PHYSICS OF ELEMENTARY PARTICLES
AND ATOMIC NUCLEI. THEORY

On Relation between Bulk, Surface and Curvature Parts of Nuclear Binding Energy within the Model of Hexagonal Clusters

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Abstract — Using the model of hexagonal clusters we express the surface, curvature and Gauss curvature coefficients of the nuclear binding energy in terms of its bulk coefficient. Using the derived values of these coefficients and a single fitting parameter we are able to reasonably well describe the experimental binding energies of symmetric nuclei with more than 100 nucleons. To improve the description of lighter nuclei we introduce the same correction for all the coefficients. In this way we determine the apparent values of the surface, curvature and Gauss curvature coefficients which may be used for infinite nuclear matter equation of state. This simple model allows us to fix the temperature dependence of all these coefficients, if the temperature dependence for the bulk term is known. The found estimates for critical temperature are well consistent both with experimental and with theoretical findings.

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1. INTRODUCTION

For several decades the statistical multifragmentation model (SMM) [1] was a good guide for theoretical and experimental studies of the nuclear liquid-gas phase transition. However, at present some of its major assumptions do not look well justified and have to be reexamined in view of new theoretical developments. Among them we would like to mention that inclusion of the Fisher exponent $\tau$ [2] into a simplified version of SMM [3] led to an understanding of a possible complicated structure of the nuclear liquid-gas phase transition on the basis of exact analytical solution [4, 5] of such a simplified model. Examination of the critical exponents of a simplified SMM made in [5] led to a conclusion that, in contrast to the Fisher droplet model [2], the nuclear liquid-gas phase transition may have not a critical endpoint, but the tricritical endpoint, if the value of exponent $\tau$ is between 1 and 2, while for $\tau \geq 2$ the critical endpoint maybe absent at all [4, 5].

The concept of surface tension induced by the interaction of nuclear fragment with the thermal medium suggested in [6] and developed further in [7, 8] allowed us to introduce into the SMM the equation of state of compressible nuclear liquid and to successfully account for the effects of the surrounding medium on the surface tension of nuclear fragments of arbitrary size in a way which obeys the L. van Hove axioms of statistical mechanics [9, 10]. In addition, this concept again brings up two questions of principal importance for theoretical modeling of nuclear liquid-gas phase transition: (i) why the curvature contribution of the binding energy of large nuclei is absent in the SMM?; and (ii) what is the temperature dependence of the proper surface and curvature parts of the nuclear binding energy to which the contributions generated by the interaction of nuclear fragment with the surrounding thermal medium should be added to?

There is an extended literature in which these main questions are discussed on the basis of different approaches and, hence, we have to apologize that here we quote only a few works directly related to our discussion. It will mainly concern the relation between the bulk $-a_v A$, surface $a_s A^{\frac{2}{3}}$ and curvature $a_c A^{\frac{1}{3}}$ terms of the binding energy of symmetric nuclei consisting of $A \geq 10$ nucleons. The empirical Bethe-Weizsäcker formula [11] successfully describes the binding of large nuclei and the major part of this energy is determined by the bulk and surface terms which are, respectively, proportional to the coefficients $a_v$ and $a_s$, while the curvature coefficient $a_c$ in this formula is set to zero. Over last five decades this formula was essentially improved [12–18] to account for various properties of more than 2700 known nuclei. In some references even two curvature terms, namely the usual one $a_c A^{\frac{1}{3}}$
and the Gauss one $a_G A^0$, are discussed [14, 15]. In fact, already in 1953 on the basis of the Fermi gas model Hill and Wheeler concluded that a curvature dependent term $a_C A^3$ should exist in the liquid-drop model of nuclei [19], but until now there is no consensus on its presence in the modified Bethe-Weizsäcker formula. Moreover, the existing versions of SMM completely ignore it and in part this can be explained by the hope that the curvature term may play a minor role in nuclear multifragmentation studies. However, in the realistic extensions of Fisher droplet model [20, 21] which are used to describe the liquid-gas phase transition the curvature term is present. Therefore, the curvature term should be present in the SMM of nuclei, but in this case the temperature dependence of surface and curvature terms should be derived simultaneously in order to have a thermodynamically consistent treatment. Unfortunately, within the mean-field approximation such a task is rather complicated even for the surface tension [14, 23], but for the statistical model like the SMM the results of mean-field approach cannot be used, since they break down the L. van Hove axioms of statistical mechanics [9, 10] and, hence, will destroy the main attractive feature of SMM, i.e. the statistical character of phase transition. Therefore, to resolve the two main questions formulated above we need a sufficiently simple model which, nevertheless, will not lead to the conflict with the L. van Hove axioms of statistical mechanics.

A recent paper [17] is devoted to an interesting discussion of the relation between the bulk and surface terms in the Bethe-Weizsäcker formula. For this purpose the authors of [17] considered a toy model of atomic nucleus which have a cubic shape and in which the nucleons are also cubic. Accounting for the interaction of nearest neighbors one ends up with the relation $a_T = a_S$ within the cubic model. At first glance this result cannot be robust due to strongly oversimplified treatment of the real physical nuclei within the model of cubic nuclei. However, even this primitive picture allows one to conclude about existence of a strong correlation between the values of $a_T$ and $a_S$ coefficients in the Bethe–Weizsäcker formula.

