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New Mass Evaluation and Its Implication for the Neutron-Rich Nucleosynthesis Product Yield

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Abstract—The binding energy of unknown nuclei far from the line of stability is calculated using local mass relations that describe proton–neutron correlations. The calculations are quite accurate, and a correction of the approximation is proposed that allows the accuracy of the estimates to be improved further. The positions of the boundaries of the existence of atomic nuclei are predicted on the basis of new estimates of the binding energies. Results from modeling the nucleosynthesis products yield in the neutron excess region depend strongly on the choice of the mass model.

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INTRODUCTION

Fundamental characteristics of atomic nuclei include their mass and the binding energy of the nucleus uniquely associated with it. The systematics of nuclear mass must be studied in order to (among other things) understand nuclear structure and model the processes of nucleosynthesis. There are many different ways of making theoretical estimates of binding energies (mass models). They can be divided into microscopic and macro-microscopic, and phenomenological approaches based on local mass relations [1, 2]. Local mass relations are arithmetic expressions that combine the binding energies of several nearby nuclei on the chart of nuclides. Garvey and Kelson pioneered this approach in the late 1960s [3]. The approach was later developed substantially: new mass relations were used, our understanding of the effects described by the relations was refined, and the number of nuclear masses known from experiments was increased greatly [4, 5]. The approach of local mass relations remains relevant today, thanks to clear and simple calculations, the availability of experimental data, and the good accuracy of existing estimates [1].

In [6–8], we calculated binding energies on the basis of local mass relations using the expression for residual neutron–proton interaction among nuclei throughout the *NZ* diagram. Due to the release of the new Atomic Mass Evaluation (AME2020) collection of experimental data [9], this work compares our earlier results to the AME2020 findings and proposes a correction to the approximating formula that allows the binding energies of unknown nuclei to be calculated more accurately. The calculations also allow the limits of the existence of nuclei to be refined.

In this work, we compare results from nuclear mass estimates made using the macro-microscopic liquid drop model with the finite range of nuclear forces (FRDM) [10] and the Weizsacker–Skyrme model (WS + RBF) [11], accompanied by microscopic calculations using the Hartree–Fock formula with the Skyrme potential (HFB-24) [12].

In the final part of this work, we calculate the cross sections and rates of reactions (n, γ), and the yields of nucleosynthesis products during the astrophysical *r*-process using new estimates of binding energies.

COMPARING EARLIER RESULTS TO AME2020

Most of the expressions used in phenomenological approaches to predicting the masses of unknown nuclei are in one way or another based on characteristics associated with neutron–proton pair correlations [4, 5]. In this work, we use the expression for the energy of *np*-pairing [13]:

$$\Delta_{np}(Z,N) = [B(Z,N) - B(Z,N-1)] - [B(Z-1,N) - B(Z-1,N-1)], \quad (1)$$

where B is the binding energy of a nucleus; Z and N are the numbers of protons and neutrons, respectively. The fourth binding energy can be calculated we have an analytical approximation of $\Delta_{np}(Z,N)$ and three binding energies are known. This allows us to make iterative calculations. Estimates of earlier iterations

Table 1. Root-mean-square deviations of binding energies estimates using different approaches from the experimental data of AME2020 [9]

Estimates		σ, keV
[6, 7]	Earlier results	381
[7]	Earlier results supplemented by means of machine learning	376
[11]	Macro-microscopic calculations using the Weizsacker–Skyrme model (WS + RBF)	298
[12]	Microscopic calculations using the Hartree–Fock model with the Skyrme potential (HFB-24)	715
[10]	Macro-microscopic calculations using the finite-radius liquid drop model (FRDM)	791

Table 2. Coefficients and root-mean-square deviations of approximations $\Delta_{np}^{\text{cal}}(A)$, obtained using AME 2003 [16], 2012 [15], 2016 [14], and 2020 [9]

	Even A				Odd A			
AME	2003	2012	2016	2020	2003	2012	2016	2020
α, MeV	29.751	26.061	25.186	28.218	44.251	24.380	25.158	17.277
β	–0.799	–0.770	–0.764	–0.789	–1.294	–1.164	–1.167	–1.076
σ, MeV	0.211	0.185	0.193	0.181	0.182	0.163	0.165	0.158

can be used as known binding energies, allowing us to move far from the area studied experimentally.

