## Introduction to the Cubic Ellipsoid Nuclear Model and its Correlation with the Atomic Covalent Radius

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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. The model contains the advantages of the liquid drop, shell, collective and cluster models and can serve as a starting point to an effective field theory process. The main goal at this stage is not necessarily to obtain more accurate results than existing models, but rather to raise the possibility of a tangible interpretation of nuclear and atomic physics and to explore different perspectives of this idea. According to the model, the nucleus generally has an ellipsoidal shape, made up of a three-dimensional lattice of protonneutron bonds (treated here as a cubic system) and nuclear shells populated by protons, which resemble the atomic shells of the periodic table. The excess neutrons (those not paired with protons) are in the nuclear envelope. First, it is shown that the model is empirically confirmed (to a good approximation) via nuclear mass calculation and a consistent development of the nuclei with filled sub-orbitals. It is then argued that the periodic system is derivable from the model. Furthermore, the spatial nuclear structure is shown to correlate with the covalent atomic radius, and this potentially implies that the nuclear structure determines the atomic properties.

#### **1** Introduction

The nucleus and the atom have a size difference of about five orders of magnitude and are governed by different forces. The nucleons are held by the (strong) nuclear force, and the atomic properties are derived from the solution of the Schrödinger equation, where the nucleus is treated as a point electric charge. Beyond that, the nucleus has almost no effect on the atom. Only for hydrogen there is an exact solution. In larger atoms there is no complete solution and corrections are added. In nuclear physics the theory is incomplete. There is no nuclear potential, only approximations and estimates through models and instead of an exact quantum field theory, an effective field theory is used.

This study claims that there is a direct relationship between the nuclear structure and the atomic properties and presents a model that supports this idea for all types of nuclei. This seemingly contradicts the common perception in physics according to which there is a separation between the two theories, therefore it is necessary to explain how this is possible and why this idea can still be viable. The separation between the nuclear structure and that of the atom is neither self-evident nor intuitive. The purpose of this research is to investigate whether there is a tangible interpretation of nuclear physics using a nuclear model that reflects the atomic properties. The development of the model is described in detail in the study itself. The model is still preliminary, referring to a static nucleus (ignoring for instance vibration and rotation) and requires extensions and improvements; nonetheless, even in this simple state it provides good results. This paper presents the research basics through two topics. The first is the model construction and its mass formula calculations for the nuclei with filled sub-orbitals. The second issue is the correlation between nuclear geometry and the atomic covalent radius. Following studies will expand the research and analyze various nuclear and astro-physical subjects in the light of the model.

## 2 Part one: the model and its mass formula

## 2.1 The requirements

The experimental data and the structure of the periodic table determine the requirements that the model must meet. These requirements allow the 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, a stable diproton atom,  $He_2^2$ , could be expected for instance.
- 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, the observation of a stable neutronium nucleus,  $n_2$ , would be expected.
- 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) to justify the model assumption.
- The same holds for the orbitals and their population sequence.
- The nuclear proton distribution shall be equal for all isotopes of the same element to justify their identical chemical behavior.
- Pauli's exclusion principle must be fulfilled.

# 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.

# 2.2 The model

From the above requirements a model was derived:

- The nuclear structure:
  - $\circ~$  The shape of the nucleus is in general an ellipsoid, which is physically reasonable.
  - It consists of a cubic system of p-n bonds with a constant distance between neighboring nucleons. The cubic system prevents n-n and p-p bonds.
  - The excess neutrons, beyond those that are paired with protons, are in the envelope of the nuclear ellipsoid.
- Properties:
  - The population of nuclear shells with protons is 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 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 and spin-down, except for only single nucleons, if their number is odd. The exact spin distribution is not essential at this point and is therefore not discussed in this article.
- $\circ$  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.
    - Compliance with Pauli's exclusion principle.

As an example, the x-y plane cross sections along the z-axis and the x-z plane cross section of the Krypton  $Kr_{36}^{82}$  nucleus are observed.

Figure 1: Kr<sub>36</sub><sup>82</sup> nucleus



*Legend: protons:* full circles according to the orbitals *S*, *P*, *D* (L = 0, 1, 2). *numbers:* principal quantum number n. *neutrons:* hollow circles with colors according to their orbital. *excess neutrons*, beyond the number equal to the protons (unpaired neutrons).