Hence, a partial success of the cubic nucleus model analyzed in [17] motivates us to formulate more elaborate model of hexagonal cluster [24]. Using an exact mathematical representation for the number of spherical particles in each filled layer we will express the coefficients $a_S$, $a_C$ and $a_T$ in terms of a single parameter $a_T$. Since our major interest is related to the equation of state of symmetric nuclear matter, then the derived parameterization of the bulk, surface and curvature terms is not applied to the description of the experimental data, but it is compared with two most successful fits of the experimental binding energies of nuclei of $A \geq 50$ nucleons and with other theoretical predictions for the coefficient $a_C$. To apply the derived model to the description of light nuclei with $A \geq 10$ nucleons, we will study the corrections of each coefficient in the spirit of leptodermous expansion. In this way we will determine the apparent values of the coefficients $a_T$, $a_S$, $a_C$ and $a_T$ which should be used in the modified SMM. Using the fact that the same relation between the coefficients $a_T$, $a_S$, $a_C$ and $a_T$ is valid for finite temperatures, we will obtain the temperature dependence of these coefficients for a single large nucleus in a vacuum and estimate the critical temperature of such nucleus above which it becomes absolutely unstable.

The work is organized as follows. In Section 2 we establish the hexagonal cluster model of nuclei and express the coefficients $a_T$, $a_S$ and $a_C$ in terms of the bulk coefficient $a_T$. Section 3 is devoted to a discussion of theoretical predictions for the curvature coefficient $a_C$. The same correction is introduced for all these coefficients and their apparent values are found. Also in this Section we establish the temperature dependence of the coefficients $a_T$, $a_S$, $a_C$ and $a_T$ using the SMM parameterization of the bulk coefficient temperature dependence. Our conclusions are formulated in Section 4.

2. SURFACE AND CURVATURE ENERGY OF HEXAGONAL CLUSTERS

As was mentioned above, a simple model developed in the paper [17] is rather unphysical. The main reason of this is that neither real nuclei nor nucleons are cubic. In order to study the relation between bulk, surface and curvature terms in the leptodermous expansion of the Bethe-Weizsäcker formula a more realistic model is required. Here we develop the geometrical model which assumes that the nuclei are the hexagonal structures of spherical nucleons. The main object of our analysis will be the main binding energy of nucleus consisting of $A$ nucleons

$$E_b(A,(a_K)) = -a_T A + a_S A^1 + a_C A^3,$$

which describes the bulk $a_T$, surface $a_S$ and curvature $a_C$ terms in the Bethe–Weizsäcker formula [11]. In particular, in our analysis we will use the two sets of [17]

\begin{align*}
\text{set I} & : E^I_b(A) = E_b(A, a_T = 15.6 \text{MeV}; a_S = 17.32 \text{MeV}; a_C = 0 \text{MeV}), \\ \text{set IV} & : E^{IV}_b(A) = E_b(A, a_T = 15.26 \text{MeV}; a_S = 15.26 \text{MeV}; a_C = 3.6 \text{MeV}),
\end{align*}

which provide an excellent fit of the experimental binding energies of nuclei for $A \in [20; 250]$. Since these sets are in a good agreement with the other fits of experimental nuclear binding energies (see, for
instance, [15] for a comprehensive review and the references therein), in what follows we will accept these sets as the two typical representatives which equally well reproduce the experimental data for the nuclei with \( A \in [50; 250] \) nucleons. Visually these two curves for \( E_\text{b}\) can be hardly distinguished from each other and, hence, we consider them equivalent to each other for the nuclei with \( A \in [50; 250] \) nucleons.

Similarly to ordinary liquids [22] one may think of the hexagonal clusters consisting of the cells in which a single particle (nucleon) is moving. The cells are formed dynamically by the other nucleons. The advantages of this model compared to cubic one are as follows. First of all, the shape of the cells is nearly spherical. At the same time the large nuclei have a shape which is approximately spherical (not cubic!), and this is in agreement with the common wisdom of modern nuclear physics. In addition the hexagonal structure of nuclei in the present model leads to their dense packing which is also in conformity with the contemporary state of knowledge. Hence, a hexagonal nucleus can be considered as a central nucleon cell covered by several layers of the other cells in which a single nucleon is moving (see Fig. 1).

