MASS DEFECT CALCULATION MODEL

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The paper analyzes the theoretical concepts of existing approaches to estimating the nuclear mass defect and creates, based on empirical data and the results of the analysis, mathematical models for calculating the energy of the nucleus and its decay. The result was the creation of a system of five components that reflect the influence of each factor on the value of the internal energy of the nucleus; the identification of the correlation of empirical data with theoretical concepts; the creation of a computer model for finding the energy of all possible simplest reactions of capture and decay of isotopes.

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INTRODUCTION

The object of the study is theoretical models of the nucleus and mathematical dependences of the properties of radioactive isotopes on their nucleon composition. The subject of the study is theoretical concepts and empirical data that underlie the calculation of the mass defect of the nucleus and its decay energies.

The work has significant scientific novelty, because in creating a system of equations for calculating the mass defect, it was possible to achieve minimal errors and at the same time combine the visual characteristics of empirical graphs of the dependence of the mass defect value on the number of protons and neutrons in the nucleus with a theoretical understanding of the components of the nuclear energies. The results of the work can be used for practical purposes: for example, for the selection of radioisotope material and engineering design parameters of radioisotope energy sources, or for predicting new stable isotopes. Also, the methodology for analyzing and comparing empirical and theoretical data developed in the work will allow in the future to improve and refine existing nuclear models.

As a result of the work, the basic nuclear properties of isotopes were studied, and the need to develop a methodology for their assessment was shown. An analysis of theoretical models of the nucleus and existing theoretical methods for assessing the mass defect of the nucleus was carried out. Based on the analysis of graphs of empirical data, an own methodology for assessing the value of the mass defect of isotopes was created, which is calculated by five components: the minimum mass defect of the element, the number of neutrons of the isotope with the minimum mass defect of the element, the parabolic coefficient, the linear coefficient, the parity coefficient. Based on the derived equations, a computational computer system was created that, when entering the number of protons and neutrons, calculates the mass defect of the nucleus and the energy of all possible simplest decay and capture reactions.

1. THEORETICAL ASPECTS

In order to understand and describe the processes occurring in nuclei, various models of the nucleus are used.

Within the framework of the droplet model of the nucleus, the first equation for finding the mass defect was created – the Weizsäcker equation, which we will consider later. This model considers the nucleus as a spherical equally charged incompressible drop. According to this model, phenomena similar to the behavior of a liquid drop are present in the nuclear system: nuclei have surface tension, combine and divide like drops [1, 2].

Also important in our work is the shell model. It considers the nucleus from the point of view of the presence of shells, which are energy levels on which nucleons are located [3, 4]. This model, unlike the droplet model, also explains the deviation of the general dependences on magic numbers, helps to take into account the correction for the pairing energy, because it includes the Pauli principle, and explains the changes in the form of the dependence that occur at certain amount of the number of nucleons.

To describe the dependence of the mass defect value on the nucleon composition of the nucleus within the framework of the droplet model, there is a Weizsäcker formula, which is semi-empirical. That is, each term of the formula was proposed theoretically, based on the droplet model of the nucleus, although later the equation was supplemented to take into account the influence of the phenomena considered by the shell model. The Weizsäcker formula has the following coefficients:

– volume coefficient, which takes into account the energy of the strong interaction between nucleons;

– surface coefficient, which takes into account the energy of surface tension;

– electrostatic coefficient, which takes into account the electrostatic repulsion between protons;

– asymmetry coefficient, which takes into account the influence of the fact that, according to the Pauli exclusion principle, identical nucleons cannot be at the same energy level. That is why the greater the difference between the number of protons and neutrons, the greater the energy compared to that which could be with such a number of nucleons;

– parity coefficient, which takes into account the fact that, according to the Pauli principle, a system with an even number of protons and neutrons has a higher energy.

So, summing up, we can note that according to the Weizsäcker equation model, the internal energy of the nucleus can be decomposed into the following components: bulk, surface, Coulomb, asymmetry energy, pairing energy.

It should be noted that there are modified models of the Weizsäcker equation that have a smaller error and have been supplemented with other refined theoretical concepts. But they are often too complex for quick practical calculation.

To create a mathematical model, previously collected data was selected, which included the main characteristics of isotopes: the number of protons, the number of neutrons, the mass of the nucleus, the mass defect of the nucleus of a given nuclide. When building the tables, we relied on data from the "Nuclear Wallet Cards" database, certified by the International Atomic Energy Agency.

