7th DRHBc mass table workshop

7.1-7.4 Gangneung

A new empirical formula for nuclear binding energies

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Supervisor: Zhongming Niu

On behalf of Q. Wu, W. F. Li, and Z. M. Niu *et al*.

Contents

01

Introduction

Introduction

Nuclear mass plays important roles not only in various aspects of nuclear physics, but also in other branches of physics, such as astrophysics and nuclear engineering.

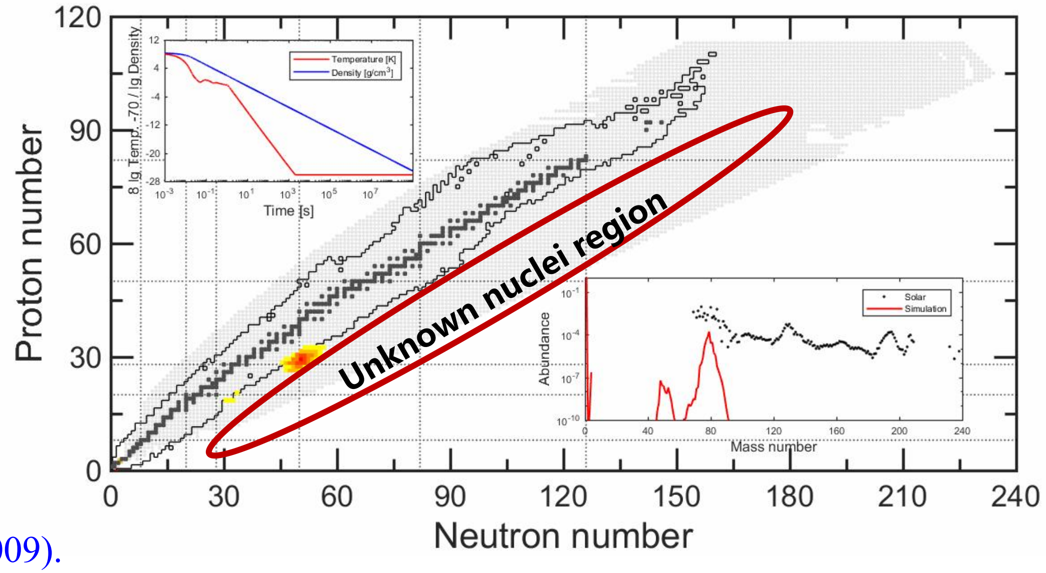
D. Lunney *et al.*, Rev. Mod. Phys. **75** 1021 (2003).
M. Bender *et al.*, Rev. Mod. Phys. **75** 121 (2003).

Application:

▲ To extract various nuclear structure information (nuclear pairing correlation, shell effect, deformation transition).

▲ Playing an important role in understanding the origin of elements in the Universe (inputs of *r*-process).

▲ The accurate mass determination is very important to test the unitarity of CKM matrix.



H. Z. Liang *et al.*, Phy. Rev. C **79** 064316 (2009).
J. C. Hardy *et al.*, Phy. Rev. C **91** 025501 (2015).

Introduction

Theoretical models of nuclear mass:

1) Macroscopic model

(i) Bethe-Weizsäcker (BW) formula

①C. F. Von Weizsäcker, Z. Phys. **96**, 431 (1935). ②M. W. Kirson, Nucl. Phys. A **798**, 29 (2008).
③H. A. Bethe *et al.*, Rev. Mod. Phys. **8**, 82 (1936).

2) Macro-microscopic model

(i) Weizsäcker-Skyrme (WS) model

①N. Wang *et al.*, Phys. Rev. C **82**, 044304 (2010). ②N. Wang *et al.*, Phys. Rev. C **81**, 044322 (2010).
③N. Wang *et al.*, Phys. Lett. B **734**, 219 (2014).

(ii) Finite-range droplet model (FRDM)

①P. Möller *et al.*, At. Data Nucl. Data Tables **59**, 185 (1995). ②P. Möller *et al.*, Phys. Rev. Lett. **108**, 052501 (2012).