In what follows we use an approximation of the nearest neighbors interaction. Namely, an interaction of each pair of nucleons contributes the energy \( \varepsilon < 0 \) to the binding energy of nucleus. The mathematical basis of our treatment is the formula which relates the number of covering layer \( k \) \( (k = 1 \) for first layer, \( k = 2 \) for second layer and so on) to the number of nucleons in it \( 10k^2 + 2 \) [24]. For example, the number of nucleons in the first layer is 12. In what follows we consider a large nuclei with \( n \gg 1 \) covering layers. Moreover, similarly to [17, 18] we neglect the effects related to the shell structure of clusters and consider \( n(A) \) as a continuous function of number of nucleons \( A \). The total number of nucleons (mass number) in such a nucleus is

\[
A = 1 + \sum_{k=1}^{n} (10k^2 + 2) = \frac{10n^3}{3} + \frac{10n^2}{2} + \frac{22n}{6} + 1. \tag{4}
\]

For \( A \gg 1 \) the third and fourth terms in Eq. (4) are negligibly small comparing to the first and the second ones. Hence we can write

\[
A \approx \frac{10n^3}{3} \left[ 1 + \frac{3}{2n2} \right]. \tag{5}
\]

From Eq. (5) it is convenient to express the number of outer (surface) layer \( n \) as

\[
n(A) \approx \left[ \frac{3A}{10} \right]^{\frac{2}{3}} \left[ 1 + \frac{3}{2n} \right]^{\frac{2}{3}} = \frac{3A^{\frac{2}{3}}}{10} \left[ 1 - \frac{1}{2n2} \right].
\]

\[
n(A) \approx \left[ \frac{3A^{\frac{2}{3}}}{10} \right]^{\frac{2}{3}} \frac{1 - \frac{1}{2} \left[ \frac{3A^{\frac{2}{3}}}{10} \right]}{2} = \frac{3A^{\frac{2}{3}}}{10} - \frac{1}{2}.
\]

where on the second step of derivation an approximation for the third power root was applied and the leading order approximation \( n = (3A/10)^{\frac{2}{3}} \) was used on the third step. A more refined expression for \( n(A) \) of Eq. (4) less than \( 10^{-3} \) for any \( A \) larger than 2.5.

Using Eq. (6) we are able to calculate the binding energy \( E_\text{b}(A) = -a_\nu A + a_s A^{\frac{2}{3}} + a_c A^{\frac{1}{3}} \) of the nucleus under consideration. Each nucleon not located on the surface has 12 nearest neighbors. At the same time each nucleon located on the surface (\( n \)-th layer) of the nucleus has three vacant positions which are not filled by nucleons. Therefore, from the bulk energy of the system

\[
-a_\nu A = 12\varepsilon A, \tag{7}
\]

one has to subtract the surface energy of three absent nearest neighbors. The latter nucleons belong to \( (n + 1) \)-th covering layer and, hence, their number is \( 10(n + 1)^2 + 2 \). Thus, one gets

\[
a_s A^{\frac{2}{3}} + a_c A^{\frac{1}{3}} = -3\varepsilon \left[ 10(n(A) + 1)^2 + 2 \right] = -3\varepsilon \left[ 10 \left( \frac{3A^{\frac{2}{3}}}{10} + \frac{1}{2} \right) + 2 \right]. \tag{8}
\]

\[
= -3\varepsilon \left[ 10 \left( \frac{3A^{\frac{2}{3}}}{10} + \frac{9}{2} \right) \right].
\]

\[
= -3\varepsilon \left[ \left( \frac{3A^{\frac{2}{3}}}{10} + \frac{9}{2} \right). \right.
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order approximation we can find that the surface term is quadratic. Finally, using the leading appears in the present model. It is linear in whereas the curvature term naturally

It is remarkable, that in contrast to the model of cubic nuclei of [17] the curvature term appears in the present model. It is linear in $\frac{1}{A}$ whereas the surface term is quadratic. Finally, using the leading order approximation we can find that

$$a_s A^\frac{1}{3} = -30 e \left( \frac{3A}{10} \right), \quad a_c A^\frac{1}{3} = -30 e \left( \frac{3A}{10} \right),$$

$$E_{B}^{th} = 12 \epsilon A - 30 e \left( \frac{3A}{10} \right) - 30 e \left( \frac{3A}{10} \right).$$

The obtained results demonstrate two advantages of the present model. First, in contrast to the cubic model of [17] one can derive in the same way not only the surface term, but the both curvature terms. Second, in contrast to the models of nuclear forces the present one does not depend on the definition of nuclear radius $R_A \approx r_n A^{\frac{1}{3}}$ and on the value of particle number density of nuclear ground state. In what follows we, however, neglect the correction $-\frac{27}{2} \epsilon = -1.125 a_f$ (the last term in Eq. (8)) which is called the Gauss curvature term [15] in order to present our main results. However, in appropriate places we will comment on how one can account for such a correction.

Using Eqs. (7) and (9) we can find that in the model of nuclei with hexagonal structure

$$a_r = \frac{4}{90^{\frac{1}{3}}} \approx 1.1204,$$

$$a_s = 0.3^{\frac{1}{3}} \approx 0.6694 \approx \frac{1}{1.4939}.$$  

Amazingly, taking the typical value of the binding energy per nucleon for zero temperature $a_r = 16$ MeV used in the statistical multifragmentation model [1], we obtain that the surface free energy coefficient is $a_s = 1.1204 a_r = 17.9248$ MeV, which is just 0.4 percent less than the typical value 18 MeV used in this profound model [1]. Taking the bulk term $a_r = 1.56$ MeV of set I of [17], from Eq. (11) one finds $a_s \approx 17.77$ MeV which differs from the corresponding value $a_s \approx 17.32$ MeV found in [17] by about 0.9 percent.