### 2.3 The Mass formula

The mass formula was built in accordance with the theory of the model, unlike the semiempirical one [7], [8], [9]:  $m_{calc_x} = Z_x \cdot m_p + N_x \cdot m_n - \frac{(E_{b_x} - E_{c_x})}{c^2}$  (1)

- $A_x$ : the atomic mass (number of nucleons) of the nucleus x.
- $m_{calc_r}$ : the calculated mass of the nucleus *x*.
- $Z_x$ : the atomic number.
- $m_p$ : the mass of the proton.
- $N_x$ : the number of neutrons  $(N_x = A_x Z_x)$ .
- $m_n$ : the mass of the neutron.
- $E_{b_x}$ : the total nuclear 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 nuclei.

(2)

•  $n_{b_x}$ : the number of nucleon-nucleon bonds in the nucleus *x*.

$$E_{c_x} = \frac{e^2}{4\pi\epsilon_0} \frac{1}{d_0} \left\{ \frac{1}{2} \sum_i^{Z_x} \sum_{j\neq i}^{Z_x} \frac{1}{d_{i,j}} \right\} = \frac{e^2}{4\pi\epsilon_0} \frac{1}{d_0} e_{c_x} \quad \text{where} \quad e_{c_x} \coloneqq \frac{1}{2} \sum_i^{Z_x} \sum_{j\neq i}^{Z_x} \frac{1}{d_{i,j}} \tag{3}$$

- $d_0$ : the minimum distance between two neighboring nucleons (assuming all nuclei have the same cubic structure and density).
- $d_{i,j}$ : the unitless distance between the protons of the indices *i* and *j* measured in multiples of  $d_0$ :  $d_{i,j} = \sqrt{(x_j - x_i)^2 + (y_j - y_i)^2 + (z_j - z_i)^2}$  (4)
- $e_{c_v}$ : the unitless total electric energy of the nucleus (sum of the reciprocal distances).

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

$$rel_err_{\chi} = \left| \frac{m_{calc_{\chi}} - m_{meas_{\chi}}}{Z_{\chi} \cdot m_{p} + N_{\chi} \cdot m_{n} - m_{meas_{\chi}}} \right| = \left| \frac{m_{calc_{\chi}} - m_{meas_{\chi}}}{mass\_defect_{\chi}} \right|$$
(5)

- $m_{meas_x}$ : 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. Note:  $rel\_err_x$  is represented here in percentage.

The mass formula depends thus only on the two variables:

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

The implementation requires two preliminary calculation steps for each nucleus:

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

Note: the exact shape of the nucleus affects the results of the mass formula.

#### 2.4 Mass calculation of nuclei with filled sub-orbitals

As mentioned above, the nuclear shape influences the mass formula results; this is caused because of the following:

- The shape of the nuclear core consists of proton-neutron pairs and affects the electric charge distribution.
- The total arrangement of the nucleons determines the number of bonds in the nucleus and therefore affects the binding energy.

These points must be considered to ensure a scientific approach and to avoid data manipulation. The nuclear core has a specific and unambiguous arrangement, so the electric energy seems to be well calculated. Unlike this, the arrangement of the excess neutrons in the nuclear envelope can be achieved in various ways and this entails a modification of the number of bonds and as a result a change of the binding energy. To address this, the nuclei with complete sub-orbitals were drawn and the excess neutrons were arranged in a consistent manner. The drawings of the nuclei with filled sub-orbitals are shown in Appendix A.

Only then the mass formula calculation was implemented on fourteen nuclei with filled suborbitals (the colors are according to the sub-orbitals: s, p, d, f):  $Ne_{10}^{20}$ ,  $Mg_{12}^{24}$ ,  $Ar_{18}^{36}$ ,  $Ca_{20}^{40}$ ,  $Zn_{30}^{70}$ ,  $Kr_{36}^{72}$ ,  $Sr_{38}^{86}$ ,  $Cd_{48}^{116}$ ,  $Xe_{54}^{128}$ ,  $Ba_{56}^{132}$ ,  $Yb_{70}^{168}$ ,  $Hg_{80}^{202}$ ,  $Rn_{86}^{214}$ ,  $Ra_{88}^{218}$ .

