EMPIRICAL ANALYSIS OF THE FORMULA FOR THE BINDING ENERGY OF NUCLEI

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UDC 539.1.01

An accurate knowledge of the properties of the nuclear energy surface is important not only for practical reasons (to calculate nuclear masses, and to predict the properties of superheavy elements and nuclei far from the β-stability line), but also to check and refine nuclear models. The well-known semiempirical formula for the binding energy due to Bethe and Weizsacker [1] has been subjected to a number of refinements and modifications in order to obtain better agreement with experiment [2-10]. The correction terms, introduced from theoretical considerations, take into account the specific features of the distribution of nucleons in the nucleus (the diffuseness of the boundary, the nonuniformity of the distribution in the inner region, and the difference between the neutron and proton densities) [2-5], the effects of deformation and compressibility of the nuclei [6-10], Coulomb exchange interaction [3, 6], etc. However, because there is no rigorous theory of the nucleus the role of the various correction terms remain unclear. As far as their empirical basis is concerned, the introduction of correction terms into the equation for the binding energy, despite the addition of new parameters, does not lead to any appreciable improvement in the agreement with experiment. Nevertheless, the introduction of purely empirical corrections to the parity and the effects of the shells considerably improves the agreement with experiment [1, 3, 6, 11].

All this stimulated us to try to clarify the features of the structure of the formula for the binding energy, without previous resource to any model representations, and based exclusively on experimental data.

It is well known that for any fixed mass number A the stability of the isobars falls, while the energy increases the further the nuclei are from the region of stability both on the neutron-excess side and on the proton-excess side. A detailed analysis of the experimental data given in [12-15], shows that within the limits of experimental error the isobar cross sections of the energy surface in the regions between the magic numbers of neutrons and protons are (for nuclei of each of the four types of parity) quadratic parabolas, so that the total energy of a nucleus with mass number A and charge Z can be represented in the form [12-14]

$$E(A, Z) = E^0(A) + \kappa (Z - Z^0(A))^2, \tag{1}$$

where κ is a constant, and Z^0 increases linearly with A in the limits between the magic numbers N and Z. When the magic numbers N (or Z) intersect, κ and Z^0 change abruptly, but such that for the system of nuclei as a whole κ decreases while Z^0 increases as A increases.

Taking this into account, the averaged equation for the binding energy of nuclei, neglecting the effects of the shells, can be written in the form*

$$B(A, Z) = \kappa(A) Z^2 + \varphi(A) Z + X(A). \tag{2}$$

In what follows it will be more convenient to write Eq. (2) in the form of a sum

$$B(A, Z) = \alpha_v(A) \cdot A - \frac{\alpha_c(A)}{A^{1/3}} \cdot Z^2 - \alpha_s(A) \cdot \frac{(A-2Z)^2}{A} + \frac{\alpha_w(A)}{2} |A - 2Z|. \tag{3}$$

* In this case $E(A, Z) = A \cdot E_n - Z \cdot E_{np} - B(A, Z)$, where E_n is the total energy of a neutron, while E_{np} is the difference between the neutron and proton energies.

M. V. Lomonosov Moscow State University. Translated from Izvestiya Vysshikh Uchebnykh Zavedenii, Fizika, No. 12, pp. 122-128, December, 1974.

This form is more convenient because when $\alpha_C(A) = \text{const}$, $\alpha_S(A) = \text{const}$, $\alpha_V(A) = \text{const} + \text{const} \cdot A^{-1/3}$ and $\alpha_W(A) = 0$, Eq. (3) reduces to the usual Bethe—Weizsacker formula. When $\alpha_W(A) \neq 0$ an additional so-called Wigner-term occurs in the formula. Interpreting $[\alpha_C(A)/A^{1/3}] \cdot Z^2$ as the Coulomb energy of the nucleus, we can calculate the relation between α_C and A using experimental data on the charge distribution in the nuclei [16]. For the Hofstadter distribution this gives (see Appendix 1)