In our previous work [6–8], this approach was used successfully to predict masses in the region of superheavy elements and estimate neutron drip-line. The power dependence on mass number A with a free term was used as approximations of Δ_{np} (1), and the array of nuclei was divided into five intervals for different values of A in making approximations. The compilation of AME2016 experimental data in [14] served as the basis for calculations.

Compared to the earlier compilation, AME2020 has a set of new experimental values for the nuclear masses. Table 1 shows the standard deviations of the binding energies in different approaches from the experimental values of AME2020. Our results in the considered approach have good accuracy that is comparable to the estimates of other models. Results obtained via machine learning are also highly accurate, confirming the effectiveness of predicting the binding energy of a given nucleus when using those of neighboring nuclei as input parameters. The corresponding approach to predictions is proposed in [7].

CORRECTING APPROXIMATIONS

A new formula for approximating (1) is a power-law dependence on mass number A with parameters α and β:

$$\Delta_{np}^{\text{cal}}(A) = \alpha \cdot A^{\beta}. \quad (2)$$

In [6, 7], the exponent was fixed at $\beta = -1$ for even A and $\beta = 0$ for odd A. In this work, we decided to use the exponent as a fitting parameter when finding a new approximation, which allowed us to not split the data array into separate ranges for A.

Points corresponding to symmetrical nuclei with $N = Z$ are excluded from the data set being approximated; they differ considerably from other values of Δ_{np} because of the additional contribution from the Wigner energy (see Fig. 1). Figure 1 also shows that points with $N = Z \pm 1$ are arranged according to the general array, so they should not be excluded. The absence of excluded values for magic nuclei in the region of medium and heavy nuclei demonstrates the low sensitivity of parameter Δ_{np} to shell effects. It also allows us not to exclude points with N and Z values corresponding to magic numbers. Values of Δ_{np} for light nuclei with $A < 40$ are excluded from approximation due to fluctuations caused by structural shell effects. As already noted, approximation is done over the array of nuclei with no division into intervals, but the values for nuclei with even and odd mass numbers are approximated separately. Coefficients of approximation obtained on the basis of AME2020 and data compilations AME2016 [14], 2012 [15], and 2003 [16] are given in Table 2. The relative constancy of the coefficients of approximation for the branch with even values of A and their substantial changes for odd A with the increased number of experimental data should be noted.

The power-law dependence of two-nucleon correlations on mass number A has been debated since the 1950s. [5]. The most common dependences include power functions of constantA^{β}, where $\beta = -1/3$ [17, 18], $\beta = -2/3$ [19], and $\beta = -1$ [20], and individual dependences with $\beta = -1$ for even A and $\beta = 0$ for odd A [5]. Dependence A^{-1} could indicate pairing forces with short radii of action when the particles participating in interaction are distributed over the volume of the nucleus [21]. The results in this work show