The following was achieved (experimental data from [1]):

- A consistent nuclear form.
- The nuclei were found to be within the stability range of their isotopes (or the range of relative longer half-life, for radioactive elements of Z > 82).

• Relative error of mass calculation: max = 4.7%, mean = 1.5%, std. dev = 1.3%.

This is within reasonable range [7], [10]. The calculation parameters of the mass formula were found as:

- $d_0 = 1.62 \pm 0.03$  fm the minimum distance between two neighboring nucleons.
- $e_b = 5.72 \pm 0.03 \text{ MeV}$  the energy of a single nucleon-nucleon bond.

this seems to be within range as well [5]. Through  $d_0 \approx (r_n + r_p)$  a rough estimate of the sum of the proton and neutron radii is obtained,

- and the relative error is estimated:
  - $r_n \approx 0.80 \text{ fm neutron radius [3]}, r_p \approx 0.84 \text{ fm proton radius [4]}.$
  - $r_n + r_p \approx 1.64 \ fm$
  - Relative deviation for  $d_0: \left| \frac{d_0 (r_n + r_p)}{(r_n + r_p)} \right| = \left| \frac{1.62 1.64}{1.64} \right| = \left| \frac{0.02}{1.64} \right| \approx 1.5\%$  (6)

This is a byproduct of the mass formula calculation, which provides an unintended result that reinforces the model assumption. Further studies will show that the main influence comes from the nuclear core of the proton-neutron pairs, so the precise deployment of the excess neutrons in the envelope is less crucial.

#### 3 Part two: the link between the nuclear geometry and the atomic properties

To confirm the model hypothesis, a direct link between the nuclear structure and the atomic properties must be shown.

#### 3.1 Nuclear covalent radius - definition and calculation

As a preparation step, two definitions are made:

- A "valance proton": the proton, that was last added to the current, in-filling process, sub-orbital of the nucleus.
- The "nuclear covalent radius": the relative geometric distances of the "valance proton" from the nuclear center.

The following illustrations demonstrate the way the "nuclear covalent radius" of the "valance proton" is calculated from the nuclear geometry via  $r_{x,y,z} = \sqrt{x^2 + y^2 + z^2}$ *Figure 2: calculating the nuclear covalent radius* 



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 might be intuitively expect.

#### 3.2 Comparison between the nuclear and atomic covalent radii

The cubic ellipsoid nuclear model was first created in search of a connection between the nuclear structure and the atomic properties. Therefore, the pattern of the atomic covalent radius is sought to compare with the "nuclear covalent radius" of the corresponding nuclear sub-orbital. Each atomic covalent radius must be associated with the correct "nuclear covalent radius". At this stage the research refers only to nuclei with filled sub-orbitals (s, p, d, f). Further study successfully expands this to about 30 symmetric nuclei. The atomic data is available for atomic number  $Z \in [1, 96]$  (from [11]); the nuclei are thus:

Row 1: *He*<sup>4</sup><sub>2</sub>

Row 2:  $Be_4^9$ ,  $Ne_{10}^{20}$ Row 3:  $Mg_{12}^{24}$ ,  $Ar_{18}^{36}$ Row 4:  $Ca_{20}^{40}$ ,  $Zn_{30}^{70}$ ,  $Kr_{36}^{72}$ Row 5:  $Sr_{38}^{36}$ ,  $Cd_{48}^{116}$ ,  $Xe_{54}^{128}$ Row 6:  $Ba_{56}^{132}$ ,  $Yb_{70}^{168}$ ,  $Hg_{80}^{202}$ ,  $Rn_{86}^{214}$ Row 7:  $Ra_{88}^{218}$ 

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 picometer  $([pm] \text{ or } 10^{-12}m)$  whereas the proton distance in relative values (the values of the adjustment parameters were found to be  $r_0 \approx 40$ ,  $a \approx 30$ ).

An apparent correlation between the two curves is observed, although the atomic curve is taken from the experimental data and the nuclear covalent radius is a geometric property, measured according to the ellipsoid model. This unexpected result is a strong hint for a link between the nuclear and atomic geometries and properties and might be the proof to the cubic ellipsoid nuclear model. Moreover, it may imply a different interpretation of the nature of a bound electron.