3) Microscopic mass model

(i) Hartree-Fock-Bogoliubov (HFB) theory

①Y. Aboussir *et al.*, At. Data Nucl. Data Tables **61**, 127 (1995).
②S. Goriely *et al.*, Phys. Rev. Lett. **102**, 152503 (2009). ③S. Goriely *et al.*, Phys. Rev. C **93**, 034337 (2016).

(ii) Relativistic mean-field (RMF) model

①L. S. Geng *et al.*, Prog. Theor. Phys. **113**, 785 (2005). ②K. Y. Zhang *et al.*, At. Data Nucl. Data Tables **144**, 101488 (2022).

4) Machine learning method

①R. Utama *et al*, Phys. Rev. C **93**, 014311 (2016). ②Z. M. Niu *et al.*, Phys. Lett. B **778**, 48 (2018).
③X. H. Wu *et al.*, Phys. Lett. B **834**, 137394 (2022). ④Z. M. Niu *et al.*, Phys. Rev. C **106**, L021303(2022).

Introduction

Empirical formula:

1）The coefficients of the empirical formula have physical significance and help to understand the related physical properties.

2) The empirical formula is simple in form, fast in calculation, and low in cost.

3) The empirical formula method has been used in the study of many physics problems.

(i) Nuclear β-decay half-lives

Y. Zhou *et al.*, Sci. China-Phys. Mech. Astron. **60** 082012 (2017).

J. G. Xia *et al.*, Acta. Phys. Sin. **73** 062301 (2024).

(ii) Neutron capture cross sections

A. Couture *et al.*, Phys. Rev. C **104** 054608 (2021).

(iii) ......

02 Theoretical framework

Theoretical framework

Bethe–Weizsäcker (BW) mass formula:

C. F. Von Weizsäcker, Z. Phys. 96, 431 (1935).
H. A. Bethe et al., Rev. Mod. Phys. 8, 82 (1936).

$$B = B_v + B_s + B_c + B_a + B_p$$
$$= a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{sym}(N-Z)^2 A^{-1} + a_p \delta A^{-1/2}$$

Volume energy B_v

Surface energy B_s

Coulomb energy B_c

Symmetry energy B_{sym}

Pairing energy B_p

Theoretical framework

Improvement of BW formula

The semi-empirical formula is improved by introducing related physical terms to the traditional BW model.

M. W. Kirson, Nucl. Phys. A 798, 29 (2008).

$$B_{\text{th}} = a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{sym}(N-Z)^2 A^{-1} + \delta a_p A^{-1/2} + B_{xc} + B_W + B_{st} + B_r + B_m \quad \text{(FK)}$$

$$B_{\text{th}} = a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{sym}(N-Z)^2 A^{-1} + \delta a_p A^{-1/2} + B_{xc} + B_W + B_{st} + B_r \quad (\text{FK}^*)$$

Exchange Coulomb term : $B_{xc} = a_{xc} Z^{4/3} A^{-1/3}$

Wigner term : $B_W = a_w |N-Z| A^{-1}$

Surface symmetry term : $B_{st} = a_{st}(N-Z)^2 A^{-4/3}$

Curvature term : $B_r = a_r A^{1/3}$

Shell effects term: $B_m = \alpha_m P + \beta_m P^2$

For simplicity, we will use FK to denote this formula and give FK* as a comparison to study the effect of the shell effects term.