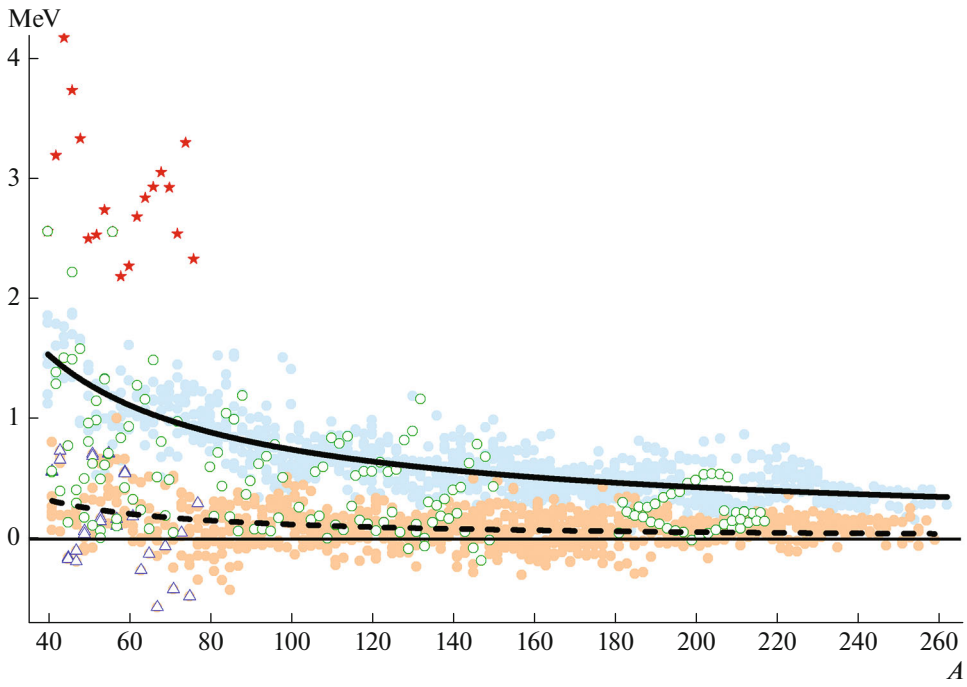

Fig. 1. Calculations of $\Delta_{np}(A)$ based on experimental data from AME 2020 [9] (even A values are marked with blue dots; odd A values are marked with orange dots; symmetrical nuclei with $N = Z$ are marked with red stars; nuclei with $N = Z \pm 1$, are marked with blue triangles; nuclei with magic numbers in N or Z are marked with white dots) and our approximation of Δ_{np}^{cal} (even A values are shown by the bold line; odd A values are given by the dashed line) (color online).

that degree of approximation (2) is close to −1 for nuclei with odd A, regardless of the database (from AME2003 to AME2020) (Table 2).

RESULTS AND DISCUSSION

To test a new approach to finding approximation $\Delta_{np}^{\text{cal}}(A)$, we estimated binding energies on the basis of AME 2003, 2012, and 2016 using two approaches (according to [6, 7] and the proposed correction). Deviations of the calculated binding energies from their values in AME2020 were calculated for new isotopes whose masses were included in AME2020 but not in earlier versions of the database. Mean deviations of estimates from the AME2020 experimental data are given in Table 3. Approximation (2) allows us to obtain more accurate results for all considered intervals A and input arrays AME.

Figure 2 shows the limits of the existence of nuclei according to different mass models. The drip-lines is determined by the nuclei for which the separation energies of proton or proton pair, neutron or neutron pair S_p, S_{pp}, S_n, S_{nn} change from positive to negative (where $S_p = B(N,Z) - B(N,Z-1)$, other separation energies are defined in a similar way). The position of neutron drip-line for nuclei with $Z > 50$ changed according to predictions of local mass relations based

Table 3. Root-mean-square deviations (keV) of AME2003 [16], 2012 [15], and 2016 [14] estimates using different approximations $\Delta_{np}^{\text{cal}}(A)$ and theoretical AME estimates from the experimental AME2020 [9] values for different ranges of nuclei

	AME2003			AME2012			AME2016		
A ≥	40	120	180	40	120	180	40	120	180
Δ_{np}^{cal} [6]	747	308	201	466	192	139	381	149	127
Δ_{np}^{cal} (this work)	664	301	201	384	190	165	372	134	108
AME estimates	455	315	178	293	169	139	223	162	169

