NUCLEAR PHYSICS AND ELEMENTARY PARTICLES

https://doi.org/10.46813/2023-148-003

NUCLEOSYNTHESIS OF NUCLEAR MATTER: ENTROPY EFFECTS

V.T. Maslyuk[1], Ye.O. Skakun[2], I.L. Semisalov[2], M.I. Romanyuk[1]
[1]Institute of Electron Physics, Nat. Acad. Sci. of Ukraine, Uzhhorod, Ukraine;
[2]National Science Center "Kharkov Institute of Physics and Technology", Kharkiv, Ukraine
E-mail: volodymyr.maslyuk@gmail.com

The work considers an alternative way of formation of chemical elements during the disintegration of nuclear matter formed during the explosion of stars. In addition to the energy parameters that determine the stability of nuclear matter and the ways of its disintegration, the entropy factor must also be considered. The calculation points to its extreme feature in the transition from symmetric to structured or asymmetric decay caused by the "inclusion" of quantum effects from nuclear shells.

PACS: 26.30.+k, 26.35.+c, 26.50.+x

INTRODUCTION

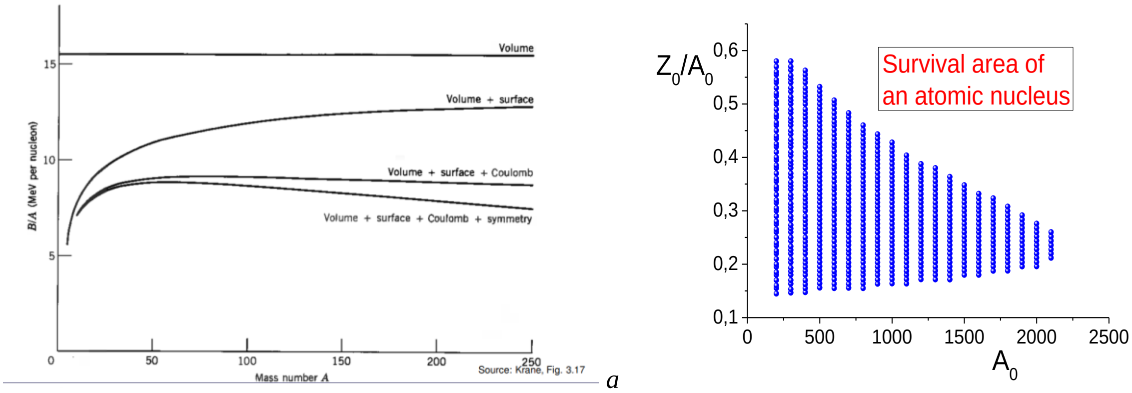
The modern theory of nucleosynthesis is based on several stages of the formation of chemical elements, the first of which includes the formation of primary nucleons from the quark-gluon plasma at temperatures above 10^{10} K, and upon its further cooling – light nuclei to lithium and beryllium [1]. The next stage is related to the processes of stellar nucleosynthesis, which occur in stars with a high density of matter ($10^{-3}…10^{-1}$) nucl. fm-3 and temperature, T, range 0.5…10 MeV, the equilibrium maintained by nuclear forces [2]. As a rule, the mass of such stars should exceed the Chandrasekhar limit of 1.4 times the mass of the Sun. These requirements are satisfied by white dwarfs and neutron stars whose evolution ends with a supernova explosion [3]. According to modern ideas, the synthesis of chemical elements occurs in stars and products of their explosions due to elementary interaction involving neutrons (s- and r-processes) and protons (p-processes) or by fusion of light nuclei [4]. Conventionally, this approach is similar to the "snowball" formation process, when all known Periodic Table's chemical elements were formed due to successive mass and charge growth. One must note such nuclear reactions are possible under the influence of strong electromagnetic fields of the ionized plasma of stellar matter, the parameters of which can be reproduced in terrestrial conditions at nuclear physics installations. However, the result of a supernova explosion can also be the fragmentation of the formed matter into clusters of different sizes, which preserves the thermodynamic parameters of the original nuclear matter. Such a multi-fragmentary array will tend to their further clustering and ultimately form the entire diversity of isotopes of chemical elements. The success of this direction of the nucleosynthesis theory requires new ideas about the stability of nuclear matter of arbitrary size and an understanding of the rules governing the processes of its transformation [5, 6].