2. MASS DEFECT PREDICTION MODEL

2.1. DEPENDENCE OF MASS DEFECT ON THE NUMBER OF NEUTRONS

At the beginning of the work, based on literature data [5], it was determined that the mass defect dependence has the form of parabolic curves. Therefore, the logical step was to estimate the parameters of these parabolas and find a certain regularity in them. In particular, let's start by constructing graphs of the mass defect dependence on the number of neutrons. We construct graphs for each element, plotting the mass defect value on the vertical axis, and the neutron value on the horizontal axis. As a result of visual analysis of the graphs and the fact that to find the value of the function at each point of the parabola, it is necessary to know only such data about the graph as the curvature coefficient and the coordinates of the vertex, it was determined that the function of the mass defect dependence on the number of protons and neutrons in the nucleus consists of the following coefficients:

– the coordinate of the vertex of the parabola on the vertical axis, i.e. the minimum mass defect among the isotopes of the element;

– the coordinate of the vertex of the parabola on the horizontal axis, i.e. the number of neutrons of the isotope with the minimum mass defect;

– parabolic coefficient: left and right branches of parabolic dependences that intersect at the point corresponding to the isotope with the smallest mass defect. In its form, the function describing the parabola resembles the asymmetry coefficient of the Weizsäcker formula, and the visual characteristic of the graph also clearly demonstrates the asymmetry coefficient, since the left branch of the parabola illustrates the dependence of energy on the degree of excess of protons, and the right branch – neutrons;

– linear coefficient: a system of piecewise-linear functions that corresponds to the influence of the shell model. Analysis of graphs illustrating the dependence for different elements showed that at some number of neutrons, sharp breaks in the curvilinear graph occur, so this – phenomenon is convenient to describe as the sum of the piecewise-linear and parabolic functions. Each such break corresponds to the filling of the shell;

– neutron parity coefficient. This coefficient, like the parity coefficient of the Weizsäcker formula, takes into account the influence of the Pauli principle, and, in particular, the effect of spin coupling, i.e., the lowering of the energy of the system with an equal number of nucleons of the same type with spins up and down, i.e., with an even number of protons and neutrons.

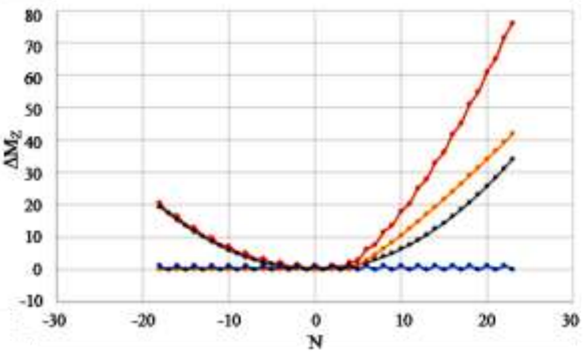

Fig. 1. Dependence of mass defect on number of neutrons for Polonium isotopes, represented by the sum of functions of parabolic coefficient, linear coefficient on parity coefficient. Orange indicates the total graph, yellow – linear coefficient, gray – parabolic, blue – parity coefficient

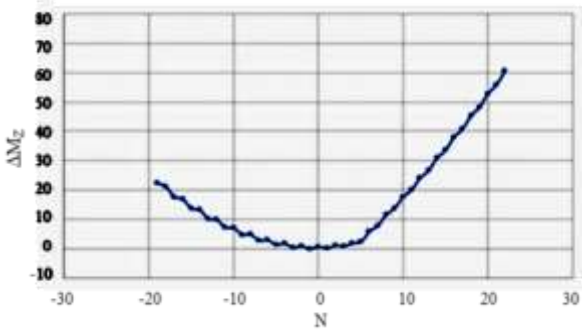

Fig. 2. Empirical graph of the mass defect versus the number of neutrons for Polonium isotopes

2.2. MODEL OF THE DEPENDENCE OF THE MINIMUM MASS DEFECT OF AN ELEMENT ON THE NUMBER OF PROTONS

In this section, we consider the dependence of the coordinate of the vertex of the graph along the axis of the minimum mass defect on the number of protons of the element. Having conducted an empirical analysis of the data from the graphs, we determined that the dependence of the value of the smallest mass defect among all isotopes of each element on the ordinal number of the element has the form of a piecewise linear function, similar to a parabolic one.