$$\alpha_c(A) = 0.673 + 0.00029 \cdot A \text{ MeV}. \tag{4}$$

To find the relations $\alpha_S(A)$, $\alpha_W(A)$ and $\alpha_V(A)$ we will start from the requirement that the mean square deviation of Eq. (3) from the experimental values should be a minimum for a minimum number of parameters introduced. We will take the approximating functions in the fairly general form

$$\alpha(A) = \sum_{\kappa} (a_\kappa + b_\kappa \cdot A)^{c_\kappa}, \tag{5}$$

where a_κ, b_κ, and c_κ are adjusting parameters. These parameters can be chosen in various ways; the best function from among those with a fixed number of parameters is taken to be that which gives the minimum mean-square deviation. Termination occurs for such a number of parameters for which the addition of one more parameter leads only to a small reduction in the mean-square deviation.

To find $\alpha_S(A)$ and $\alpha_W(A)$ it is convenient to use β-decay data. If the isobar cross section of the nuclear energy surface is a quadratic parabola, then, according to Eq. (2), $^1/_4$ of the difference in the β^--decay energies $E^-(A, Z) \equiv E(A, Z) - E(A, Z + 1)$ and $E^-(A, Z + 2) = E(A, Z + 2) - E(A, Z + 3)$ of the isobars (A, Z) and (A, Z + 2) must be equal to the curvature of the parabola

$$\kappa(A) = \frac{1}{4}\{E^-(A, Z) - E^-(A, Z+2)\}. \tag{6}$$

In this case $\kappa(A)$, according to Eqs. (2) and (3), is related to $\alpha_S(A)$ by the equation

$$\kappa(A) = \frac{4\alpha_s(A)}{A} + \frac{\alpha_c(A)}{A^{1/3}}. \tag{7}$$

The position of the minimum of the isobar parabola $Z^0(A)$ is found from the condition $[\partial E(A, Z)/\partial Z]_{Z = Z^0(A)} = 0$, or from the equivalent condition (see [12, 14]) $E^-[A, Z^0(A)] = E^+[A, Z^0(A)]$ [where $E^+(A, Z) = -E^-(A, Z - 1)$ is the energy of the β^+-decay of the nucleus (A, Z) into the nucleus (A, Z − 1)]. Taking into account also the linear dependence on Z of the energies $E^\pm(A, Z)$, that follows from Eq. (2), we can express $Z^0(A)$ in terms of the energy of the β decay of the isobars (A, Z) and (A, Z + 2)

$$Z^0(A) = Z + 2\left\{1 + \frac{E^+(A, Z+2) - E^-(A, Z+2)}{E^-(A, Z) - E^+(A, Z)}\right\}^{-1}. \tag{8}$$

On the other hand, it also follows from Eqs. (2) and (3) that $Z^0(A)$ is related to $\alpha_W(A)$ by the equation

$$Z^0(A) = -\frac{\varphi(A) + E_{np}}{2\kappa(A)} = \frac{2\alpha_s(A) + \alpha_w(A) + \frac{1}{2}E_{np}}{\frac{\alpha_c(A)}{A^{1/3}} + \frac{4\alpha_s(A)}{A}}. \tag{9}$$

Using the experimentally measured β-decay energies of the isobars and using Eqs. (6) and (8) we can determine the "experimental" values of $\kappa(A)$ and $Z^0(A)$. If the isobar curves were accurate parabolas the values of $\kappa(A)$ [and similarly $Z^0(A)$], obtained using various isobars, would be the same for the same A. As seen from Figs. 1 and 2 this is in fact the case everywhere the magic numbers N and Z do not intersect. This confirms the correctness of the choice of the dependence of B on Z in the form of Eqs. (2) and (4).*

Starting from the requirement that the mean-square deviation for $\kappa(A)$ calculated from Eq. (7) should be a minimum for the minimum number of parameters in the expression for $\alpha_S(A)$, we find that the dependence of α_S on A should be linear, and numerically

$$\alpha_s(A) = 13.1635 + 0.04450 \cdot A \text{ MeV}. \tag{10}$$

* Attempts to choose the dependence of B on Z in a form different from Eq. (2) does not improve the agreement with the experimental values of κ and Z^0.