This work examines the role of entropy factors in such transformations. Special attention is paid to nuclear clusters of transitional sizes, having atomic mass A within several thousand to values of A ~ 300…500, when nuclear shells are formed, and quantum effects are manifested. The proposed theory goes beyond the droplet model and can be applied to a nuclear cluster of arbitrary size. As the first stage, this paper considers the case of two-fragment fragmentation of a nuclear cluster of arbitrary size.

1. THE STABILITY OF NUCLEAR MATTER: ENERGY FACTORS

The basic element of modern nuclear physics is the drop model, when the nucleus is considered as a drop of charged liquid, the energy of which consists of volume, surface, symmetric, and electrostatic components. The macroscopic method, which is the basis of this approach, allows us to estimate nuclei's mass and specific binding energy, to study the energetic conditions of their fission and α- and β-transformations. The mathematical design of this approach contains Bethe-Weizsäcker's semi-empirical formula, which, based on experimental data, formalizes the numerical coefficients of the indicated components of the nuclear energy, Fig. 1,a. Further development of the macroscopic approach was obtained in works [7 - 9], which supplement the Weizsäcker formula by taking into account the shell corrections associated with the magic numbers of protons 2, 8, 14, 20, 28, 50, 82, 108, 124 and neutrons, respectively 2, 8, 14, 20, 28, 50, 82, 124, 152, 202. This method makes it possible to describe the values of the binding energies of known nuclei with an accuracy of a percent and estimate their stability depending on the sizes. Fig. 1,b presents the result of assessing the stability region of atomic nuclei, performed within the framework of the droplet model based on the formula [7]. As can be seen, the graph demonstrates that at A> 2200, there are no nuclear formations with negative binding energy, which is a condition for their stability. The droplet model gave rise to the macroscopic direction of the theory of the nucleus, which later underwent many modifications [10]. Subsequently, the theory considered the energy constants obtained based on the single-particle Yukawa potential, shell corrections, spin-dependent parameters, and restrictions related to the locality of the nuclear droplet. These modifications made it possible to say about creating a macro-microscopic direction of the theory. They gave a new impetus to calculating the characteristics of the ground state of nuclei up to the values of A ~ 339 [11]. Interest in this kind of calculation is also due to the search for an island of stability – hypothetical super heavy nuclei with filled proton and neutron shells, the lifetime of which is longer than that of neighboring transuranic isotopes. The further development of the core theory is connected with the development of computer technologies – the possibilities of GRID technologies and the increase in the speed of computer calculations. Recent successes in computational techniques are associated with the microscopic approach, the mathematical apparatus that considers nucleon degrees of freedom and internucleon forces. An example is the nuclear density functional theory, which uses appropriate single-particle orbitals, is based on effective nucleon-nucleon interactions, and allows the calculation of self-consistent mean fields for nucleons [12 - 14].

Thus, the current state of theoretical research is limited to studying the stability and transformation of atomic nuclei for A less than 300…400 at.un. [15, 16]. Phenomenological models, modified by considering microscopic components as shell corrections, indicate the possibility of stable formations for nuclear objects up to A0 ~ 4000 [17]. However, such values are much smaller than the characteristic sizes of nuclear fragments formed during explosions of supernovae and neutron stars. Therefore, it is vital to search for new theoretical possibilities for describing the stability of nuclear conglomerates of arbitrary sizes using general ideas about ordering many-particle systems.



a *b*

Fig. 1. Factors forming the binding energy of atomic nuclei according to the Weizsäcker formula (a); stability region of hypernuclei for different ratios between their atomic mass A_0 and charge Z_0 (b)

2. THE METHOD OF STATISTICAL ENSEMBLES IN THE THEORY OF NUCLEAR MATTER

In the works [18, 19], a method of statistical ensembles is proposed, which is based on color statistics and allows to study of the thermodynamic ordering after splitting arrays of nuclei-fragments of the original nucleus of arbitrary mass (A) and charge (Z). Its basis is using thermodynamic functions oriented to study the stability of a system of many particles.