Note: the covalent atomic radius is not necessarily the "farthest point" on the "surface of the atom" (which probably corresponds better to the van der Waals radius) but the point corresponding to the "valence proton".



*Graph 1: the nuclear vs. atomic covalent radius* 

#### 4 Discussion

This model is still in an early stage; however, it obtains a good estimate of the nuclear mass and the sum of the proton and neutron radii  $r_p + r_n$ . The model justifies the periodic table in terms of energy levels, order of electronic population and orbitals, as well as an explanation of why different isotopes of the same element have similar chemical properties. The study revealed a correlation between nuclear geometry and the atomic covalent radius, which strengthened the research hypothesis. In a following study the mass formula calculation will be expanded to more than 350 stable nuclei (or heavy ones with a relative long half-life). Further studies will deal with nuclear phenomena that are mainly affected by the electric energy, which depends on the nuclear core (the nucleus without the excess neutrons) therefore the effect of the excess neutrons is secondary for the purpose of analyzing the principles. These studies will include, among others: the nuclear charge radius; the instability of heavy nuclei and the short half-life of superheavy nuclei; the nuclear fission mechanism, products and energy; nuclear magic numbers; astro-physical phenomena. It is emphasized that although the model still requires further development, its generality and good estimates seem to support its feasibility.

#### **5** Conclusion

The research offers a simple and logical semi-classical interpretation of the nuclear structure and links it to the atomic properties. The model offers an alternative that contains the advantages of the currently existing models and shows a clear connection between the nuclear geometry and the atomic covalent radius. Within this interpretation issues that are considered abstract become tangible and self-evident, and explanations that require complex calculations are obtained naturally. Follow-up studies will explain various phenomena considering the model.

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### Appendix A: drawing the nuclei with filled sub-orbitals in a consistent form

In the following section the nuclei of closed sub-orbital S, P, D, F are shown in a consistent form that describes their development, so a feeling can be developed to the guidelines for a stable nucleus.

The fact that such a consistent structure can be generated and that the represented nuclei for each of the observed elements lie within the range of their stable isotopes (or long-lived ones in the case of heavy nuclei beyond Pb) may be a strong confirmation of the model.

It is emphasized again that first the nuclei of filled sub-orbitals are created, in a consistent manner and only after that their mass formula is checked, meaning that it was not an iterative process, and so this is not a result of some data manipulation.

A clear pattern of nuclear growth can be followed with distinct positions where the excess neutrons are added.

## The nuclei with filled sub-orbitals according to their row in the periodic table

Row 1:  $He_2^4$ Row 2:  $Be_4^9$ ,  $Ne_{10}^{20}$ Row 3:  $Mg_{12}^{24}$ ,  $Ar_{18}^{36}$ Row 4:  $Ca_{20}^{40}$ ,  $Zn_{30}^{70}$ ,  $Kr_{36}^{72}$ Row 5:  $Sr_{38}^{86}$ ,  $Cd_{48}^{116}$ ,  $Xe_{54}^{128}$ Row 6:  $Ba_{56}^{132}$ ,  $Yb_{70}^{168}$ ,  $Hg_{80}^{202}$ ,  $Rn_{86}^{214}$ Row 7:  $Ra_{88}^{218}$ ,  $No_{102}^{254}$ ,  $Cn_{112}^{284}$ ,  $Og_{118}^{296}$ 

The first two nuclei of closed sub-orbitals,  $He_2^4$  and  $Be_4^9$ , are too small to show a specific pattern, therefore the list begins with  $Ne_{10}^{20}$ .

The drawings describe cross sections of the nuclei in the x-y planes along the z axis. For visibility only the upper (or left) half of the nuclei is shown.





Four atomic mass parameters are shown:

- A: the atomic mass of the nucleus referred to in the drawing.
- min: the minimum atomic mass for a stable nucleus (or with a relatively longer halflife, for nuclei with Z > 82).
- opt: the most abundant atomic mass.
- max: the maximum atomic mass for a stable nucleus.

