{R_c}}{\sqrt[3]{\boldsymbol{2 \cdot Z}}}$ *vs.* $\boldsymbol{Z}$ *for more than 800 nuclei.*

Following table summarizes the calculations of the above data. Charge radius data from [2].

	$\frac{R_c}{\sqrt[3]{A}}$	$\frac{R_c}{\sqrt[3]{2 \cdot Z}}$
slope	$-6 \cdot 10^{-4}$	$-6 \cdot 10^{-5}$
Δ = max – min	0.102	0.085
standard dev.	0.016	0.013

This strengthens the model assumption and could explain, why different isotopes of the same element have the same chemical behavior, because the excess neutrons do not affect their electric charge distribution.
Remark: in another different article, that is dedicated to this subject solely, we also show how the nuclear geometry makes good assessments to the radii of the light nuclei: H_1^2, H_1^3, He_2^3, He_2^4 and of the noble gases.

The radioactivity of heavy and super-heavy nuclei

The radioactivity hypothesis

The mechanism that is assumed to determine radioactivity of heavy nuclei, beyond Lead (Pb_{82}), according to the model, is the electric energy, that overcomes the binding energy (of the strong nuclear force) between the nucleons.
The instability is assumed to occur in the middle of the nuclear ellipsoid, where the electric energy reaches its maximum value; when we get to nuclear fission, this idea will be discussed further.

The calculations provide a rough prediction of the nuclear stability. We find that for nuclei larger than Lead (Pb_{82}) and up to approximately Rutherfordium (Rf_{104}) six nuclear bonds are required to keep the central protons stable.

The model hypothesis is that due to movements or fluctuations within the nucleus there is some probability that these six bonds are temporarily reduced to five bonds every certain period for a certain timespan; as a result the central proton becomes unstable, possibly ending with a radioactive emission; after several radioactive steps of this type the nucleus is transformed to Pb_{82}, where five bonds are sufficient to keep the central protons stable and radioactivity ends.
The probability for this to occur and the timespan this lasts, determines the half-life of the nucleus.
We explain this from a different point of view as well: the central proton has six bonds also for most nuclei smaller than Pb (due to the nuclear geometry), but for these nuclei only five nuclear bonds are required at most, and so even if one bond is missing for a short while, there is redundancy, so radioactivity doesn't occur; the probability for a simultaneous lack of two bonds is probably too low and so these nuclei are practically stable.
On the other hand also for nuclei beyond Lead, this phenomena might have a low probability, leading by some isotopes with $Z > 82$ to half-life in the range of even millions of years.

For nuclei beyond Rutherfordium (Rf_{104}) even six bonds are not enough to keep the central protons stable, meaning that they are inherently unstable, and therefore these nuclei have, in general, a short half-life of not more than hours, and usually much less.

Remark: the focus here is the verification of the model feasibility, so that only a very rough estimate of the radioactivity process by heavy nuclei is given, without deepening into the mechanism that governs this.

Maximum electric energy as a function of the number of nuclear bonds

According to the model mass formula the binding energy of the proton $\boldsymbol{k}$ in the nucleus $\boldsymbol{x}$ is: $E_{\boldsymbol{b}_k} = e_{\boldsymbol{b}} \cdot n_{\boldsymbol{b}_k}$ where:

- $n_{\boldsymbol{b}_k}$ is the number of nucleon-nucleon bonds of the proton $\boldsymbol{k}$ in the nucleus.
- $e_{\boldsymbol{b}} = 5.72\ MeV$: (as found via the mass formula calculation) the energy of a single nucleon-nucleon bond in the nucleus (assuming they are equal for all bonds in all nuclei).

The electric energy of the proton $\boldsymbol{k}$ in the nucleus $\boldsymbol{x}$ is:

$$E_{c_k} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{d_0}\left\{\sum_{j\neq k}^{Z_x}\frac{1}{d_{k,j}}\right\} = \frac{e^2}{4\pi\epsilon_0}\frac{1}{d_0}\, e_{c_k} \quad \text{with} \quad e_{c_k} := \sum_{j\neq k}^{Z_x}\frac{1}{d_{k,j}}$$

- $d_0 = 1.62\ fm$: (as found via the mass formula calculation) the minimum distance between two neighboring nucleons (assuming all nuclei have the same structure of cubic bonds and the same distance between their nucleons).
- $d_{k,j}$: the unitless distance between the protons of the indices k and j measured in multiples of d_0: $d_{k,j} = \sqrt{(x_j - x_k)^2 + (y_j - y_k)^2 + (z_j - z_k)^2}$
- e_k: the unitless relative electric energy of the proton $\boldsymbol{k}$ in the nucleus (sum of the reciprocal distances).

We analyze the maximum electric energy that the proton $\boldsymbol{k}$ can have, in dependency on the number of its bonds. The condition for proton bond stability is $E_{\boldsymbol{b}_k} \geq E_{\boldsymbol{c}_k}$:

$$(E_{\boldsymbol{b}_k} - E_{\boldsymbol{c}_k}) \geq 0 \quad \text{or} \quad (e_{\boldsymbol{b}} \cdot n_{\boldsymbol{b}_k} - \frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{d_0}\, e_{c_k}) \geq 0$$

this means for a single bond:

$$\frac{e^2}{4\pi\epsilon_0} \cdot \frac{1}{d_0}\, e_{c_k} \leq e_{\boldsymbol{b}}$$

Following table lists this equation for the maximum values of e_{c_k}:

n_{b_k}	e_{c_k} max. value	E_b [Joule]	E_c [Joule]	E_b -E_c [Joule]
1	6.43	9.2E-13	9.2E-13	0.00
2	12.87	1.8E-12	1.8E-12	0.00
3	19.30	2.7E-12	2.7E-12	0.00
4	25.73	3.7E-12	3.7E-12	0.00
5	32.16	4.6E-12	4.6E-12	0.00
6	38.60	5.5E-12	5.5E-12	0.00

the maximum relative electric energy as a function of the number of nuclear bonds

This means that a proton with a single nuclear bond can sustain, at most, a relative electric energy of 6.43; a proton with two bonds, 12.87 and so on; a proton with six nuclear bonds can bear at most a relative electric energy of 38.60.

Begin of instability of heavy nuclei - transition from five to six bonds

We see that the transition from five to six bonds occurs in the region where nuclei radioactivity begins and make the following assumption:

- if six bonds are required for the stability of the central proton (to overcome the electric repulsion) and:
- if there is a certain probability that one bond breaks for a short while
- then the nucleus is expected to be radioactive.