In the case of the two-fragment fission scheme, the parameters determining the equilibrium condition for each of the investigated post-fission ensembles of nuclear fragments are derived from the state of the minimum thermodynamic potential of constant pressure, which for the i-th nuclear cluster has the form:

$$G_i = \varepsilon_i - TS_i + PV_i\,, \qquad (1)$$

where ε_i is the internal energy, and V_j, respectively, the volume of the cluster of two fragments, j=1, 2, containing $N^j_{p,i}$ protons and $N^j_{n,i}$ neutrons, For different nuclear clusters, its spectrum $\{\varepsilon_i\}$ is an additive quantity:

$$\varepsilon_i = \sum_{j=1,2} B(N^j_{p,i}, N^j_{n,i})\,. \qquad (2)$$

Here $B(N^j_{p,i}, N^j_{n,i})$ are the binding energies of the j-th nucleus fragment from the i-th cluster. The probability of realization of two-fragment clusters $\{N^i_{p,1}, N^i_{p,2}, N^i_{n,1}, N^i_{n,2}\}$ from the initiate nucleus with mass A_0 and charge Z_0 is defined as:

$$Y(N^i_{p,1}, N^i_{p,2}, N^i_{n,1}, N^i_{n,2}) = \omega_i \exp\{-(\varepsilon_i + PV_i)/T\}/z. \qquad (3)$$

Here – ω_i is the degeneration of the spectrum (2) of a cluster with two fragments, which is determined through the combinatorics of colored balls, and the function z, a statistical sum, is defined as:

$$z = \sum_i \omega_i \exp\{-(\varepsilon_i + PV_i)/T\}\,. \qquad (4)$$

The entropy factor S_i in (1) is calculated due to the ω_i degeneration of the energy states ε_i and takes into account the statistical nonequivalence of nucleons having different binding energies in the fission fragments:

$$S_i = \ln(\omega_i)\,. \qquad (5)$$

Where taking into account the emission of fission neutrons:

$$\omega_i = A_0!/(\prod_{j=1,2} K(n^i_j)(N^i_{p,j}!(N^i_{n,j} - n^i_j)!). \qquad (6)$$

Here n^i_j is the number of fission neutrons of the j-th fragment of the i-th cluster, $K(n^i_j) = 1/n^i_j!$, $\prod_{j=1,2} x_j! = x_1!x_2!$. As seen from (6), with increasing temperature T, the entropy term in (1) is responsible for the symmetrization of fission products of the initial nucleus.

The obtained formulas (1) - (6) allow us to study the peculiarities of the disintegration of nuclear conglomerates of arbitrary size. As seen from (1), the way of such disintegration is determined by the minimum thermodynamic potential (1). At a constant value of work, term

PV, this is achieved at the minimum of the energy term [20]

$$Z = A/(1.98 + 0.015 \times A^{2/3}). \quad (7)$$

The entropy term is another factor that can act on ordering processes during the fragmentation of nuclear matter. Formula (5) is related to the degeneration of the energy state of the i-th nuclear cluster of the type. We believe such a cluster was formed during the fission of a nuclear conglomerate of arbitrary mass A and charge Z, or the ratio "A/Z". In the future, the task is reduced to establishing the nuclear conglomerates' evolution ways. This paper investigates how many ω_i sets can create the "A/Z" nuclear conglomerate to realize all possible two-fragment clusters. In other words, it is essential to estimate the entropy factor associated with forming an array of two-fragment clusters from the nuclear conglomerate of arbitrary volume and composition, which generally correspond to the conditions of the bound states of the cluster nucleons.

3. RESULTS AND DISCUSSIONS

For calculations, we limit ourselves to the scheme of 2-fold splitting and the Bethe-Weizsäcker formula [8], considering shell corrections and pairing effects to find the spectrum (2). In Fig. 2 shows the calculation data of the charge spectra of hypothetical nuclei in the mass range of 1000…400. At large values of A, hypothetical nuclear conglomerates divide symmetrically, forming fragments of equal mass and charge. Quantum effects are "turn on" for nuclear conglomerates starting from A ~ 600…800. For these and smaller values of A, there are ranges of values of the charges of fission fragments Z_i, at which quantum effects lead to an asymmetric yield of fission fragments. This regularity intensifies as the value of A decreases.