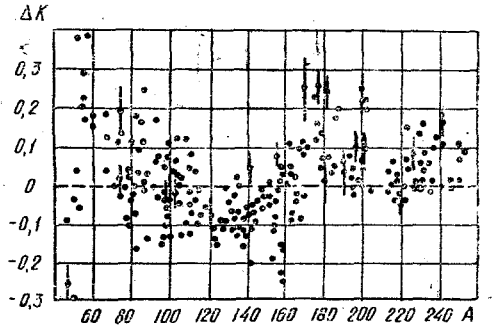

Fig. 1. The difference between the experimental and calculated values of κ.

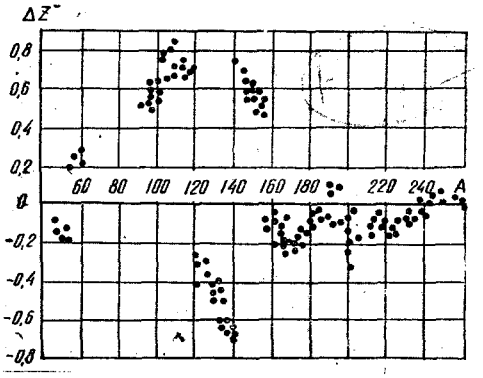

Fig. 2. Difference between the calculated and experimental values of Z^0.

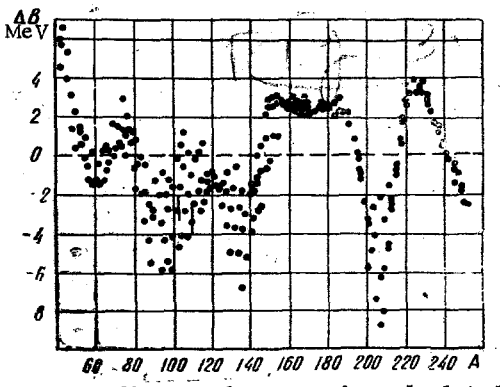

Fig. 3. Difference between the calculated and experimental values of B(A, Z).

In a similar way, from the requirement that the values of $Z^0(A)$ calculated from Eq. (9) should agree with the experimental values, we obtain that

$$\alpha_w(A) = 3{,}500 - 0{,}00924 \cdot A \text{ MeV}. \quad (11)$$

The data on the β-decay energies were taken from tables [18]. The difference between the values of $\kappa(A)$ calculated from Eq. (7) taking Eq. (10) into account, and the experimental values is shown in Fig. 1 as a function of A; in Fig. 2 a similar graph is drawn for the difference between Z^0 calculated from Eq. (9) taking Eq. (11) into account and the experimental values. As is seen from Figs. 1 and 2, the difference between the calculated and experimental values is not systematic and is due to the effect of the shells.

The relation between α_V and A was found from the requirement of minimum mean-square deviation of the binding energy [calculated from Eq. (3) taking Eqs. (4), (10), and (11) into account] from the experimental values of B(A, Z) [18] for the minimum number of parameters in the approximating equation (5). It turned out that $\alpha_V(A)$, unlike $\alpha_C(A)$, $\alpha_S(A)$, and $\alpha_W(A)$, depends on the parity of the nuclei, whereas for even—even (Z-even, N-even) nuclei

$$\alpha_v(A) = 6{,}9750 \cdot A^{0{,}117} \text{ MeV}. \quad (12)$$

If, as assumed, we isolate the correction on the parity, then when changing from even—even to even—odd nuclei we must add to the expression for B(A, Z)

$$\delta_{ee}^{eo}(A) = 11{,}74 \cdot A^{-0{,}494} \text{ MeV}, \quad (13)$$

For odd—even and odd—odd nuclei the corrections will be

$$\delta_{ee}^{oe}(A) = -11{,}02 \cdot A^{-0{,}469} \text{ MeV}. \quad (14)$$

$$\delta_{ee}^{oo}(A) = -32{,}01 \cdot A^{-0{,}566} \text{ MeV}. \quad (15)$$

In this case B(A, Z) for even—even nuclei will be given by

$$B_{ee}(A, Z) = 6{,}9750 \cdot A^{1{,}117} - (13{,}1635 + 0{,}04450 \cdot A) \times \frac{(A-2Z)^2}{A} - (0{,}673 + 0{,}00029 \cdot A) \cdot \frac{Z^2}{A^{1/3}} + (3{,}500 - 0{,}00924 \cdot A)\,|A - 2Z| \text{ MeV}. \quad (16)$$