On the other hand the value of the curvature term found in [17] $a_c = \frac{-2.6}{15.26}$ for the set IV is essentially lower than the result of Eq. (12). From Fig. 2 one can see that the derived curvature term does not provide a good description of the set I binding energy. Moreover, the increased bulk term value $a_r = 16.7$ MeV does not essentially improve the description quality for $A < 50$ as it is seen from Fig. 2. To quantify the mean deviation from the set I per nuclear mass number let us introduce the following integral

$$\Delta_A = \frac{1}{(250 - A)} \int_A^{250} dx \left( E_B^I(x) - E_B^{th}(x) \right),$$

where the binding energy of set I is $E_B^I(A)$ (corresponds to Eq. (2)) and the one of Eq. (10) with the derived coefficients, i.e. $E_B^{th}(A) = a_r (A + 1.1204 A^\frac{2}{3} + 1.1204 \times 1.4934 A^\frac{1}{3})$. From Table 1 (the third row from above) one can see that the binding energy $E_B^{th}(A)$ with the derived coefficients $a_s$ and $a_c$ and a single free coefficient $a_r = 16.7$ MeV provides a reasonable description for large nuclei with $A \geq 100$ only, while it fails completely for $A < 50$. One more possibility is to fix the ratio $a_c / a_s$ (12) and vary independently the bulk and surface terms, i.e. to employ the following parameterization

$$E_B^{th2} = -a_r A + a_s \left[ A^\frac{2}{3} + 1.494 A^\frac{1}{3} \right].$$

For the parameters $a_r \approx 15.8$ MeV and $a_s \approx 14.564$ MeV with the fixed ratio $a_c / a_s = 1.494$ one can essentially improve the original fit quality as it is.
seen from the fourth row from above in Table 1 for $A \geq 25$, while for $A < 25$ it still looks unsatisfactory. Of course, one can just ignore the derived curvature term and get a perfect description of the set I, but then one will face the problem with the Gibbs–Thomson approach to the surface tension of spherical nuclei. In order to understand the source of problem, we have to use the results of refined theoretical analysis of [18].

3. THEORETICAL PREDICTIONS FOR THE CURVATURE TERM

In [18] on the basis of the Gibbs–Thomson approach there was developed a refined theoretical model which accounts for many subtleties of finite nuclei and, as a result, it successfully determines the relation of surface and curvature terms. It employs several parameterizations of Skyrm interaction [25, 26] given in [16]. It also estimates the Tolman length $\xi$ via the surface tension coefficient $\sigma(R_A) = \sigma_0 \left(1 - \frac{2\xi}{R_A}\right)$, (15)

which is negative $\xi = -0.36$ fm and it weakly depends on the Skyrm model parameterization [18]. Equation (15) relates the surface tension $\sigma(R_A)$ of a nucleus of a radius $R_A$ with the one of infinite nucleus $\sigma_0$, which has no electrical charge. In what follows we employ the relation $R_A = R_0 A^{1/3}$ where the average value of the parameter $R_0 = 1.2$ fm is taken from [15].

In order to get the relation to the coefficients $a_S$ and $a_C$ discussed above, we have to find the free energy change from the generalized Laplace pressure $P = \frac{2\sigma(R_A)}{R_A} + \frac{\partial \sigma(R_A)}{\partial R_A}$ (see [18] for details):

$$\Delta F(A) = \int dV P(R) = \int_0^R 4\pi r^2 \sigma_0 \left(1 - \frac{\xi}{r}\right) = 4\pi \sigma_0 \left(R_0^2 - 2\xi R_0\right),$$

(16)

Using the relation $R_A = R_0 A^{1/3}$, from Eq. (16) we find the $a_S$ and $a_C$ coefficients as

$$a_S = 4\pi \frac{\sigma_0 R_0^2}{A^{2/3}} \approx 16.65 \text{ MeV},$$

(17)

$$a_C = -8\pi \frac{\sigma_0 R_0^2}{A^{1/3}} \xi = -8\pi \sigma_0 \xi R_0 \approx 10 \text{ MeV},$$

(18)

where in the last step of evaluation we substituted $\sigma_0 = 0.92$ MeV fm$^{-2}$ found in [18] for SkM Skyrm interaction [25, 26] parameterized according to [16].

This model was chosen for numerical comparison, since it is the main model of [18] and since it provides the surface energy $a_S$ which is close to the one of set IV, but the other Skyrm models considered in [18] give similar results.

From Eqs. (17) and (18) one can find the curvature term as

$$a_C = 0.6 a_S,$$

(19)

which is 40% of the ratio $a_C/a_S$ obtained within the hexagonal model Eq. (12). If one takes the results for SkM interaction found in a comprehensive review [14] (see Table 8 therein), then one gets $a_C/a_S = 12.19/16.6 = 0.734$ for this ratio, which is about 50% of the value derived above in a simple way. We believe that taking into account the fact that the hexagonal model does not contain any information about the complexity of nuclear interaction its findings are remarkable. It is, however, appropriate to stress here that, to our best knowledge, all theoretical estimates of the coefficient $a_C$ are essentially larger than the best fit with the curvature term obtained in [17] for the set IV, i.e. $a_C/a_{SIV} \approx \frac{3.6}{15.26} \approx 0.24$.