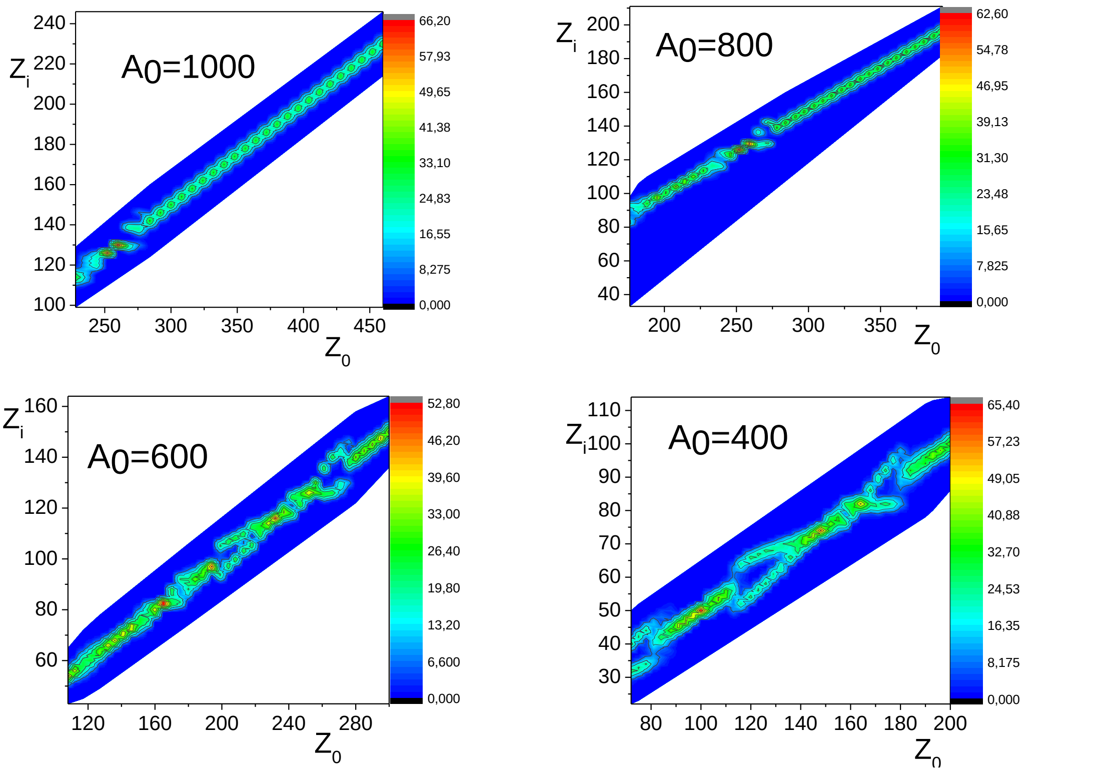


Fig. 2. There is charge two-fragment spectra of fission fragments of nuclear conglomerates with mass A_0 and Z_0. As can be seen, the decrease in the mass number A_0 expands the area of formation of asymmetric nuclei-fragments yield

Thus, the following stages of disintegration of nuclear matter of arbitrary mass can be distinguished: multifragmentation with the formation of nuclear clusters of approximately the same mass/charge; around A ~ 1000, the inclusion of quantum effects and the beginning of scission into asymmetric fragments; from A ~ 600 and less – quantum effects govern the fission of atomic nuclei, the dominance of asymmetric fission fragments.

The next stage is the consideration of the entropy factor in the separation of nuclear conglomerates. For this, the number of possible combinations that can form stable 2-fragment clusters should be investigated, for example, from the Z/A ratio of the original nucleus. In Fig. 3 shows the data of such a calculation for hypothetical nuclei in the interval 200…2200, obtained at T=1 MeV. It can be seen that, depending on Z_0/A_0, there are various combinatorial possibilities for the formation of stable 2-fragment clusters, which, along with the energy factors, determine the entropy factors of the fragmentation of nuclear matter. As one can see, the calculation shows the presence of features of the entropy factor. First, the number of combinations for the realization of the 2nd fragment cluster, or the degeneration of the nuclear system, depending on the ratio of their protons/neutrons, differs from expression (7) for establishing the equilibrium values of Z_0/A_0. Another feature is the singularity of the degeneracy factor around the values of $Z_0 \sim 440$, $A_0 \sim 1600$, the nature of which is still unknown and may be related to the choice of the expression for finding the binding energies of atomic nuclei in the form [8], which takes into account shell corrections. Such a singularity may indicate the "switch on" of quantum effects that appear during the formation of atomic nuclei of significant size. Therefore, it is advisable to test the methodology when choosing other systematics of mass formulas such as [8]. Furthermore, the calculation also shows the dependence of the indicated singularity on the temperature of the initial nuclear conglomerate, which is not contained in (7).