Theoretical framework

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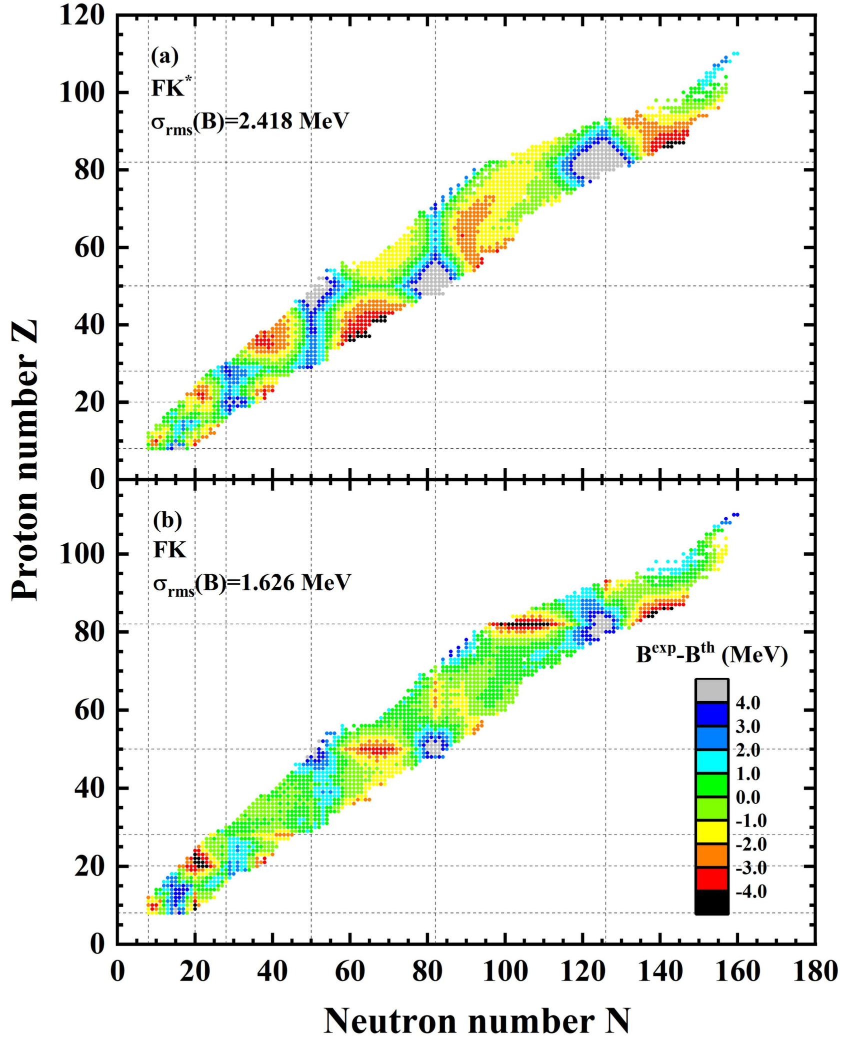