In order to demonstrate the depth of this problem let us quantify the deviation between theoretical predictions and the set IV fit of [17] using the Tolman length $\xi$. The latter can be expressed in terms of the
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Fig. 3. Comparison of the binding energy per nucleon of sets I and IV from [17] (solid black curve) with the hexagonal model with ansatz I (short dashed curve) and ansatz II (long dashed curve). For more details see the text.

discussed ratio $\frac{a_c}{a_s}$. Indeed, from Eqs. (17) and (18) we find the Tolman length as:

$$\xi = - \frac{a_c}{2a_s} r_0. \quad (20)$$

The sets I and IV of [17] obtained from the fit of data give us, respectively, $\xi_{set\, I} = 0$ fm and $\xi_{set\, IV} = -0.14$ fm. On the other hand, similarly to essentially larger value $\xi_{set\, T} = -0.36$ fm found in [18], the present model gives us $\xi_{hex} = -0.14$ fm. Although the value $\xi_{set\, IV} = -0.14$ fm is found from the fit of nuclear binding energies, it looks too small to be the true Tolman length of large nuclei. In fact, the latter value means that on the surface of nucleus its density decreases too abruptly (for details, see a discussion and figures in [18]), while the larger theoretical values look more adequate from the physical point of view. Thus, we face a severe theoretical problem: on the one hand, a very successful fit of the data corresponds to an unphysically small value of Tolman length for large nuclei, but on the other hand, the larger values of curvature term $a_c$ found in theoretical models do not allow one to successfully describe the experimental data.

Therefore, the first main question addressed in the present work can be reformulated as follows: is it possible to modify the framework outlined above and the one developed in [18] (and in similar models) in order to achieve an agreement between theoretical models and the analysis of experimental data (set IV) in such a way that the models would simultaneously provide a good description of the data and would at the same time correspond to a physically adequate value of Tolman length?

The physically motivated and sufficiently general way to improve the treatment of light nuclei is to introduce the corrections to the binding energy per pair of interacting nucleons (ansatz I, hereafter) which depend on the powers of $A^{\frac{1}{3}}$

$$\varepsilon(A) = \varepsilon_0 \left[ 1 + \frac{q_1}{A^{\frac{1}{3}}} + \frac{q_2}{A^{\frac{2}{3}}} + \frac{q_3}{A} + \ldots \right], \quad (21)$$

where the parameters $q_1$, $q_2$, and $q_3$ are the constants which should be determined from the best description of the experimental data, whereas the uncorrected binding energy of the nucleon pair is $\varepsilon_0$. Note that the ansatz I is just the leptodermous expansion. It is well known that these corrections naturally appear for finite nuclei from such an expansion [14], but compared to the approach used in [14] the advantage of the ansatz I is that it modifies all coefficients $a_\nu$, $a_s$, $a_c$ and $a_c$ simultaneously, thus, keeping the minimal number of fitting parameters.

Apparently, such an assumption allows us to compensate the most part of curvature term by the proper choice of parameters $q_\nu$. Assuming that $q_{k>3} = 0$ and substituting Eq. (21) into expression for the derived binding energy (10), one can express the coefficients $q_1$ and $q_2$ via the coefficients $q_\nu$:

$$q_1 = 5 \left[ \frac{3}{10} \right] \frac{a_c}{a_\nu} \approx 0.1204,$$

$$q_2 = 5 \left[ \frac{3}{10} \right] \left[ \frac{3}{10} \right] \frac{a_c}{a_\nu} \approx 1.5725. \quad (22)$$

However, it is more instructive to consider the parameters $q_1$ and $q_2$ as the fitting parameters to refine the derived expression for binding energy (10). As one can see from Fig. 3, the parameters $q_1$ and $q_2$ given in the second row of Table 2 provide essentially better description of the set IV. A quantitative analysis shows (see Table 1) that the deviation $\Delta$ calculated for the ansatz I is about one order of magnitude smaller, than without it. Visually, from Fig. 3 one can see that Eq. (21) allows us to perfectly reproduce the set IV for $A \geq 40$, and reasonably well for $A \in [20, 40]$, while for $A \leq 20$ this ansatz fails. Usually, for ordinary nuclei such corrections are playing an auxiliary role, but for studying the nuclear matter properties they are
important. To show this let us estimate the values for the apparent coefficients

\[ a^{app}_S = a_S - a_V q_1 \approx 1.444 a_V = 22.46 \text{ MeV}, \quad (23) \]

\[ a^{app}_C = a_C - a_V q_2 + a_S q_1 \]

\[ \approx -2.758 a_V \approx -42.88 \text{ MeV}, \quad (24) \]

\[ a^{app}_G = a_G - a_V q_3 + a_S q_2 + a_C q_1 \]

\[ \approx 4.021 a_V \approx 62.52 \text{ MeV}, \quad (25) \]

which are obtained after reordering the terms of binding energy, if one accounts for the corrections given in Eq. (22). These numbers are obtained for the coefficients given in the second row of Table 2 assuming \( a_G = 0 \). From this example one can see that the corrections given in Eq. (22) may essentially modify the binding energy of large nuclei. It is an interesting question whether the apparent coefficients (23), (24) and (25) used within the SMM will essentially modify its results or not, since the larger value of \( a^{app}_S \) coefficient maybe compensated by negative value of the \( a^{app}_C \) coefficient.