The half-life depends on the probability for the above to occur, meaning how often a bond is broken and for how long and on the processes that happen then, once a bond is broken.

nucleus	Z	max. half-life	bonds	max. e_{c_p}		
Pt	78	stable	5	31.30		
Au	79	stable	5	31.62	1.7%	deviation from the limit value 32.16
Hg	80	stable	5	31.87	0.9%	
Tl	81	stable	5	32.09	0.2%	
Pb	82	stable	6	32.29		
Bi	83	y	6	32.40		begin of instability
Po	84	y	6	32.73		
At	85	h	6	32.54		

The transition from five to six bonds that are required for the stability of the central proton.

Superheavy - very unstable nuclei - transition from six to more than six bonds

We assume similarly to the previous section, that:

- if more than six bonds are required for central proton stability
- then the nucleus is inherently unstable.

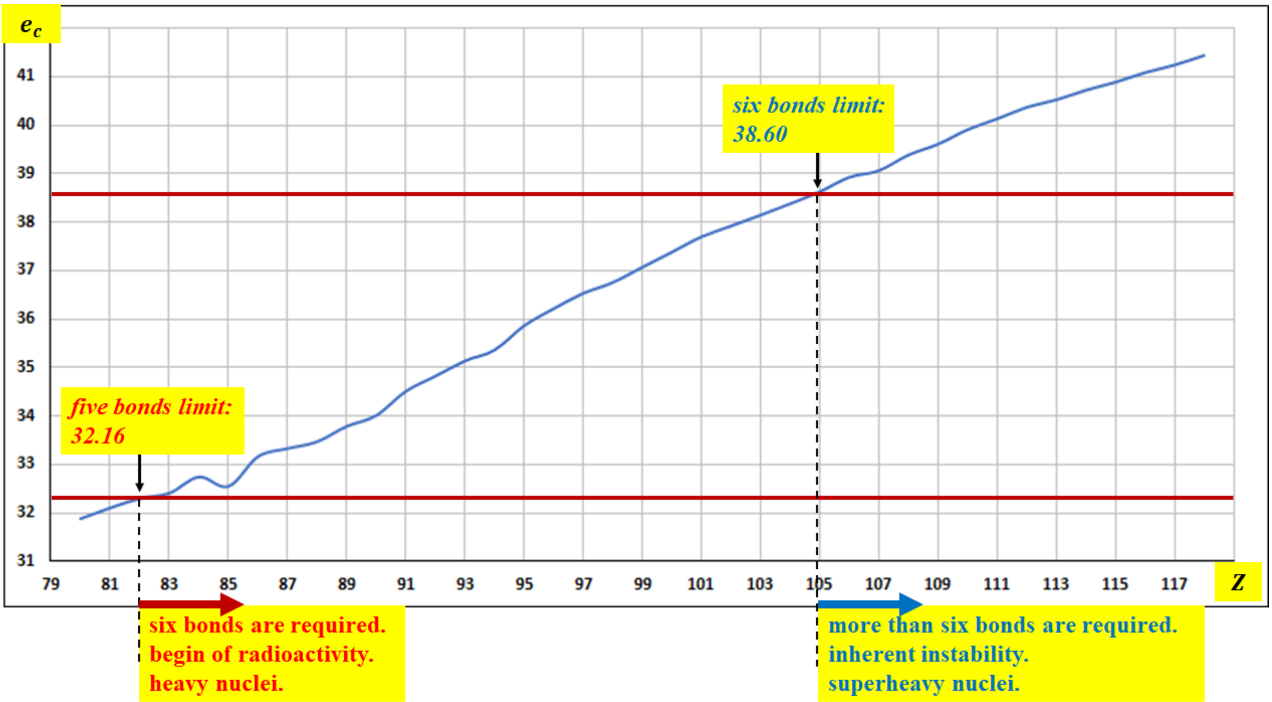
This occurs around $Z = 104$. We expect their half-life to be much shorter.

nucleus	Z	max. half-life	bonds	max. e_{c_p}		
Md	101	d	6	37.69		
No	102	m	6	37.91	1.8%	deviation from the limit value 38.60
Lr	103	h	6	38.14	1.2%	
Rf	104	m	6	38.37	0.6%	
Db	105	h	6<	38.62	0.1%	
Sg	106	m	6<	38.92		
Bh	107	m	6<	39.06		begin of superheavy nuclei
Hs	108	m	6<	39.38		
Mt	109	s	6<	39.60		

The transition from six to more than six bonds required for the stability of the central proton.

Results: the number of bonds vs. the relative electric energy

The following graph illustrates the data from the above table.
We see that radioactivity is expected to begin around Lead (Hg_{80}) and the superheavy nuclei (those that are very unstable with short half-life) are expected to begin around Dubnium (Db_{105}).



Limits of radioactive nuclei (six nuclear bonds) and superheavy nuclei (beyond six bonds)

The nuclear fission

the fission hypotheses

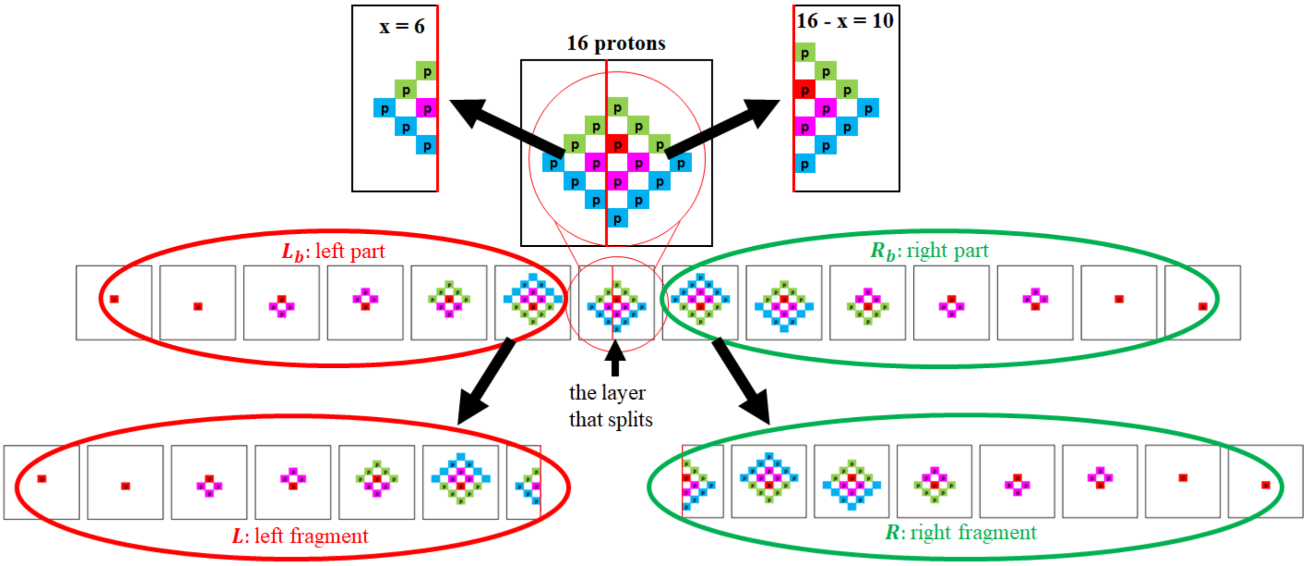
We raise the following hypotheses regarding the fission mechanism:

- A necessary but not sufficient condition for fission is that the nucleus is larger than Lead (Pb) and so has an unstable core.
- The split of the nucleus occurs in one of the two central (innermost) layers.
- The number of protons of each fission product (fragment) is the number of protons in the original nucleus from its outermost side to its fission point.
- The number of neutrons must be a bit lower than the relatively more stable isotope of the nucleus; for example, for Uranium the more stable isotope is U_{92}^{238}, so the unstable isotope is smaller. The assumption here is that this lack of several neutrons enables some movement of the nucleons in the nucleus and so after radioactivity occurs in the center of the nucleus, a rearrangement of the inner parts enables the split and the creation of the fragments.

In the following sections we describe the fission mechanism according to the model, explain how to calculate the size of the fragments and then demonstrate it with examples.

The fission mechanism

The nuclear split occurs according to the model at one of the central nuclear layers (see illustration). For nuclei with even number of protons it doesn't matter if we select the right or left center as the one that splits, but for nuclei with odd number of protons, the two possibilities shall be considered separately.



The fission and the definition of the fragments

We define (see illustration):

- P : number of protons of the nucleus that undergoes fission.
- R_b: the number of protons of the right part of the nucleus till its center.
- L_b: as R_b, for the left part without its most inner layer (of 16 protons).
- x: the number of protons (out of 16) from the left side of the layer that splits.
- R: the number of protons of the right fragment.
- L: the number of protons of the left fragment.

calculate their values as follows:

- $P := \begin{cases} 2m+1 & P\ odd \\ 2m & P\ even \end{cases}$ with m integer
- $R_b := \frac{P}{2} = m$ (integer division)
- $L_b := \frac{P}{2} - 16 + remainder\left(\frac{P}{2}\right) = \begin{cases} m-16+1 & P\ odd \\ m-16 & P\ even \end{cases}$
- $R := R_b + 16 - x$
- $L := L_b + x$

and get that the sum of the fragments is equal, as required, to the total number of protons P:

- $R + L = (m + 16 - x) + \begin{cases} m-16+1+x \\ m-16+x \end{cases} = \begin{cases} 2m+1 & P\ odd \\ 2m & P\ even \end{cases} = P$

We take $x \in [6,16-6] = [6,10]$ and get the most probable fission product. We could expand it to $x \in [1,15]$, if we want to get additional potential fission products.

Fission products (fragments)

The following table shows the results of the above calculation for the nuclei from Thorium (Th_{90}) to Fermium (Fm_{100}) with the x values $x \in [6,10]$ (and in each subsequent column the *16-x* values).

nucleon	x=6	10	x=7	9	x=8	8	x=9	7	x=10	6
Th_{90}	Sb_{51}	Y_{39}	Te_{52}	Sr_{38}	I_{53}	Rb_{37}	Xe_{54}	Kr_{36}	Cs_{55}	Br_{35}
Pa_{91}	Sb_{51}	Zr_{40}	Te_{52}	Y_{39}	I_{53}	Sr_{38}	Xe_{54}	Rb_{37}	Cs_{55}	Kr_{36}
U_{92}	Te_{52}	Zr_{40}	I_{53}	Y_{39}	Xe_{54}	Sr_{38}	Cs_{55}	Rb_{37}	Ba_{56}	Kr_{36}
Np_{93}	Te_{52}	Nb_{41}	I_{53}	Zr_{40}	Xe_{54}	Y_{39}	Cs_{55}	Sr_{38}	Ba_{56}	Rb_{37}
Pu_{94}	I_{53}	Nb_{41}	Xe_{54}	Zr_{40}	Cs_{55}	Y_{39}	Ba_{56}	Sr_{38}	La_{57}	Rb_{37}
Am_{95}	I_{53}	Mo_{42}	Xe_{54}	Nb_{41}	Cs_{55}	Zr_{40}	Ba_{56}	Y_{39}	La_{57}	Sr_{38}
Cm_{96}	Xe_{54}	Mo_{42}	Cs_{55}	Nb_{41}	Ba_{56}	Zr_{40}	La_{57}	Y_{39}	Ce_{58}	Sr_{38}
Bk_{97}	Xe_{54}	Tc_{43}	Cs_{55}	Mo_{42}	Ba_{56}	Nb_{41}	La_{57}	Zr_{40}	Ce_{58}	Y_{39}
Cf_{98}	Cs_{55}	Tc_{43}	Ba_{56}	Mo_{42}	La_{57}	Nb_{41}	Ce_{58}	Zr_{40}	Pr_{59}	Y_{39}
Es_{99}	Cs_{55}	Ru_{44}	Ba_{56}	Tc_{43}	La_{57}	Mo_{42}	Ce_{58}	Nb_{41}	Pr_{59}	Zr_{40}
Fm_{100}	Ba_{56}	Ru_{44}	La_{57}	Tc_{43}	Ce_{58}	Mo_{42}	Pr_{59}	Nb_{41}	Nd_{60}	Zr_{40}

Table of the expected fission fragments from Th_{90} *to* Fm_{100} *for* $x \in [6,10]$