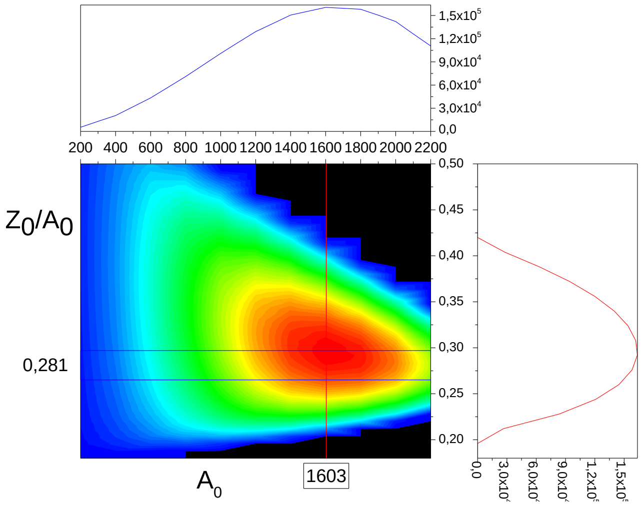


Fig. 3. The probability of 2-fragment fission of a hypothetical nucleus of mass A_0 for different values of its charge Z_0

The obtained data indicate the existence of priority channels of disintegration of nuclear matter, which are focused on the formation of actinide mother nuclei, the decay of which formed more than 300 quasi-stable nuclei, which are the basis for the creation of chemical elements of the Earth's crust and stellar bodies. This fact also explains the existence of heavy nuclei in them, the formation of which is unlikely in any other way, for example, through the "snowball" mechanism.

CONCLUSIONS

As can be seen, the proposed theoretical approach can be applied to the study of the stability and decay channels of nuclear conglomerates of arbitrary mass and offers an alternative to the classical scheme of the formation of a variety of atomic nuclei and isotopes of the Earth and celestial bodies. Such studies indicate that stellar nucleosynthesis of known isotopes and chemical elements can also occur through a cascade of formed nuclear matter decay processes. However, the proposed theory does not contain fitting parameters and proposes the establishment of such decay channels for nuclear conglomerates of arbitrary size.

Currently, the calculation possibilities are limited to the reliable establishment of the binding energy and the decay channels of hypothetical nuclei up to A ~ 400 at.un. Further theoretical studies of nuclear conglomerates of greater mass are available for research within the framework of only phenomenological approaches, which establish their stability regions. Therefore, we can say that solving this problem requires taking into account, in addition to the energy factor, the entropy factor as a factor of the stability of nuclear conglomerates to establish probable channels of their disintegration.

ACKNOWLEDGEMENTS

The authors are grateful to V.Yu. Denisov for his support during the preparation of this work.

REFERENCES

1. R. Tayler. Intorduction to Big Bang nucleosynthesis: open and closed models, anisotropies // *Philosophical Transactions of the Royal Society of London. Series A, Mathematical and Physical Sciences.* 1982, v. 307, p. 3-17. http://doi.org/10.1098/rsta.1982.0096.
2. G. Wallerstein et al. Synthesis of the elements in stars: forty years of progress // *Rev. Mod. Phys.* 1997, v. 69, iss. 4, p. 995. DOI: https://doi.org/10.1103/RevModPhys.69.995.
3. F.-K. Thielemann, M. Eichler, I.V. Panov, B. Wehmeyer. Neutron Star Mergers and Nucleosynthesis of Heavy Elements // *Annual Review of Nuclear and Particle Science*. 2017, v. 67, № 1, p. 253-274. https://doi.org/10.1146/annurev-nucl-101916-123246.
4. Bradley S. Meyer. The r-, s-, and p-processes in Nucleosynthesis // *Annu. Rev. Astron. Astrophys.* 1994, v. 32, p. 153-90.
5. V.T. Maslyuk. The mass (charge) spectrum of superheavy nuclei fission fragments: the new perspectives for the theory of nucleosynthesis // *International Conference on Current Problems in Nuclear Physics and Atomic Energy* (NPAE-Kyiv 2012). Proceedings Part I and Part II.
6. A.S. Botvina, I.N. Mishustin. Statistical approach for supernova matter // *Nuclear Physics A*. 2010, v. 843, issue 1-4, p. 98-132. https://www. sciencedirect.com/science/article/pii/S0375947410005099.
7. P.R. Chowdhury, C. Samanta, D.N. Basu. Modified Bethe-Weizsacker mass formula with isotonic shift and new driplines // *Mod. Phys. Lett*. 2005, A 20, p. 1605-1618. https://doi.org/10.1142/S021773230501666X.
8. Cameron, Alastair Graham. Walter and Richard Michael Elkin. Role of the symmetry energy in atomic mass formulas // *Canadian Journal of Physics.* 1965, v. 43, p. 1288-1311.