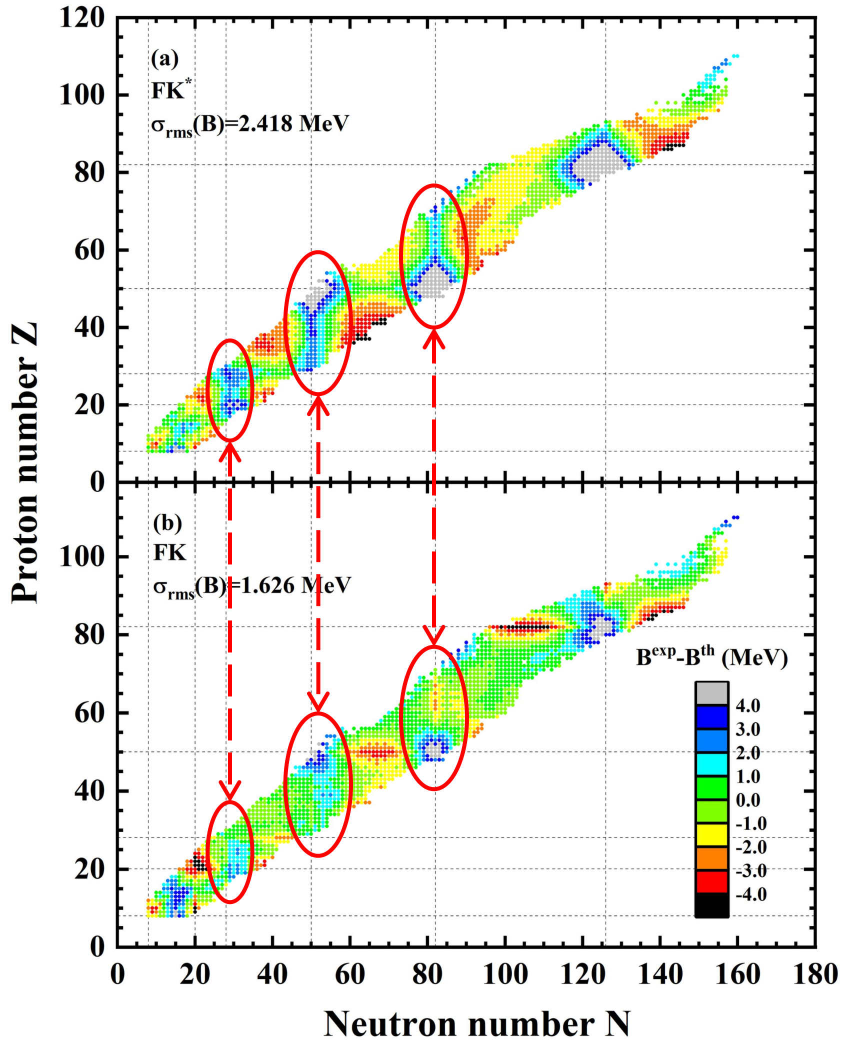
Fig.1 Binding energy differences between the experimental data with the FK* and FK predictions.

▲ **The inclusion of the shell effects term** reduces the rms deviation of binding energies from **2.418 MeV** to **1.625 MeV**.

▲ Compared to FK*, the FK significantly improves the binding energy predictions for some neutron magic numbers and other partial nuclear regions, such as around $Z = 30 - 45$, $N = 90 - 110$.

▲ FK has a relatively poor description of the binding energy of Z in the region around 50 and 82.

Theoretical framework



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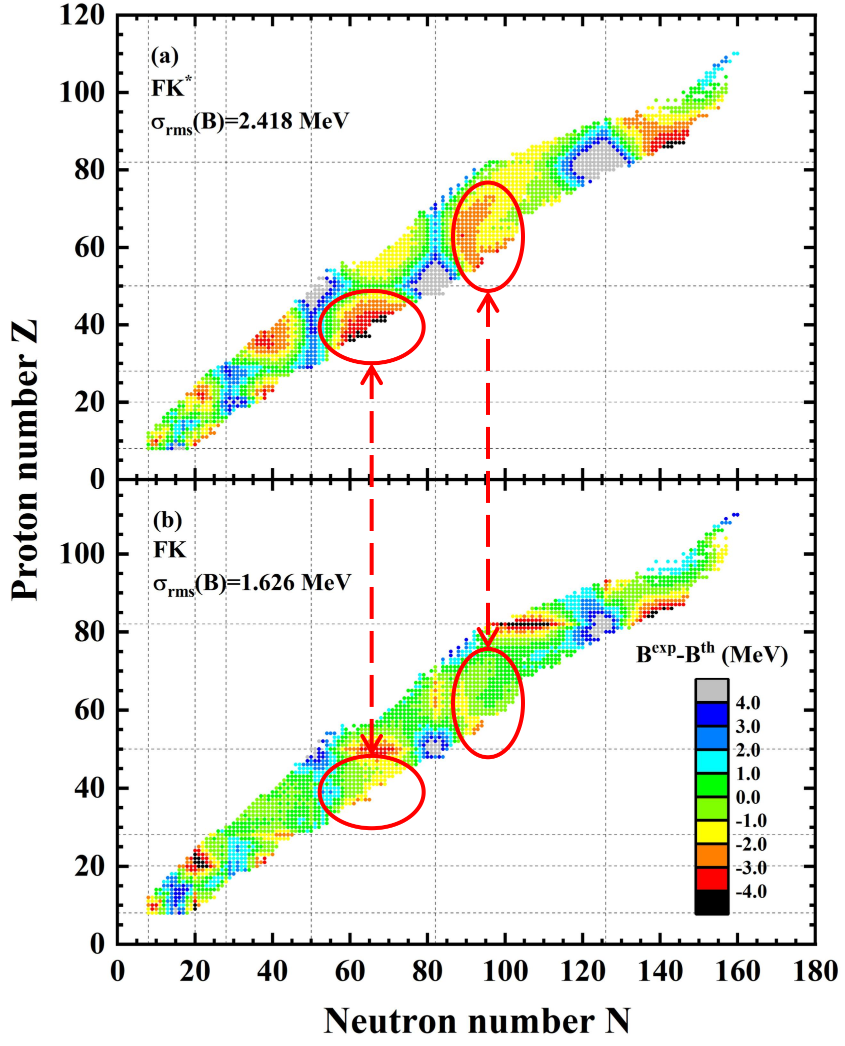