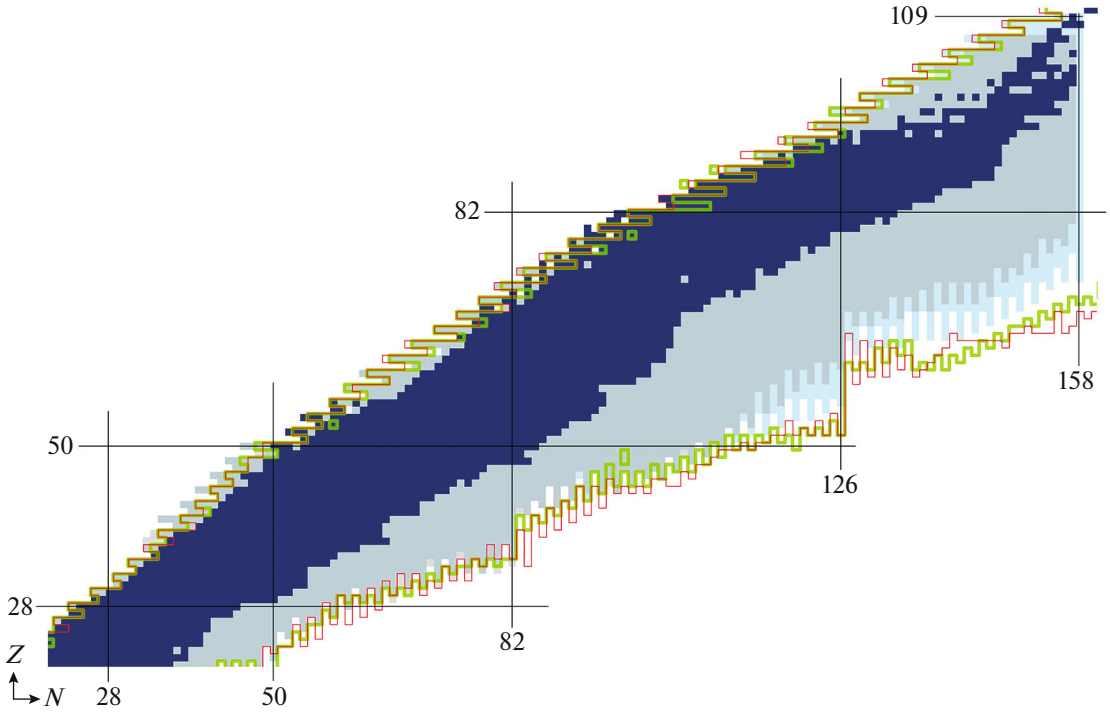

Fig. 2. Drip-lines based on various approaches to mass predictions. The dark blue area presents experimental values of AME2020 [9], the grey area shows earlier results [6, 7], and the light blue area is the results from this work. Results from using the WS + RBF model [11] are shown by the green line; results from using the HFB-24 model [12] are shown by the red line (color online).

on the transition to new approximation Δ_{np} and became closer to the macro-microscopic models estimates. The changes can be explained by the approach's large number of iterations (up to 30–40) required for predictions in this region. An increase in the number of steps weakens the connection between estimates and experimental data and increases the dependence on the choice of approximation. Another reason could be the change in the actual values of Δ_{np} for neutron-rich nuclei, even though the approximation is based on experimentally studied nuclei close to the line of stability. Despite the above factors of a possible drop in the predictive ability of the approach in the considered area, the estimates correctly reproduce the magic features of nuclei (the sensitivity of the neutron drip-line to magic number $N = 126$) even if there are no shell corrections to the approximation.

Due to topological features of formula (1) and the availability of experimental data, the region of estimates based on Δ_{np} is limited by nuclei with $Z \le 109$ and $N \le 158$. We can enter the region of heavier nuclei using additional estimates based on experimental values of the energies of α-decay or other means (e.g., machine learning algorithms). Corresponding calculations based on AME2016 data were presented in [6–8].

NUCLEOSYNTHESIS CALCULATIONS

The astrophysical *r*-process is now considered to be the main source of heavy elements in the Universe [22]. However, this process can be studied only theoretically, due to the conditions critical for its occurrence. The modeling of the *r*-process is largely based on data on nuclear masses. Experimental values of nuclear masses are not available in the region of the process, so the choice of how we predict the masses of unknown nuclei becomes important.