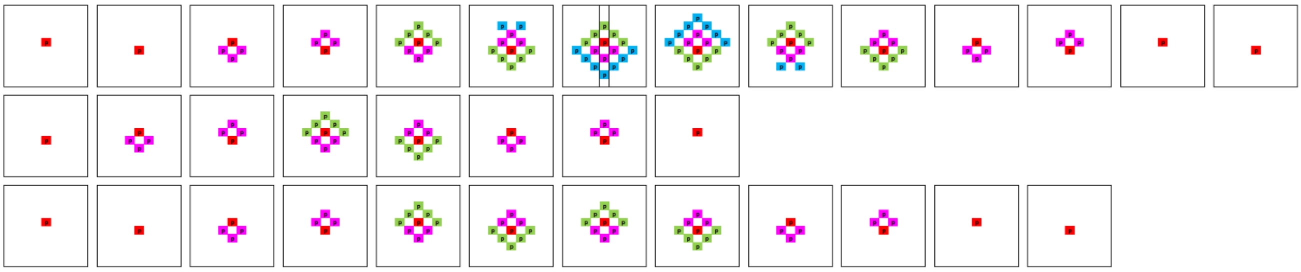
These results show the main fragments [13]; in order to get additional fragments x could be taken from a wider range (e.g. $x \in [3,13]$ or even $x \in [1,15]$).

Fission examples: observation of the protons solely

First we want to observe only the protons involved in the process; we choose for Uranium and Plutonium products [12], that have higher probability to appear and see first that according to the number of protons, the fission shall occur at one of the two center layers, as the model predicts.
The area of the split in one of the center layers is marked with two lines.

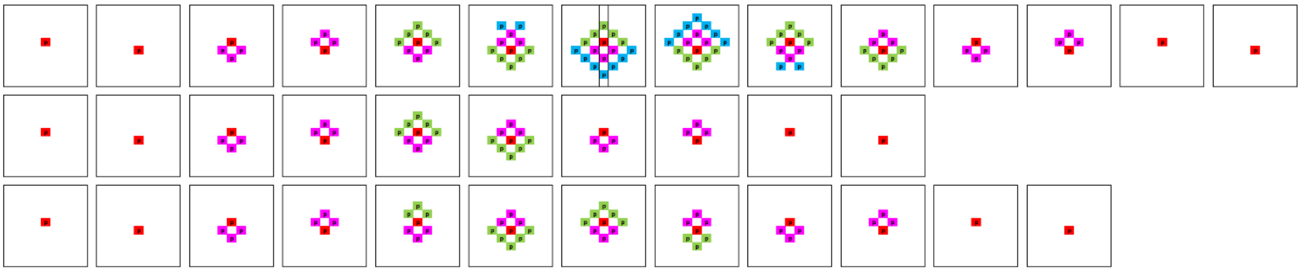
Uranium

$U_{92} \Rightarrow Kr_{36} + Ba_{56}$



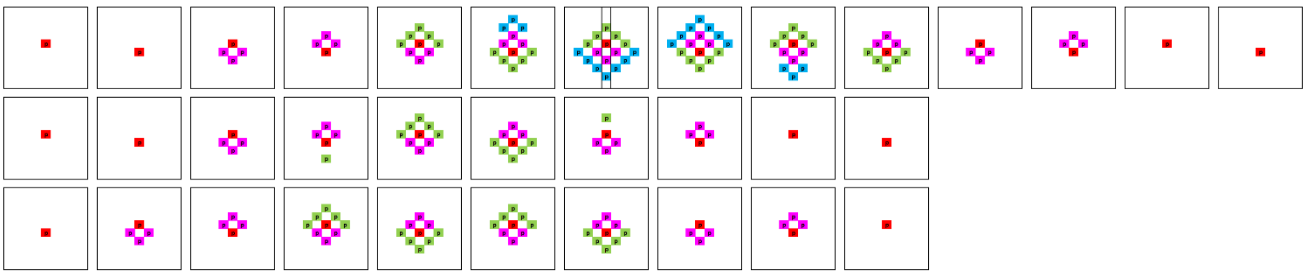
p**: protons according to the orbitals **S**, **P**, **D**, **F

$U_{92} \Rightarrow Zr_{38} + Te_{52}$



Plutonium

$Pu_{94} \Rightarrow Zr_{40} + Xe_{54}$

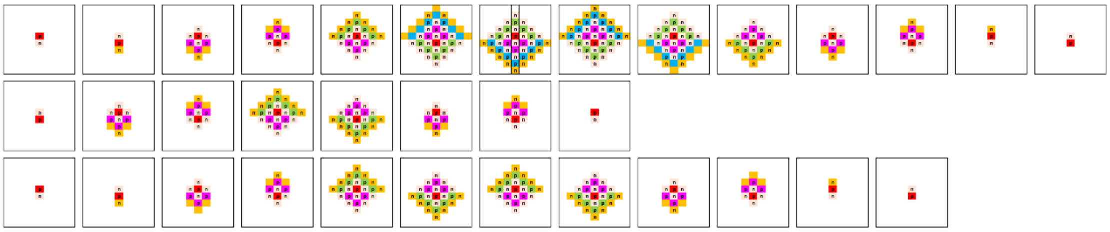


Fission examples: the full fragments

Now we consider the above nuclei as a whole [23].
We see that for the nucleus that undergoes fission and also for the product nuclei almost all potential excess neutron positions are occupied.
The area of the split in one of the center layers is marked with two lines.
The number of neutrons in the fission region corresponds to the number of neutrons in the fission products, even though we only chose it based on the number of protons in it. This is possibly a reinforcement for the model and the fission hypothesis.

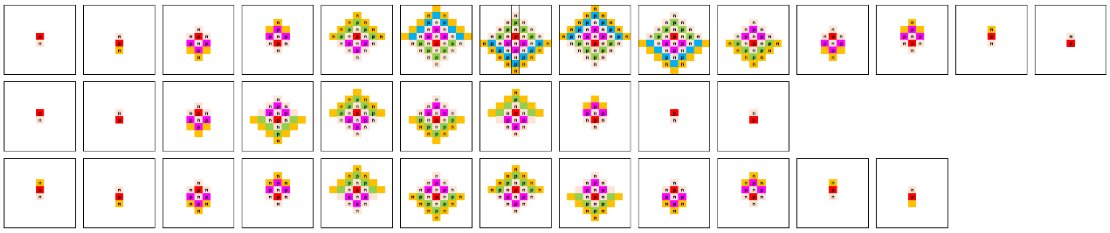
Uranium

$$U_{92}^{235} + n_0^1 \Rightarrow Kr_{36}^{90} + Ba_{56}^{144} + 2 \cdot n_0^1$$