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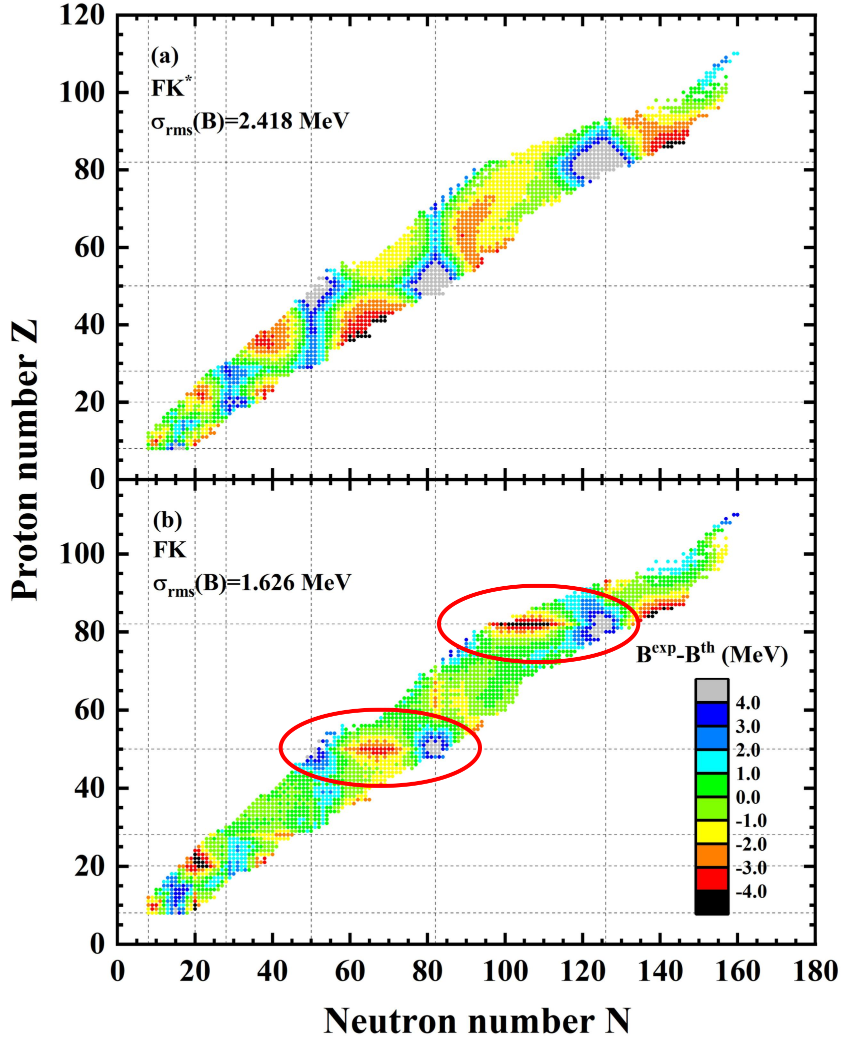