From the point of view of writing the formula for the binding energy in the form (3) the smoothed formula obtained contains 6 independent parameters for nuclei of each of the types of parity (including the four common parameters), i.e., as many as the Bethe—Weizsacker formula (taking into account in the latter the corrections on the parity and the index 2/3 in the term for the surface energy). However the agreement between the Bethe—Weizsacker formula and experiment is much worse than Eq. (16), which is easily seen

TABLE 1. Comparison of the Different Versions of the Formula for the Binding Energy

	σ_κ	σ_{Z^0}	σ_B (for o-e. nuclei)
Green [2]	0,270	0,459	3,05
Mozer [9]	0,126	0,430	3,08
Cameron [3]	0,204	0,445	2,88
Kodama [10],	0,137	0,448	2,73
Swiatecki [8]	0,163	0,432	2,81
Formula [16]	0,115	0,401	2,89

from Table 1, where we have given: a) the mean-square deviations from the experimental values for the curvature of the isobar parabolas σ_K, b) the mean-square deviations σ_{Z0} for Z^0, and c) the mean-square deviations σ_B for the binding energy B(A, Z). The structure of the Bethe—Weizsacker formula is such that it is impossible simultaneously to ensure the correct form of the β-stability line of $Z^0(A)$, and the correct dependence on A of the curvature coefficient of the isobar cross sections $\kappa(A)$.

The introduction into the Bethe—Weizsacker formula of a surface symmetry term [7] [which corresponds in Eq. (3) to $\alpha_S(A)$ of the form $a_S - b_S A^{-1/3}$] agrees qualitatively with our conclusions [see Eq. (10)] regarding the increased role of the symmetry energy in heavy nuclei, and gives better agreement with the experimental values of $\kappa(A)$. However, the assumption that the whole part of the energy which is linear in Z is contained in the symmetry energy leads either to an increase in $\kappa(A)$ for light and medium nuclei [3], or to a reduction for heavy nuclei [8, 9]. In addition the β-stability line also differs somewhat from the experimental line in the region of heavy nuclei. Hence, the introduction of the Wigner term is necessary in order to give a better description of nuclei far from the β-stability line, and also of superheavy nuclei. The positive role of the Wigner term is discussed in [8]. A characteristic feature of Eq. (16) is the absence of the surface term in explicit form. Qualitatively, the dependence of α_V on A, according to Eq. (12), acts in the same way as the introduction of the surface-energy term, but the quantitative agreement between Eq. (12) and experiment is better (σ_B is less), than when the surface term is introduced. Moreover, in the last case $\alpha_V(A)$ an extraneous parameter is introduced, namely,

$$\alpha_v(A) = a_v - b_v A^x, \tag{17}$$

where $x = -1/3$, and a_V and b_V are positive constants. Using a variational procedure we will attempt to find the best value of x in Eq. (17). It turns out to be -0.45, and consequently, the quasisurface term has the form $\text{const} \cdot A^{0.55}$, and not $\text{const} \cdot A^{2/3}$, as is assumed in the liquid-drop model. This result can be interpreted in the language of the liquid-drop model as a fall in the surface tension as A increases. The need to re-examine the surface term was recently pointed out in [17].

Finally, the procedure of separating the terms which depend only on A is not completely unique, since instead of the Wigner term, one could isolate simply the term proportional to the first power of Z, or disturb the symmetry in the symmetrical energy term by replacing $A - 2Z$ by $A - \alpha'_S(A) \cdot Z$. However, in neither of these versions is the "classical" form of the surface term a better approximation. The assumed formula for the binding energy of nuclei gives better agreement with experiment for the least number of parameters (see the table) compared with other formulas, for nuclei far from the β-stability line, and for heavy nuclei. A further improvement can be obtained by introducing local shell corrections.