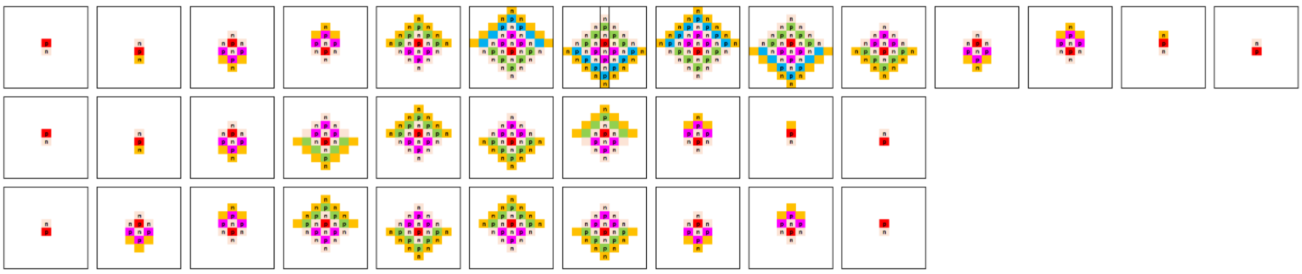
***p**: protons according to the orbitals **S**, **P**, **D**, **F**.*
***n**: neutrons (excess neutrons have a **background**)*
no letters: empty position

$$U_{92}^{235} + n_0^1 \Rightarrow Zr_{38}^{94} + Te_{52}^{139} + 3 \cdot n_0^1$$



Plutonium

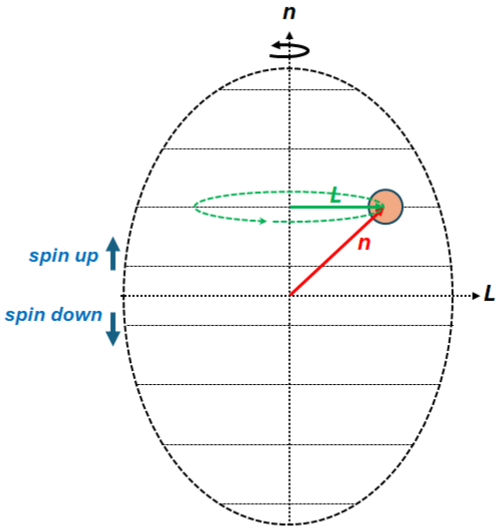
$$Pu_{94}^{239} + n_0^1 \Rightarrow Xe_{54}^{134} + Zr_{40}^{103} + 3 \cdot n_0^1$$



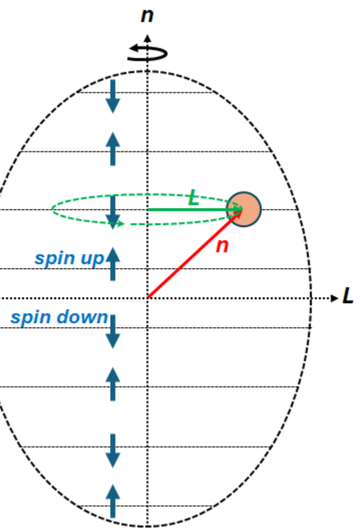
The nuclear spin

There are different possibilities for the spins of the nucleons to be distributed in the nucleus. At this stage of the research it is not decisive, but we give two options as an example to clarify the discussion points. The requirement is only to have a fully symmetric distribution of the spin of the nucleons in the nucleus.

<u>**First example**: an equal spin for each ellipsoid half</u>
The upper half of the ellipsoid is referred to as spin-up and the lower part as spin-down.



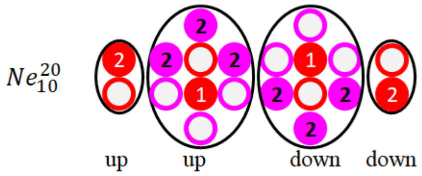
<u>**Second example**: an equal spin for each ellipsoid x-y layer</u>
(not to be confused with nuclear shell)

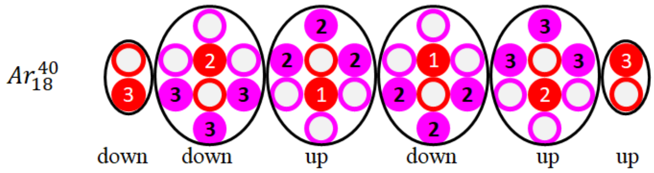


Next we discuss this second example.

We begin with the Helium He_2^4 in the following illustration of two proton-neutron pairs:

We define the spins of the left pair, where the proton appears above the neutron, as spin-up, and the one on the right as spin-down.
Now we expand this idea to Neon Ne_{10}^{20} and Argon Ar_{18}^{36}:





In general, we see that each layer of the ellipsoid consists either of spin-up or spin-down nucleons.
Neighboring layers of similar outermost sub-orbitals have opposite spins; e.g. for Argon the layers from the second till the fifth have an outermost sub-orbital P and so their spins change **d-u-d-u**; this doesn't necessarily hold for the first and second layers (or the sixth and fifth), where the outermost sub-orbitals are S and P respectively.
This arrangement possibly partly enables the order of proton-neutron pairs in clusters of alpha particles and may also play a role in the determination the so-called nuclear magic numbers, where clustering may influence the nuclear energy.
This idea shall still be processed in following studies and possibly also be analyzed if it has to do with the Hund rules and the population sequence of atomic states, but at this point we don't further discuss it.

Astrophysics

The hypotheses of constant tangential velocity and minimum atomic size

We raise two hypotheses, that shall support our following research steps.