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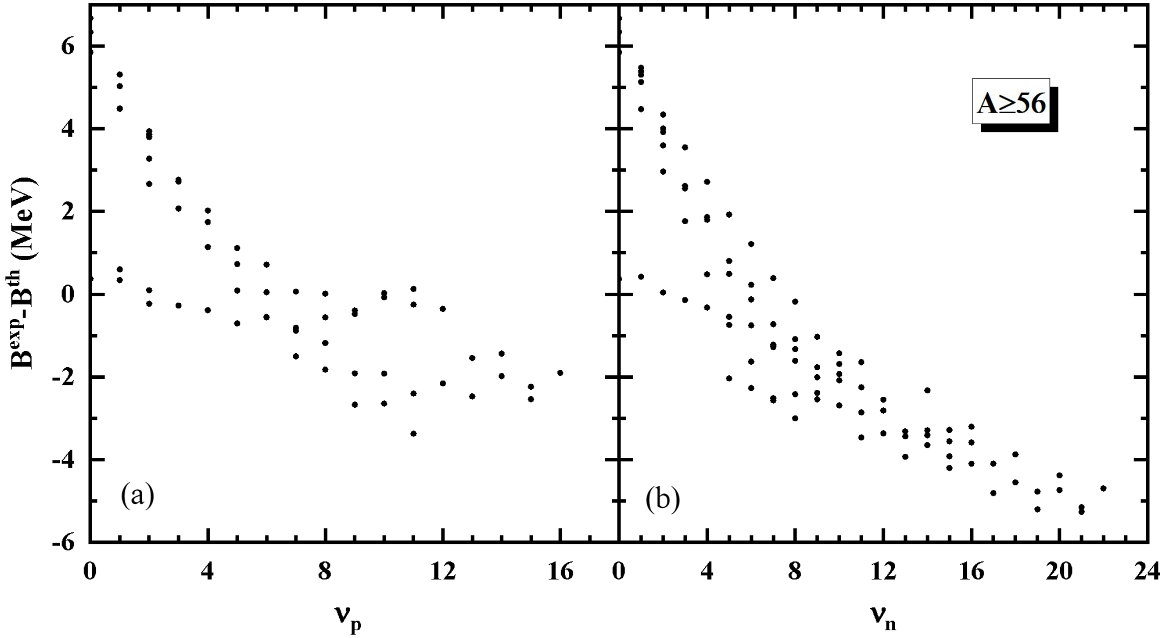

Fig.2 Binding energy differences between the experimental data with the FK predictions for nuclei with $A \geq 56$ as a function of the v_p (a) and v_n (b).

▲ The binding energy differences between the experimental data with the FK predictions decrease with increasing v_p and v_n.

▲ It may be possible to improve the description of the nuclear binding energy by introducing linear terms related to v_p and v_n in the formula.

$$B_{th} = a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{sym}(N-Z)^2 A^{-1} + \delta a_p A^{-1/2} + a_{xc} Z^{4/3} A^{-1/3} + a_w |N-Z| A^{-1} + a_{st}(N-Z)^2 A^{-4/3} + a_r A^{1/3} + \alpha_m P + \beta_m P^2 + c_m(v_p + v_n) \quad \text{(F1)}$$