Figure 3 shows the mass distributions of *r*-isotopes in the canonical model, based on results from calculations in SkyNet [23]. Calculated rates of neutron capture reactions (n, γ) at temperatures of 0.1–10 GK, obtained using the TALYS software [24] and different mass models, were used. A preliminary discussion of the effect the choice of statistical model parameters has on isotope yields in the *r*-process can be found in [25]. The discrepancies in the results on the distribution of isotopes for some mass numbers A exceed three orders of magnitude. There are also qualitative differences. Micro-macroscopic FRDM and WS + RBF models for $A = 70$–90 predict several noticeable dips not observed in estimates based on Δ_{np} and HFB-24. FRDM results predict an increased yield of isotopes with $A = 100 - 170$, relative to other models. In con-

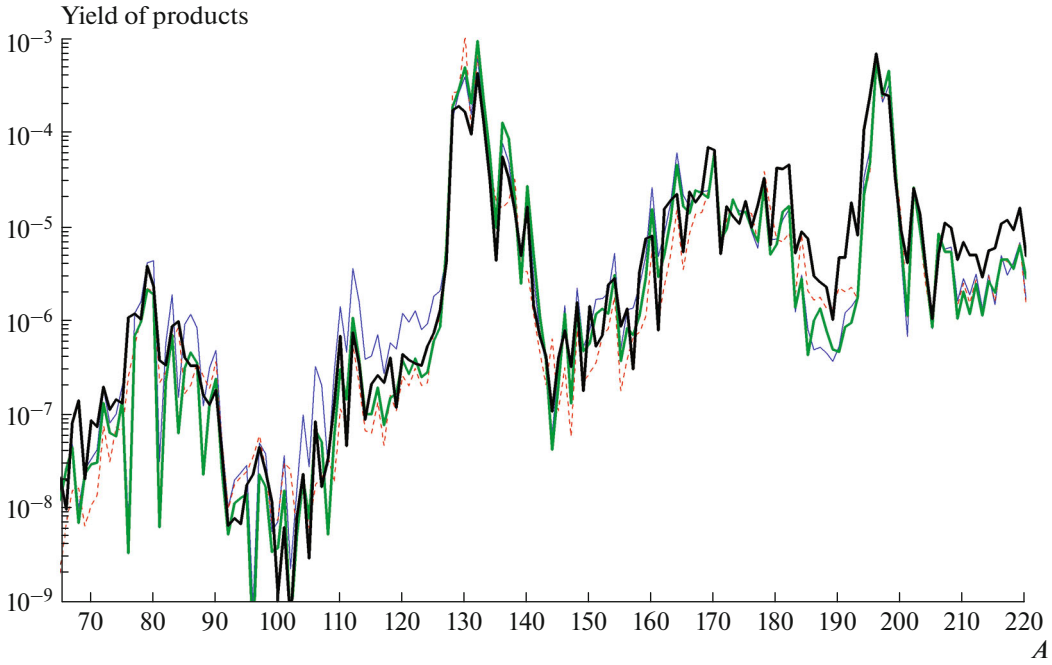

Fig. 3. Results for the yield of the *r*-process when calculating rates of the (n, γ) reaction, based on different estimates of the binding energies. The results from this work are marked by the black line; WS + RBF results [11] are marked by the green line; HFB-24 results [12] are marked by the red dashed line; FRDM results [10] are marked by the blue line (color online).

trast, the FRDM concentration of isotopes with $A > 180$ is lower.

CONCLUSIONS

Binding energies predicted using local mass relations based on the formula for residual neutron–proton interaction (1) demonstrate high accuracy comparable to that of the models most widely used in nuclear physics. The idea proposed in [7] of using machine learning algorithms to predict binding energies with those of several neighboring nuclei serving as input parameters has good predictive ability.

Correcting the approach to approximating residual neutron–proton interaction according to expression (2) allows us to improve the accuracy of predictions even more. It may therefore be recommended for further use for mass predictions. The corrected approximation and experimental data of AME2020 allowed us to obtain new estimates of binding energies for nuclei with $Z \leq 109$ and $N \leq 158$, and to refine the positions of limits of the existence of atomic nuclei.

The high sensitivity of the results from modeling the *r*-process to the choice of the mass model was demonstrated. Considerable qualitative and quantitative differences between the resulting distributions of isotopes testify to the relevance of further studies on the sources of the observed differences.

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CONFLICT OF INTEREST

The authors declare that they have no conflicts of interest.

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