One can also reproduce the set IV with the same quality, if the Gauss curvature term, \( -\frac{27}{2} a_V \) or the last term in Eq. (8) is taken into account. The corresponding parameters are given in the third row of Table 2.

The reason of why a simple leptodermous-like correction of Eq. (21) fails to reproduce the binding energy for \( A < 20 \) is apparent. At small \( A \) values the correction provided by Eq. (21) is not small and, hence, it dramatically changes the \( A \)-dependence of expression (10). In order to avoid such a problem for the nuclei with masses in the range \( A \in [10;50] \) we employ a less sophisticated form of correction, the ansatz II afterwards,

\[ \varepsilon(A) = \varepsilon_0 \left[ 1 + \frac{q_2}{A^{2/3}} + \frac{q_3}{A^{4/3}} \right], \quad (26) \]

which has two parameters only, but a higher \( A \)-power of the term next to the \( A^{-2/3} \) correction. Its advantage is that by construction such an ansatz does not affect the surface coefficient \( a_S \), but modifies the higher order terms. We also analyzed the two parametric version of Eq. (21) with \( q_1 \approx 0 \), when the parameters \( q_2 \) and \( q_3 \) were used to fit the set I, and found that the ansatz II provides an essentially better description of the sets I and IV. As one can see from Table 1, compared to the ansatz I, this ansatz with one less parameter provides a better description of the set I for \( A \geq 10 \) both without the Gauss curvature term and with it. The values of corresponding parameters are given in Table 2. For the case \( a_G = 0 \) the ansatz II generates the following apparent coefficients for nuclear matter

\[ a^{app}_S = 1.1204 a_V \approx 17.44 \text{ MeV}, \quad (27) \]

\[ a^{app}_C = a_C - q_2 a_V \approx 0.24 a_V \approx 3.82 \text{ MeV}, \quad (28) \]

\[ a^{app}_G = q_2 a^{app}_S \approx 1.602 a_V \approx 25.15 \text{ MeV}. \quad (29) \]

Comparing these coefficients with the ones found for the ansatz I, one can conclude that (i) their values strongly depend on the quality of light nuclei description; (ii) the ansatz II coefficients \( a_V \) and \( a^{app}_S = 1.1204 a_V \) almost coincide with the ones of the set I and with the usual SMM values [1], while the curvature coefficient \( a_G \) almost matches the corresponding coefficient of the set IV; (iii) for the both ansatze the Gauss curvature coefficient is sizably larger than the bulk one. In Fig. 3 we compare the ansatz I obtained from fitting the set I with the sets I and IV. This is done in order to demonstrate that for a high quality fit a tiny difference between the sets I and IV observed at \( A > 50 \) matters.

Including in the treatment the Gaussian curvature term \( -\frac{27}{2} a_V \), we obtain no change for the bulk and surface coefficients, only a slight numerical shift for the coefficient \( q_2 \) and an essential increase of the coefficient

### Table 2. Different sets of parameters used to modify the hexagonal model results in order to better reproduce the sets I and IV. The details can be found in Table 1. The first column refers to the corresponding parameterization. The second, the fourth and the sixth rows do not account for the Gauss curvature term, while the third, the fifth and the seventh ones account for it.

| Ansatz | \( a_V \), MeV | \( q_1 \) | \( q_2 \) | \( q_3 \) |
|--------|----------------|---------|---------|---------|
| I: Eqs. (10), (21) | 15.55 | -0.324 | 4.075 | 0 |
| I: Eq. (10) and Gauss, Eq. (21) | 15.50 | -0.494 | 5.05 | 1.5 |
| II: Eqs. (10), (26) | 15.70 | 0 | 1.43 | 20.5 |
| II: Eq. (10) and Gauss, Eq. (26) | 15.70 | 0 | 1.35 | 31.25 |
| III: Eqs. (10), (30) | 15.35 | 0 | 2.3 | -3.86 |
| III: Eqs. (10) and Gauss, Eq. (30) | 15.26 | 0 | 2.65 | -4.604 |

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q}. Consequently, the coefficient $a_{c\, app}^{app\, II} = 5.07$ MeV is increased only by 25\%, while the coefficient $a_{G\, app}^{app\, II} \approx 41.41$ MeV gained the contribution from the Gaussian term $\frac{27}{24} a_{\varphi}$ of hexagonal cluster model. Thus, ansatz II not only provides the best description of the nuclear binding energy with three parameters only, but, compared to the ansatz I, it also demonstrates a stability of the apparent values of all coefficients. Therefore, we consider the ansatz II as the most successful one.