Theoretical framework

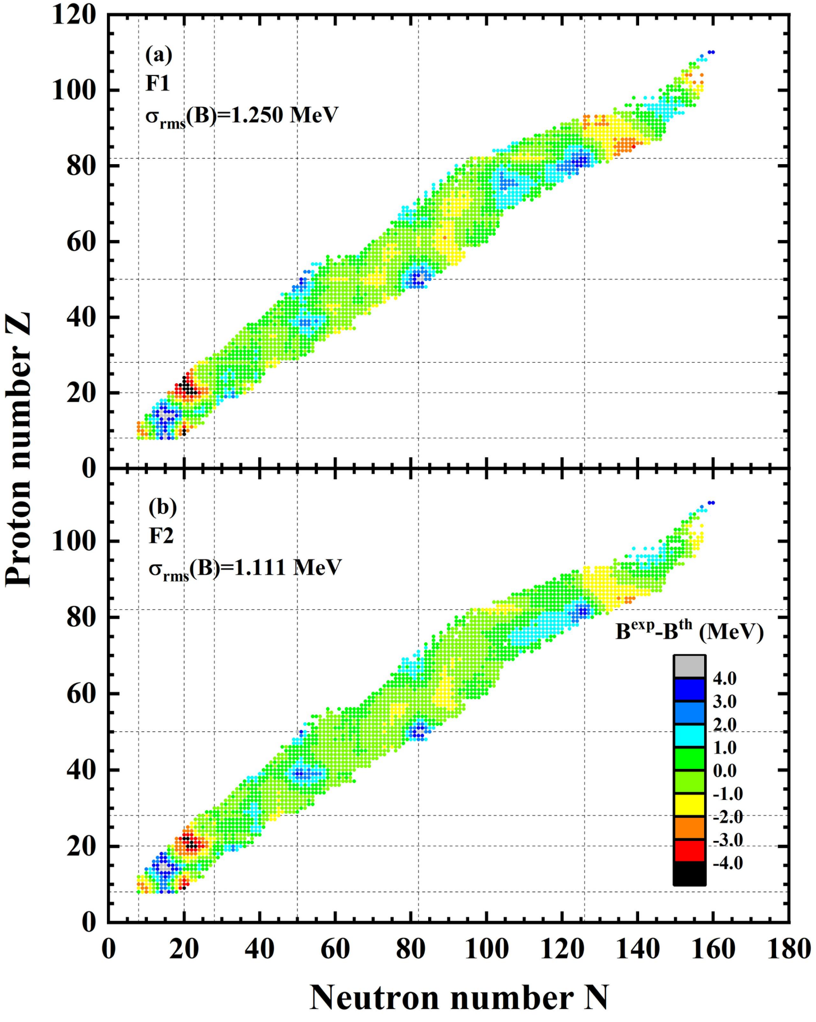

Fig.3 Binding energy differences between the experimental data with the F1 and F2 predictions.

▲ The introduction of a linear term for v_p and v_n improves the formula predictive ability in regions near the magic numbers.

▲ The $|\Delta B|$ decrease with increasing the distance from the doubly magic nuclei. For this property, the introduction of exponential functions related to v_p and v_n may help to improve the description of the binding energy.

$$B = a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{xc} Z^{4/3} A^{-1/3} + a_r A^{-1/3} + \alpha_m P + \beta_m P^2 + \delta a_p A^{-1/2} + a_{sym} (N-Z)^2 A^{-1} + a_w |N-Z| A^{-1} + a_{st} (N-Z)^2 A^{-4/3} + c_m (\nu_p + \nu_n) \quad \text{(F1)}$$

N. Wang *et al.*, Phys. Lett. B 734, 219 (2014).

$$B = a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{xc} Z^{4/3} A^{-1/3} + a_r A^{-1/3} + \alpha_m P + \beta_m P^2 + \delta_{np} a_p A^{-1/3} + a_{sym} I^2 A f_s + c_m (\nu_p + \nu_n) + e_{m1} e^{e_{m2}(\nu_n^2 + \nu_p^2)} \quad \text{(F2)}$$