The constant tangential velocity of bound electrons and nucleons

Hypothesis: the tangential velocity of nucleons in a nucleus is constant; this might be the case also for bound electrons in an atom.
To calculate the tangential velocity, we analyze the nuclear rotation via its angular momentum:
$L \approx \hbar \cdot l \approx p \cdot r = m \cdot v \cdot r = m \cdot (\omega \cdot r) \cdot r = m \cdot \omega \cdot r^2.$
in our model we assume that the orbital radius of the nucleus is roughly linear and grows by a constant value, r_0, while moving from one orbital to its next neighbor:
$r = l \cdot r_0$ with $l: \{0, 1, 2, 3\}$ for the orbitals $L: \{S, P, D, F\}$
we get: $L \approx \hbar \cdot l \approx m \cdot (\omega \cdot l \cdot r_0) \cdot l \cdot r_0$
which means: $v = \omega \cdot l \cdot r_0 = constant$
we define: $v_0 = \omega_0 \cdot r_0$ and $\omega_0 = \frac{\hbar}{m \cdot r_0^2}$ and so $\omega = \frac{\omega_0}{l}$ using:

- $r_0 = d_0 = 1.62 \cdot 10^{-15} m$: the distance between neighboring nucleons.
- $m_p = 1.67 \cdot 10^{-27} kg$: the nucleon mass (for a rough estimate, we consider the proton and neutron mass as equal).

we get:

- tangential velocity: $v_0 = \omega_0 \cdot d_0 \approx \frac{\hbar}{m_p \cdot d_0} = \frac{1.05 \cdot 10^{-34}}{1.67 \cdot 10^{-27} \cdot 1.62 \cdot 10^{-15}} \approx 3.8 \cdot 10^7 \ \frac{m}{s}$

The minimum volume of a bound electron

Hypothesis: the minimum volume occupied by a bound electron defines a lower limit for the atomic volume; or the same statement in the opposite direction: the minimum size of an atom is determined by the minimum volume occupied by a bound electron.
We calculate it by comparing the angular momentum of the electron and the proton under the assumption of a constant tangential velocity of the bound particles:
$L_e \approx \hbar \approx L_p \quad \rightarrow \quad m_e \cdot r_e \approx m_p \cdot r_p \quad \rightarrow \quad r_e \approx \frac{m_p \cdot r_p}{m_e} \approx 1.5 \cdot 10^{-12} \ m$
which is in the range of its de-Broglie wavelength.
The meaning of this bound electron is assumed to be a minimum atomic size, before the proton and electron are fused to become a neutron; we assume that this is the case in the limit between white dwarfs and neutron stars.

Neutron star and the TOV limit

We want to assess the size and mass of a neutron star, and assume that the star is an expansion of the nuclear model, so we treat it as if it were a large nucleus.
A basic particle in the star is assumed to have the mass of a nucleon m_p and a basic cell size is derived from the distance between two neighboring nucleons in the star:
$d = 2 \cdot r = d_0 \approx 1.62 \cdot 10^{-15}\ m.$
A cubic bond is expected, so the volume of the basic cell and its density are:

- $V_{cell} = d^3 \approx 4.3 \cdot 10^{-45}\ m^3.$
- $\rho = \frac{m_p}{V_{cell}} \approx 3.9 \cdot 10^{17}\ \frac{kg}{m^3}$ this is within expected range [14].

The gravitational pressure in the center of the star is $P = \frac{2 \cdot \pi \cdot G \cdot \rho^2 \cdot R^2}{3}$ [17] with R the star radius and the force on the central nucleon in the star is about $F = P \cdot S$, with $S = 4 \cdot \pi \cdot r^2$ the surface of the nucleon.
We get:

- $F = \frac{8 \cdot \pi^2 \cdot G \cdot \rho^2 \cdot R^2 \cdot r^2}{3}$ the force on the cell in the center of the star.
- $R = \sqrt{\frac{3 \cdot F}{8 \cdot \pi^2 \cdot G \cdot \rho^2 \cdot r^2}}$ the star radius.
- $M = \rho \cdot V = \frac{\rho \cdot 4 \cdot \pi \cdot R^3}{3}$ the star mass.

Based on data from [5] we assume that the maximum force a nucleon can bear is about:

- $F_{max} \approx [3.0, 4.0] \cdot 10^4\ N$ maximum tolerable force in the star center.

this means:

- $R \approx [1.3, 1.5] \cdot 10^4\ m$, $M \approx [3.6, 5.6] \cdot 10^{30}\ kg$

and with $M_{sun} = 2 \cdot 10^{30}\ kg$ we get: $\frac{M}{M_{sun}} \approx [1.8, 2.8]$

which delivers a rough estimation to the maximum star mass, before it collapses to become a black hole; this is in the range of the Tolman-Oppenheimer-Volkoff limit [16].
We summarize the process:

- from the assumption of constant cubic arrangement, we get the density ρ.
- assuming the maximum force a nucleon can bear is F_{max} we get the star radius R through the gravitational pressure P in the center of the star.
- via R we get the star volume V.
- the star mass M is calculated using the star volume and density.

Remark: the main assumptions here are that the neutron star is a kind of large nucleus with a constant density and a rough estimate of the maximum force a nucleus can bear.

White dwarf and the lower limit of atomic size

The discussion of white dwarfs is done in a somewhat similar way to that of neutron stars above.
Hypothesis: there is a maximum pressure that atoms inside a white dwarf can bear, beyond this they collapse, and their electron and proton are fused to form a neutron.
Via the constant tangential velocity assumption, we make a rough estimate of the minimum basic cell radius for an atom to be in the range of $r_e \approx r_p \cdot \frac{m_p}{m_e} \approx 1.5 \cdot 10^{-12}\ m$.
Another assumption is that the star was created by light elements, so each basic cell consists of one electron, one proton and one neutron [18] meaning the atomic mass is about $A = 2$.
The star consists of atoms, so unlike the cubic arrangement in the neutron star, here the basic cell volume is assumed to be a sphere and not a cube.
Assuming a typical white dwarf radius and mass:

- $R \approx 1 \cdot 10^7\ m$ [18]
- $M \approx 0.5 \cdot M_{sun} = 1.0 \cdot 10^{30}\ kg$ [18]

We get:

- $V = \frac{4 \cdot \pi \cdot R^3}{3} \approx 4.2 \cdot 10^{21}\ m^3$ white dwarf volume.
- $\rho = \frac{M}{V} \approx 2.4 \cdot 10^8\ \frac{kg}{m^3}$ white dwarf density.
- $V_{cell} = \frac{m}{\rho} = \frac{A \cdot m_p}{\rho} \approx 1.4 \cdot 10^{-35}\ m^3$ white dwarf basic cell volume.
- $r_{cell} = \sqrt[3]{\frac{3 \cdot V_{cell}}{4 \cdot \pi}} \approx 1.5 \cdot 10^{-12}\ m$ white dwarf basic cell radius.

We see that the result for r_{cell} is in the range of r_e.

This strengthens the hypothesis, that there is a minimum atom size, beyond which the electron and proton are fused to form a neutron.