This ansatz perfectly matches the sets I and IV for $A > 20$, but for $A = 10 - 14$ nucleons the typical deviation from these sets is about 3–6 MeV per nucleon. Therefore now we concentrate on improving the description of light nuclei with the minimal number of parameters. To complete this task and to demonstrate that a better quality of light nuclei (with 10–20 nucleons) description may essentially affect the apparent values of the curvature and Gauss terms, we consider the correction with two parameters, the ansatz III,

$$
\epsilon(A) = \epsilon_0 \left[ 1 + \frac{q_2}{A^\frac{2}{3} + q_3} \right] \rightarrow \epsilon_0 \left[ 1 + \frac{q_2}{A^\frac{2}{3} - \frac{q_3 q_3}{A^\frac{2}{3}} + \ldots} \right], \quad (30)
$$

where in the limit $A \gg 10$ we expanded the denominator to get an asymptotic form of the ansatz III. As one can see from Table 1 this ansatz provides the best description of the set IV for $A \geq 10$ both without the Gauss curvature term and with it although it has a pole at $A < 10$. The values of corresponding parameters are given in Table 2. For the case $a_c = 0$ this gives the apparent values of the nuclear matter coefficients

$$
a_{c\, app\, III} = 1.1204 a_{\varphi} \approx 17.2 \text{ MeV}, \quad (31)
$$

$$
a_{c\, app\, III} = a_c - q_3 a_{\varphi} \approx -0.6274 a_{\varphi} \approx -9.62 \text{ MeV}, \quad (32)
$$

$$
a_{c\, app\, III} = q_3 a_{c\, app\, III} \approx 2.5774 a_{\varphi} \approx 39.56 \text{ MeV}. \quad (33)
$$

Although this ansatz perfectly matches the sets I and IV for $A \geq 10$, one can see that the found value of the apparent curvature coefficient does not reproduce either the set I value $a_c = 0$ or set IV result $a_c = 3.6$ MeV. If the Gaussian curvature term $\frac{27}{24} a_{\varphi}$ is included into the treatment, one finds that the coefficients $a_{c\, app\, III} \approx -14.9$ MeV and $a_{c\, app\, III} \approx 62.93$ MeV are increased in about one and half times, i.e. in contrast to the ansatz II both of these coefficients are modified essentially.

Of course, we analyzed the other forms of corrections and surprisingly found that the ones, which have simple pole provide a better description of the sets I and IV with a smaller number of parameters. In particular, despite an inadequate behavior at $A < 10$ the ansatz III provides the best description of set I with the minimal number of parameters. We believe that for small nuclei with less than 20 nucleons the present model cannot be applied and the point that the derived parameterization of binding energy has to be supplemented by the corrections with the pole is a reflection of the fact that the binding energy of small nuclei should be corrected differently than it is done for the larger ones.

A similar way to improve the coefficient $a_c$ given by Eq. (18) cannot, however, be used, since it is already obtained from the leptodermous expansion of the Skyrm interaction [18]. Our educated guess is that one possible solution of this problem is related to the fact that the radius of nucleus of $A$ nucleons can be modified as

$$
R(A) = r_0 A^\frac{1}{2} \left[ 1 + q_4 A^{-\frac{1}{2}} \right]. \quad (34)
$$

In this case the free energy (16) generated by the Laplace pressure can be written as

$$
F(A) = 4 \pi \sigma_{\varphi} \left[ R^2(A) - 2 \xi R(A) \right] \approx 4 \pi \sigma_{\varphi} \left[ r_0^2 A^2 + 2 (r_0 q_4 - \xi) r_0 A^{\frac{1}{2}} + \ldots \right], \quad (35)
$$

where on the right hand side we neglected the terms proportional to $A^0$. Apparently, such an assumption allows one to reduce the coefficient $a_c$ to its value found in [17] without modifying the true Tolman length, if one chooses $q_4 = \frac{\xi}{\frac{2 \pi \sigma_{\varphi}}{r_0^2}} \approx -0.183$.

The suggested approach allows us to easily elucidate the temperature dependence of the coefficients $a_S$, $a_c$ and $a_{c\varphi}$, if the corresponding dependence of the bulk term $a_v(T)$ is known. Taking the usual SMM parameterization of the bulk term as $a_v(T) = \frac{a_v(0)}{\xi_f} + \frac{T^2}{\xi_f^2}$ (where $\xi_f \approx 16$ MeV [1]) which accounts for the Fermi motion of nucleons at non-vanishing temperature $T$, one can find

$$
a_{\varphi}(T) = a_{\varphi}(T) \frac{a_{\varphi}(0)}{a_v(0)}, \quad \text{with } B \in \{S, C, G\}, \quad (36)
$$

since by construction all these coefficients can be expressed in terms of temperature dependent binding energy per pair of nucleons $\epsilon = -a_{\varphi}(T)$ at the temperature