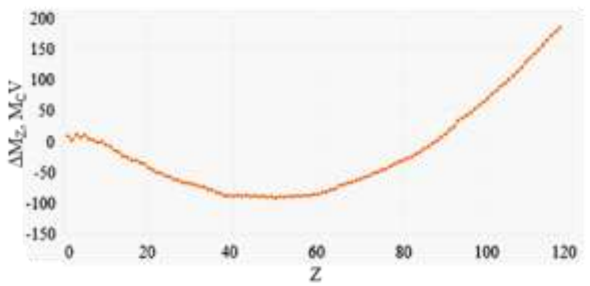

Fig. 3. Empirical dependence of the smallest mass defect among isotopes of an element on the element's ordinal number

Based on the constructed graphs, we determined the following empirical equation:

$$\Delta M_z = 12{,}96 - 3.41 \cdot |Z - 3.5| + k_i \cdot (Z, Z_i)^{1,2} + 1.02 \cdot P(Z), \quad (1)$$

where $P(Z) = Mod(Z, 2)$ – parity function, (2)

$$H_i(Z, Z_i) = \frac{|Z - Z_i| + (Z - Z_i)}{2}, \quad (3)$$

Z_i – the initial value of each line segment of the function; k_i – the slope of each linear segment of the function.

Calculated values of Z_i and k_i are presented in the table below.

Table 1

Z_i	23	38	57	82	106
k_i	0.75	0.86	1.03	1.03	0.43

2.3. DEPENDENCE OF THE NUMBER OF NEUTRONS VS PROTONS OF AN ISOTOPE WITH A MINIMUM MASS DEFECT VALUE

At this stage, we need to determine the dependence of the number of neutrons of the isotope with the lowest mass defect value on the ordinal element, that is, determine the lowest energy isotopes of each element.

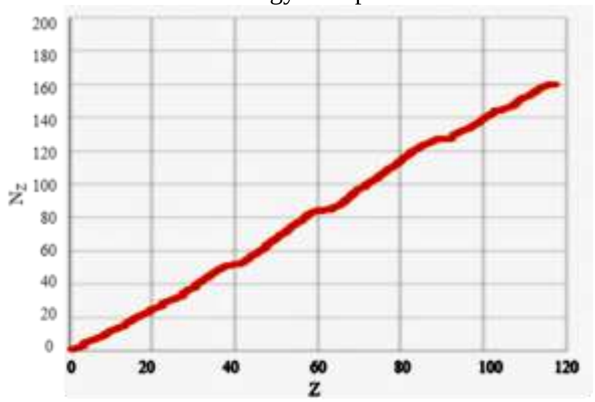

Fig. 4. Dependence of the number of neutrons of an isotope with the minimum mass defect value on the number of protons

Fig. 4 shows an example for an isotope. It can be seen that this dependence is very close to linear. Mathematical modeling allowed us to develop the following formulas for a more accurate description of this graph:

$$N_z = 1 + n_i \cdot T(Z, Z_{a_i}, Z_{a_i+1}), \quad (4)$$

$$T(Z, Z_{a_i}, Z_{a_i+1}) = H(Z - Z_{a_i} 0) + H(Z - Z_{a_i+1}, Z - Z_{a_i}). \quad (5)$$

The n_i coefficient values are given in the Table 2.

Table 2

Z_{a_i}	1	25	39	42	61	64	85	90	92	118
n_i	1.25	1.75	0	1.75	0	1.75	1	0	1.3	0

2.4. THE PARABOLIC COEFFICIENT

The graphs of the dependence of the mass defect on the number of neutrons on the range of all elements consist of two parabolic branches that diverge from the reference point to the left and right, that is, in the direction of increasing the shortage and excess of neutrons in the nuclei, respectively, as well as piecewise linear functions that appear for some ranges of elements. The parabolic component is represented by the formula:

$$G(Z, N, N_Z) = \left(K_l \cdot H_i(-N, -N_Z)\right)^2 + \left(K_r \cdot H_i(N, N_Z)\right)^2. \quad (6)$$

In this equation, the coefficients K_l and K_r depend on the number of protons and are the curvature coefficients of the parabola for the left and right branches, respectively. Due to the function H, the coefficient K_l appears only when the number of neutrons is less than the vertex coordinate, that is, only when there is a shortage of neutrons, and the coefficient K_r, on the contrary, appears only when there is an excess of neutrons.

$$K_l = \frac{1.738}{1 + 0.105Z} + 0.065, \quad (7)$$

$$K_r = \frac{0.072}{1 + 0.107Z} + 0.179. \quad (8)$$

2.5. PIECEWISE LINEAR COEFFICIENT AND PARITY FUNCTION FOR NEUTRONS

In addition to the main parabolic coefficient, the function of the mass defect dependence on the number of neutrons is influenced by the piecewise-linear coefficient. It consists in the manifestation of a linear slope of the parabolic dependence at some neutron ranges.