9. D. Benzaid, S. Bentridi, A. Kerraci, et al. Bethe-Weizsäcker semiempirical mass formula coefficients 2019 update based on AME2016 // *Nucl. Sci. Tech.* 2020, v. 31, p. 9. https://doi.org/10.1007/s41365-019-0718-8.
10. Michael Bender et al. Future of nuclear fission theory // *J. Phys. G: Nucl. Part. Phys*. 2020, v. 47, p. 113002. DOI: 10.1088/1361-6471/abab4f.
11. P. Möller, A.J. Sierk, T. Ichikawa, H. Sagawa. Nuclear ground-state masses and deformations: FRDM(2012), Atomic Data and Nuclear Data Tables. 2016, v. 109-110, p. 1-204. https://doi.org/10.1016/j.adt.2015.10.002.
12. J.M. Pearson, N. Chamel, A.F. Fantina, S. Goriely. *Symmetry energy: nuclear masses and neutron stars*. https://doi.org/10.48550/arXiv.1309.2783.
13. V.Yu. Denisov. Shell Corrections, Magic Numbers, and Mean Field // *Physics of Atomic Nuclei*. 2007, v. 70, № 2, p. 244-257. DOI: 10.1134/S1063778807020056.
14. F.A. Ivanyuk, C. Ishizuka, M.D. Usang, and S. Chiba. The temperature dependence of the shell corrections // *Phys. Rev. C.* 2018, v. 97, № 6, p. 054331-1-10.
15. W.J. Huang et al. The AME2020 atomic mass evaluation (I). Evaluation of input data, and adjustment procedures // *Chinese Phys. C.* 2021, v. 45, № 3. DOI 10.1088/1674-1137/abddb0.
16. M. Wang et al. The AME 2020 atomic mass evaluation (II). Tables, graphs and references // *Chinese Phys. C.* 2021, v. 45, № 3. DOI 10.1088/1674-1137/abddaf.
17. V.T. Maslyuk, O.O. Parlag, M.I. Romanyuk, O.I. Lendyel, T.J. Marinetc. The features of the fission fragments yields formation of the actinide nuclei on example of uranium isotopes // *EPL (Europhysics Letters).* 2017, v. 119, № 1, p. 12001. https://doi.org/10.1209/0295-5075/119/12001.
18. V. Maslyuk et al. Transformations of actinides fission product yields due to post-scission emission of nuclear particles: ^{232}Th // *Canadian Journal of Physics.* 2021, v. 99, № 1. https://doi.org/10.1139/cjp-2020-0356.
19. V. Denisov and V. Plyuyko. *Problems of nuclear physics and nuclear reactions.* 2013, v. 45, iss. 41. Kyiv University Publishing and Printing Center, Kyiv, Ukraine. 430 p. https://inis.iaea.org/collection/NCLCollectionStore/Public/45/091/45091761.pdf.

Article received 24.07.2023

НУКЛЕОСИНТЕЗ ЯДЕРНОЇ МАТЕРІЇ: ЕНТРОПІЙНІ ЕФЕКТИ

В.Т. Маслюк, Є.О. Скакун, І.Л. Семісалов, М.І. Романюк

Робота пропонує альтернативний шлях утворення хімічних елементів при дезінтеграції ядерної матерії, утвореної під час вибуху зірок. Показано, що окрім енергетичних параметрів, що визначають стійкість ядерної матерії та шляхи її дезінтеграції, необхідно враховувати і ентропійний фактор. Розрахунок вказує на його екстремальну особливість в області переходу від симетричного до структурованого чи асиметричного розпаду, обумовленого «включенням» квантових ефектів від ядерних оболонок.