All nuclei were found to be in the range:  $min \le A \le max$ , which is a reinforcement to the model (data from [1]).





p: protons **p p p** according to the orbitals S, P, D, F n: neutrons ; n: excess neutrons



n: neutrons ; n: excess neutrons

#### Appendix B: the ellipsoids of the nuclei with filled sub-orbitals

To better understand the model, the ellipsoids of the filled sub-orbitals are shown and arranged as they appear in the periodic table. The orbitals grow from left to right and the layers grow from top to bottom; the colored arrows refer to the sub-orbital that was last filled.



Figure 5: cross sections in the x-z plane of the ellipsoids with filled sub-orbitals

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.

#### Appendix C: the mass formula calculation data

The values reached by the mass formula calculation:

- $d_0 = 1.62 fm$
- $e_b = 5.72 MeV$

The legend of the table below is given according to its position from left to right:

- *nuc*.: the nucleus (symbol).
- $Z_x$ : atomic number of the nucleus x; the number of protons.
- $A_x$ : mass number of the nucleus x; the number of nucleons.
- $N_x := A_x Z_x$ : the number of neutrons of the nucleus *x*.
- $n_k$ : the number of nucleon-nucleon bonds in the nucleus as it was calculated by the relevant Excel file.
- *e<sub>c</sub>*: total relative electric energy of the nucleus as it was calculated by the relevant Excel file.
- *measured [amu]*: measured mass [1] of the nucleus in [amu].
- *base mass:*  $Z_x \cdot m_p + N_x \cdot m_n$  [*amu*]: base mass in [amu]:

number of protons  $\cdot$  proton mass + number of neutrons  $\cdot$  neutron mass

- *calculated mass [amu]*: calculated mass according to the mass formula in [amu]  $m_{calc_x} = Z_x \cdot m_p + N_x \cdot m_n - \frac{(E_{b_x} - E_{c_x})}{c^2}.$
- $\Delta_I$ : [amu] calculated measured: calculated mass minus measured mass in [amu]
- $\Delta_2$ : [amu] base measured: base mass minus measured mass in [amu]
- relative error  $\Delta_1$ :  $\Delta_2$ : the relative error in percent: relative error =  $|\frac{calculated mass-measured mass}{base mass-measured mass}|$

Table 1.	mass f	òrmula	calcul	lation	data
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nuc.	$Z_x$	$A_x$	n <sub>k</sub>	e <sub>c</sub>	measured mass [amu]	calculated mass [amu]	relative error $\Delta_1: \Delta_2$	$\begin{array}{ll} \text{base} & \text{mass} \\ Z_x \cdot m_p + N_x \cdot m_n \\ [\text{amu}] \end{array}$	$\Delta_1$ : calculated minus measured	$\Delta_2$ : base minus measured
Ne	10	20	32	26	19.9924	19.9878	2.8%	20.1594	-0.0046	0.1670
Mg	12	24	38	34	23.9850	23.9905	2.6%	24.1913	0.0054	0.2063
Ar	18	36	66	74	35.9675	35.9526	4.7%	36.2869	-0.0149	0.3194
Ca	20	40	72	86	39.9626	39.9584	1.2%	40.3188	-0.0042	0.3562
Zn	30	70	132	185	69.9253	69.9310	0.9%	70.5649	0.0056	0.6396
Kr	36	82	160	254	81.9135	81.9200	0.9%	82.6605	0.0065	0.7471
Sr	38	86	166	271	85.9093	85.9318	2.9%	86.6924	0.0226	0.7832
Cd	48	116	236	421	115.9048	115.8910	1.3%	116.9385	-0.0137	1.0337
Xe	54	128	264	508	127.9035	127.8978	0.5%	129.0341	-0.0058	1.1306
Ba	56	132	270	531	131.9051	131.9147	0.8%	133.0660	0.0097	1.1610
Yb	70	168	354	796	167.9339	167.9443	0.7%	169.3585	0.0104	1.4246
Hg	80	202	432	1014	201.9706	201.9541	1.0%	203.6392	-0.0166	1.6686
Rn	86	214	460	1132	213.9954	213.9904	0.3%	215.7349	-0.0050	1.7395
Ra	88	218	466	1162	218.0071	218.0140	0.4%	219.7668	0.0069	1.7596