Pulsar - the lower limit of the rotation period

To analyze pulsars, we assume also here that a neutron star acts somewhat as a giant nucleus and as such maintains some of the nuclear properties, and discuss it in the light of the model. The elements formed in a star before undergoing supernova are assumed to be mainly up to the fourth row of the periodic table.

The lower limit of the rotation period

In order to calculate the pulsar angular velocity, we use the assumption made above regarding the constant tangential velocity, in the ideal situation in which all nuclei lie parallel to each other and so their superposition leads to a maximal angular and tangential velocity.

Data of a pulsar:

- The minimum radius: $R \approx 1.5 \cdot 10^4\ m$ [21]
- the minimum rotation period: $T \approx 10^{-3}\ s$ [15]

We use the tangential velocity found above:

- $v = \omega \cdot R \approx 3.8 \cdot 10^7\ \frac{m}{s}$

and get a rough estimation for the angular velocity:

- $\omega = \frac{v}{R} \approx \frac{3.8 \cdot 10^7}{1.5 \cdot 10^4} = 2.5 \cdot 10^3\ s^{-1}$

this implies a lower limit to the rotation period of pulsars:

- $T = \frac{2 \cdot \pi}{\omega} \approx 2.5\ ms$

which provides a rough estimate for the currently known data of about $T \approx 1.4\ ms$ [20].

The longer periods, or shorter angular velocities, are assumed to be due to a less parallel arrangement of the nuclei (or a smaller relative part with parallel nuclei) or of older pulsars that slowed down with time.

Remark: the constant tangential velocity hypothesis, delivers only a rough estimate of the real velocity. If we have a factor of 2 in the calculation, we get to $v \approx 7.5 \cdot 10^7\ \frac{m}{s}$ and the results are different, yet the focus here is to make initial usage of the model.

Atomic physics

The first ionization energy

Constructing the atomic first ionization energy function

The atomic ionization energy function should not only be adjusted mathematically, but also have a physical meaning. The process we take is not precise, yet it seems to deliver results that are good enough to assess the idea.
According to the model, the nuclear and atomic shells correspond to each other, and are as they appear in the periodic system.
We define:

- Z: the atomic number of the atom observed.
- Z_{orbit_last}: the atomic number of the atom, that closes the previous sub-orbital in the shell.
- $Z_{shell,orbit} = Z - Z_{orbit\_last}$: the number of electrons in the sub-orbital that is currently being filled.
- E_{orbit}: $\{E_S, E_P, E_D, E_F\}$: offset energy in $[\frac{kJ}{Mol}]$
- a_{orbit}: $\{a_S, a_P, a_D, a_F\}$: energy slope in $\left[\frac{kJ \cdot m}{Mol}\right]$

and estimate the energy that the outermost nuclear shell exerts on the outermost atomic shell:

- E decreases with r: $E \sim \frac{1}{r}$
- E grows with the number of atoms in the sub-orbital $Z_{shell,orbit}$: $E \sim Z_{shell,orbit}$

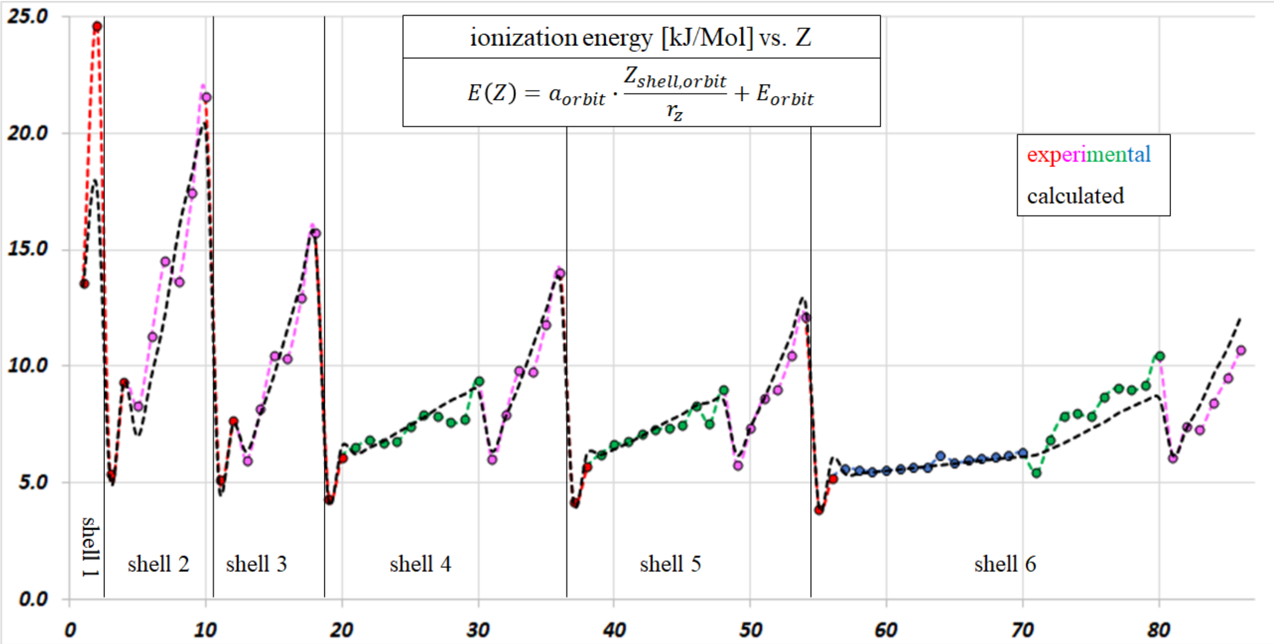
We therefore try the simplified function: $E(Z) = a_{orbit} \cdot \frac{Z_{shell,orbit}}{r_z} + E_{orbit}$
and obtain by tests the values:

- E_{orbit}: $\{E_S, E_P, E_D, E_F\} \approx \{2.1, 5.0, 6.0, 5.5\}$ $[\frac{kJ}{Mol}]$
- a_{orbit}: $\{a_S, a_P, a_D, a_F\} \approx \{550, 170, 40, 10\}$ $\left[\frac{kJ \cdot m}{Mol}\right]$

we define: $a_{orbit} \approx \frac{b}{a^{-l}}$
with: l: $\{l_S, l_P, l_D, l_F\} = \{0, 1, 2, 3\}$ the azimuthal quantum number of the sub-orbital
and get: $a \approx 4$, $b \approx 550$
the meaning of a and b is not clear yet, but we see that the function depends on the sub-orbital population and its angular momentum.