$$
T_c = \left[ \frac{a_{\varphi}(0) \xi_f}{12} \right]^{\frac{1}{2}} \in [15.6; 16.4] \text{ MeV}, \quad (37)
$$

the surface tension coefficient $a_{\varphi}(T)$ together with the bulk and curvature ones vanish and, hence, at this temperature and above it the stable clusters cannot exist. The obtained range of $T_c$ in Eq. (37) is found by taking the values of the bulk coefficient $a_v(0)$ given in...
the second column of Table 1. It is remarkable that such a range of $T_c$ values is consistent with the values of the critical endpoint (CEP) temperature found for the nuclear matter from the analysis of experimental data [27]. Also this range of $T_c$ values fits very well into the estimates of CEP temperature obtained within the mean-field equation of state with the realistic hardcore repulsion between the nucleons which allows one to go beyond the popular Van der Waals approximation [8]. Moreover, as one can see from Fig. 3 of [8] such a range of CEP temperatures is consistent with the range of the nuclear matter incompressibility constant $K_S \in [270;315]$ MeV determined recently in [28, 29].

Note that an explicit temperature dependence of the surface tension coefficient

$$a_5(T) = 1.1204 \left[ a_0(0) - \frac{T^2}{\varepsilon_f} \right] = a_0(0) \left[ 1 - \frac{T^2}{T_c^2} \right],$$  

(38)

is, on the one hand, absolutely identical to the $T$-dependence of surface coefficient deduced in [30] from the analysis of nuclear multifragmentation data. Clearly, the temperature dependence of the curvature coefficients is the same as in Eq. (38). Due to the fact that the corrections given by Eq. (21) or Eq. (26) have the same $T$-dependence, then such a $T$-dependence should be also valid for the corresponding apparent coefficients defined by Eqs. (23)—(25) or by Eqs. (27)—(29). Although the $T$-dependence of $a_0(T)$ coefficient (38) was criticized in [27] as poorly consistent with the multifragmentation data, we should stress that the analysis of Eq. (38) made in [27] does not take into account the presence of the curvature terms and, hence, it cannot be applied to the framework suggested here.

Besides, in the vicinity of $T_c$ the surface tension coefficient $a_5(T)$ (38) linearly depends on temperature which is not only similar to the Fisher droplet model [2], but also to the result obtained within the exactly solvable model of surface partition of large nuclear clusters [31, 32]. Therefore, the found values of $T_c$ may be considered as a realistic estimate for the CEP temperature of nuclear matter.

Of course, it is possible that the $T_c$ values shown above will get slightly larger, if one takes into account the surface tension induced by the repulsive and attractive interaction of large nuclear matter clusters with the thermal medium [6, 8], but to estimate such effects one needs more elaborate model than the present one.

4. CONCLUSIONS AND PERSPECTIVES

Based on the saturation property of nuclear interaction we developed here a hexagonal model of large nuclei in which all the coefficients of leptodermous expansion of nuclear binding energy are expressed in term of the binding energy of a pair of nearest neighboring nucleons. It is remarkable that at zero temperature such a model reproduces the asymptotic ratio surface to bulk binding energy coefficients known from the traditional Bethe-Weizsäcker formula [11], and that with the deviation of 40–50% it also reproduces the ratio of the curvature to surface tension leptodermous coefficients obtained within sophisticated parametrizations of Skyrme interaction between nucleons [14, 18]. In addition, the suggested approach allows one to derive the Gauss curvature term. In our opinion, this is very good result for the geometrical model which does not contain any information about the complexity of nuclear interaction.

The two major advantages of the hexagonal model are that it is very simple and that it does not rely on the value of the nuclear density of ground state and on the relation between the radius of nucleus $R(A)$ and the number of nucleons $A$ in it. Due to these advantages we were able to simultaneously determine the corrections to the surface and curvature coefficients and estimate their apparent values which should be used to evaluate the properties of symmetric nuclear matter. Surprisingly, the leptodermous-like corrections (ansatz I) do not provide the best result even for a larger number of parameters. Excluding the ansatz III which has a pole at number of nucleons below 10, the best correspondence to the data is provided by the ansatz II whose bulk and surface coefficients are very close to the usual SMM values. However, in addition this ansatz generates the both curvature terms which should be included into the SMM and studied in details. Furthermore, the advantages of the suggested model allowed us to express the temperature dependence of all these coefficients in terms of the temperature dependent bulk one. The found range of critical temperature $T_c$ obtained for a single large nucleus in a vacuum is in a very good agreement with theoretical and experimental values of this quantity. Of course, in addition to the values of proper surface and curvature coefficient discussed here one has to account for their modification in the thermal medium in a spirit of approach suggested in [6].

It is clear that for a more reliable determination of the apparent values of the coefficients $a_0, a_5, a_\zeta$ and $a_\zeta$ from the experimental binding energies one has to take into account all the terms in Bethe-Weizsäcker formula, but in this case the hexagonal model should be also improved by considering a more realistic interaction between nucleons. Furthermore, we believe that such an approach will be interesting to estimate the properties of molecular clusters in real gases, but such an analysis is out of the scope of present work.
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