$$L(Z, N) = \left[k_i \cdot F\left(Z, Z_{c_i}, Z_{d_i}, Z_{f_i}, Z_{g_i}\right) \cdot H\left(N, N_{k_i}\right)\right]^2, \quad (9)$$

where $F\left(Z, Z_{c_i}, Z_{d_i}, Z_{f_i}, Z_{g_i}\right) =$

$$\frac{H\left(Z, Z_{c_i}\right) - H\left(-Z, -\frac{Z_{d_i}\left(Z_{c_i} + Z_{d_i} + Z_{f_i} + Z_{g_i} - Z\right)}{Z_{g_i}}\right)}{Z_{d_i}^{\ 2}}.$$

The calculated coefficients are presented in the Table 3 (left branch) and Table 4 (right branch).

Table 3

Coefficients for calculations at the left branch

N_{Li}	k_{li}	Z_s	Z_l	Z_d	Z_r
125	0.3	87.4	4.0	6.0	4.0
105	0.0	62.0	4.1	6.0	6.0
82	0.8	59.5	4.6	10.0	6.0
50	1.3	36.0	6.0	8.0	6.0
28	3.8	18.6	18.1	10.0	6.0
18	0.9	16.4	1.5	0.7	1.9
14	1.4	10.1	2.6	10.0	6.0
8	1.8	5.6	2.0	10.0	6.0
4	0.5	0.0	2.0	6.0	6.0
0.0	0.0	-1.0	1.0	1.0	3.0

Table 4

Coefficients for calculations at the right branch

N_{Li}	k_{li}	Z_s	Z_l	Z_d	Z_r
125	1.2	74.9	5.1	3.7	9.4
105	0.8	57.4	4.0	6.4	11.8
82	1.0	41.8	6.0	10.0	7.1
50	1.0	24.6	5.1	7.2	4.7
28	0.6	15.0	5.1	2.7	4.9
18	0.7	9.6	3.0	3.1	2.3
14	1.0	6.9	1.4	2.1	2.9
8	1.6	3.3	3.0	0.0	2.4
4	2.3	1.9	2.3	0.0	1.5
0	2.5	0.0	0.8	0.8	2.1

The parity function of the number of neutrons is analogous to the parity function of the number of protons.

$$P(N) = Mod(N, 2). \qquad (10)$$

3. RESULT ANALYSES

The final formula for calculation of the mass defect could be represented as follows:

$$\Delta M(N.Z) = \Delta M_z(Z) + G\big(Z, N, N_Z(Z)\big) + \\ +L(Z, N) + P(N). \qquad (11)$$

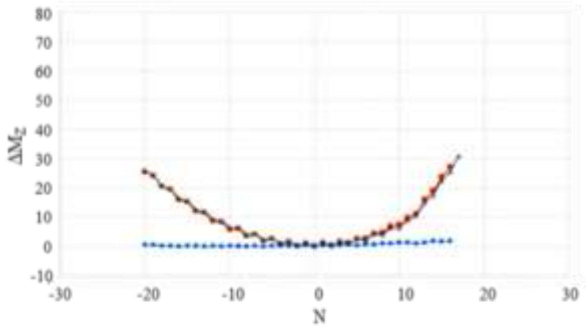

Fig. 5. Dependence of mass defect on the number of neutrons for mercury isotopes

At the Fig. 5 the gray line shows the empirical data, the orange line shows calculated data, and the level of the errors is shown in blue.

As shown at the Fig. 5, the error of calculations according to this system is 1.1 MeV for all elements. The error for elements with $54 < Z < 86$ is 0.6 MeV. The estimate of the error in this range is very important, because it is this region that gives the greatest error when calculating according to the Weizsäcker equation [5], because it consists of non-spherical nuclei that do not obey the droplet model well. Also, isotopes of these elements are widely used in obtaining energy from natural decay reactions.

CONCLUSIONS

As a result of the work, the basic nuclear properties of isotopes were studied and the need to develop a methodology for their evaluation was shown.

An analysis of theoretical models of the nucleus and existing theoretical methods for estimating the mass defect of the nucleus was carried out.

Based on the analysis of graphs of empirical data, an own methodology for estimating the mass defect value of isotopes was created, which is calculated using five components: the minimum mass defect of the element, the number of neutrons of the isotope with the minimum mass defect of the element, the parabolic coefficient, the linear coefficient, and the parity coefficient.

Based on the derived equations, a computational computer system was created that, when entering the number of protons and neutrons, calculates the mass defect of the nucleus and the energy of all possible simplest decay and capture reactions, as well as evaluates possible reactions and predicts stable isotopes.

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