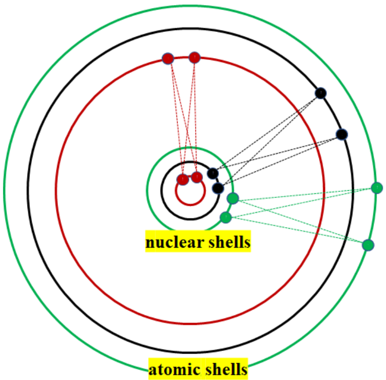
Analysis of the atomic first ionization energy function

The atomic first ionization energy function agrees well with the experiment. The variation could be due to shielding effects, that are not taken directly into account by the function.



***graph**: experimental data of the atomic first ionization energy (**S**, **P**, **D**, **F** sub-orbitals) dotted line: calculated function. Data from* [19]

Surprisingly it seems that the influence is only within the sub-orbital and the protons appear to have no effect on electrons beyond their correlated atomic orbital. According to the function the ionization energy is linear in the number of protons in the sub-orbital.
We get to the conclusion, that according to this simplified model at least, each atomic shell and orbital is influenced only by its correlated nuclear shell and orbital.
The following illustration depicts this idea.



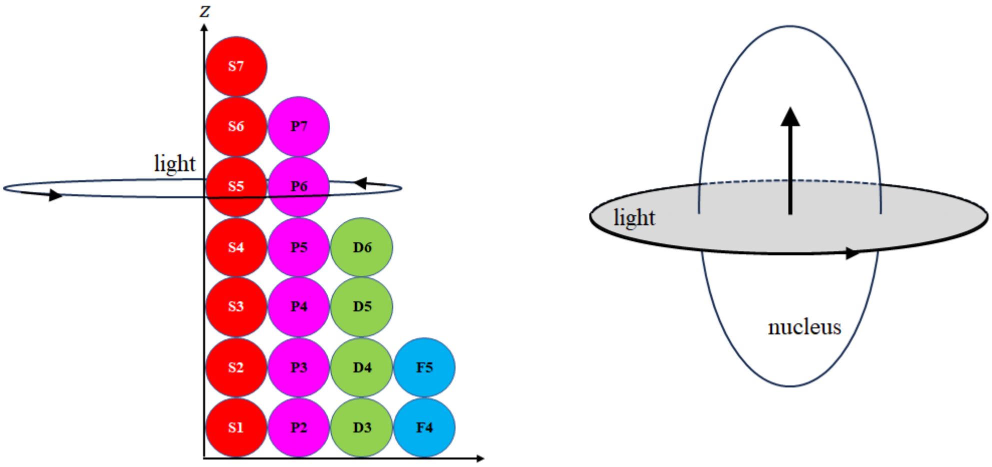
each nuclear shell and orbital affects only its corresponding atomic shell and orbital

This is also true for electronegativity, because these phenomena arise from the same source.

Electronic transition selection rules

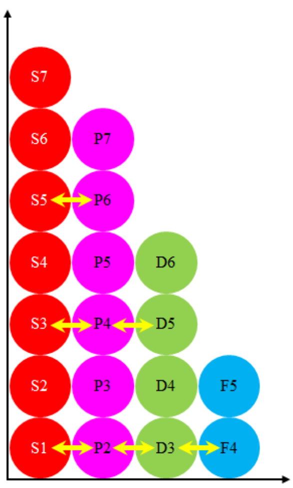
We assume that the atomic structure is somewhat similar to the nuclear geometry. According to the cubic nuclear model the ionization energy depends on the number of electrons in the sub-orbital, we therefore expect that the electron transition occurs by some sort of orbital completion via the absorbed light, that emulates a transition to the next orbital in the same plane, which is the x-y plane.

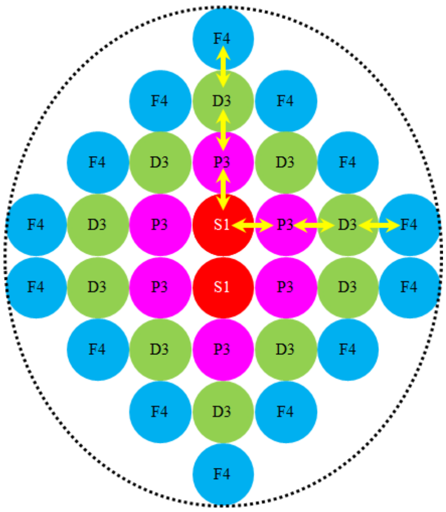
light absorption by the atom:



side vies: light absorption occurs in the x-y-plane (perpendicular to the z-axis)

electronic transitions as a result of light absorption:





side view - $\Delta n = \pm 1,\ \Delta L = \pm 1$
cross section in the x-z plane

top view - $\Delta n = \pm 1,\ \Delta L = \pm 1$
cross section in the x-y plane

Assuming the dipole transitions occur in the x-y plane, perpendicular to the z axis, we get from the illustrations above:

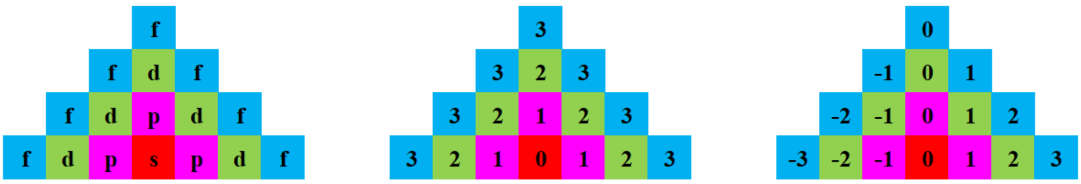
- Δn: each orbital in the x-y-plane has a principal quantum number larger than its predecessor).
- ΔL: moving toward the nuclear envelope the angular momentum increases.
- Δm: the magnetic quantum number can be read through the symmetry of the model; it grows from left to right.

and so we get the selection rules:

- $\Delta n = \pm 1$
- $\Delta L = \pm 1$
- $\Delta m = 0,\ \pm 1$

In accordance with the theory [24].
Following illustrations depict this through half an x-y layer to explain the rule for the magnetic quantum number as well.

sub-orbitals *L: angular momentum* *m: magnetic quantum number*



$\Delta L = \pm 1$ $\Delta m = 0,\ \pm 1$

The conclusion is that the selection rules are a simple consequence of the atomic structure and are essentially an inherent part of the model.

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