APPENDIX 1

Calculation of the Coulomb Energy

The usual expression for the Coulomb energy of a charge distributed with density $Ze\rho(\mathbf{r})$ ($\int \rho(\mathbf{r}) d^3r = 1$)

$$E_c = \frac{(Ze)^2}{2} \cdot \int \frac{\rho(r_1)\,\rho(r_2)}{|r_1 - r_2|}\, d^3r_1 \cdot d^3r_2 \tag{1.1}$$

in the case when the charge distribution is spherically symmetric, can be written as

$$E_c = \frac{(4\pi Ze)^2}{2} \int_0^\infty \rho(r_1)\, r_1\, dr_1 \left\{ \int_0^\infty \rho(r_2)\, r_2^2\, dr_2 - \int_{r_1}^\infty \rho(r_2)\, r_2 (r_2 - r_1)\, dr_2 \right\}.$$

This expression can be integrated by parts to give

$$E_c = \frac{(Ze)^2}{2} \cdot \int_0^\infty dr \left(4\pi \int_r^\infty \rho(r_1)\, r_1\, dr_1\right)^2 = (Ze)^2 (4\pi)^2 \int_0^\infty \rho(r)\, r^2\, dr \int_r^\infty \rho(r_1)\, r_1\, dr_1 = (Ze)^2 (4\pi)^2 \int_0^\infty \rho(r)\, r\, dr \int_0^r \rho(r_1)\, r_1^2\, dr_1. \tag{1.2}$$

The integrals in Eq. (1.2) can easily be evaluated numerically. Thus, for the Hofstadter density $\rho(r) = \rho_0 \cdot [1+\exp(r-c/a)]^{-1}$, where $c = 1.08 \cdot A^{1/3}$ F, and $a = 0.53$ F [16], E_C becomes

$$E_c = \alpha_c(A) \cdot \frac{Z^2}{A^{1/3}}, \tag{1.3}$$

where

$$\alpha_c(A) = 0{,}673 + 0{,}00029 \cdot A. \tag{1.4}$$

To evaluate E_C approximately it is convenient to express E_C in terms of the formfactor of the charge distribution $\rho(r)$. Representing $|r_1 - r_2|^{-1}$ in Eq. (1.1) in the form of the integral $1/2\pi^2 \cdot \int d^3\varkappa/\varkappa^2 \cdot e^{i\varkappa(r_1-r_2)}$ and expanding $e^{i\varkappa r_1}$ in series, and integrating, we obtain

$$E_c = \frac{(Ze)^2}{4\pi^2} \cdot \int \frac{d^3\varkappa}{\varkappa^2} \int \rho(r_2)\, e^{-i\varkappa r_2}\, d^3 r_2 \left\{1 + \sum_{n=1}^{\infty} \frac{(-1)^n \cdot \varkappa^{2n} \langle r^{2n}\rangle}{(2n+1)!}\right\}.$$

Hence, assuming that $\int \frac{d^3\varkappa}{\varkappa^2} \cdot e^{-i\varkappa r_2} \cdot \varkappa^{2n} = \frac{2\pi^2}{r_2}$ when $n = 0$, and $(-1)^{n+1} \cdot 8\pi^3 \cdot \nabla^{2(n-1)} \delta(r_2)$ when $n > 0$, we obtain

$$E_c = \frac{(Ze)^2}{2} \left\{\left\langle \frac{1}{r} \right\rangle - \sum_{n=1}^{\infty} \frac{\langle r^{2n}\rangle}{(2n+1)!} \cdot 4\pi \left| \nabla^{2(n-1)} \rho(r) \right|_{r=0}\right\}, \tag{1.5}$$

where

$$\langle r^{2n}\rangle = \int \rho(r)\, r^{2n}\, d^3 r. \tag{1.6}$$

Hence, in particular, for the Hofstadter distribution we have with a high degree of accuracy

$$E_c = \frac{(Ze)^2}{2} \left\{\left\langle \frac{1}{r} \right\rangle - \frac{4\pi\rho(0)\langle r^2\rangle}{6}\right\}. \tag{1.7}$$

Numerical calculation using Eq. (1.7) leads to results that are practically identical with those obtained using the accurate formula (1.2).

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