Theoretical framework

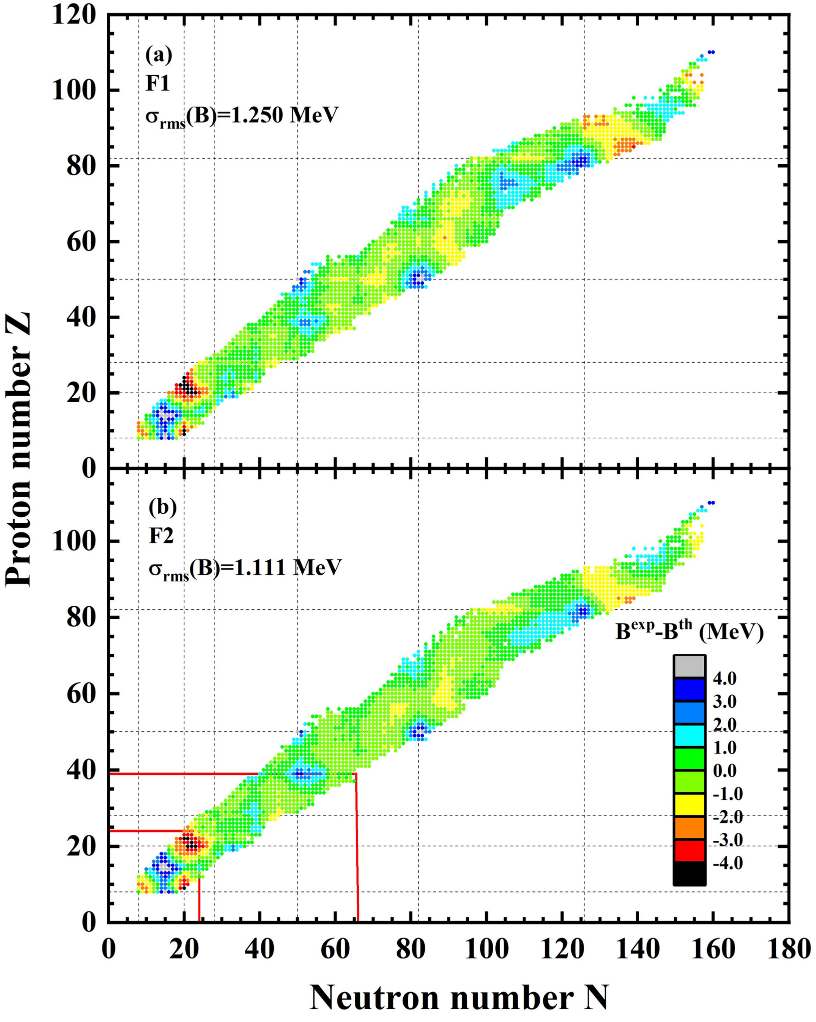

Fig.3 Binding energy differences between the experimental data with the F1 and F2 predictions.

▲ Interestingly, the sign of ΔB is not consistent for different nuclear doubly magic number regions. Apparently, formula F2 fails to reflect the different regional conditions of different doubly magic number nuclei.

▲ We introduce a coefficient δ_{shell} in the exponential term to obtain the new formula F3.

$$B = a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{xc} Z^{4/3} A^{-1/3} + a_r A^{-1/3} + \alpha_m P + \beta_m P^2 + \delta_{np} a_p A^{-1/3} + a_{sym} I^2 A f_s + c_m(\nu_p + \nu_n) + e_{m1} e^{e_{m2}(\nu_n^2 + \nu_p^2)} \quad \text{(F2)}$$

$$B = a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{xc} Z^{4/3} A^{-1/3} + a_r A^{-1/3} + \alpha_m P + \beta_m P^2 + \delta_{np} a_p A^{-1/3} + a_{sym} I^2 A f_s + c_m(\nu_p + \nu_n) + e_{m1} \delta_{shell} e^{e_{m2}(\nu_n^2 + \nu_p^2)} \quad \text{(F3)}$$

$$\delta_{shell} = \begin{cases} -1 & Z, N \in [8, 24] \\ 0 & Z \in (24, 39] \ \& \ N \in [8, 66]; Z \in [8, 24] \ \& \ N \in (24, 66] \\ 1 & \text{else} \end{cases}$$

03

Results and discussion

Results and discussion

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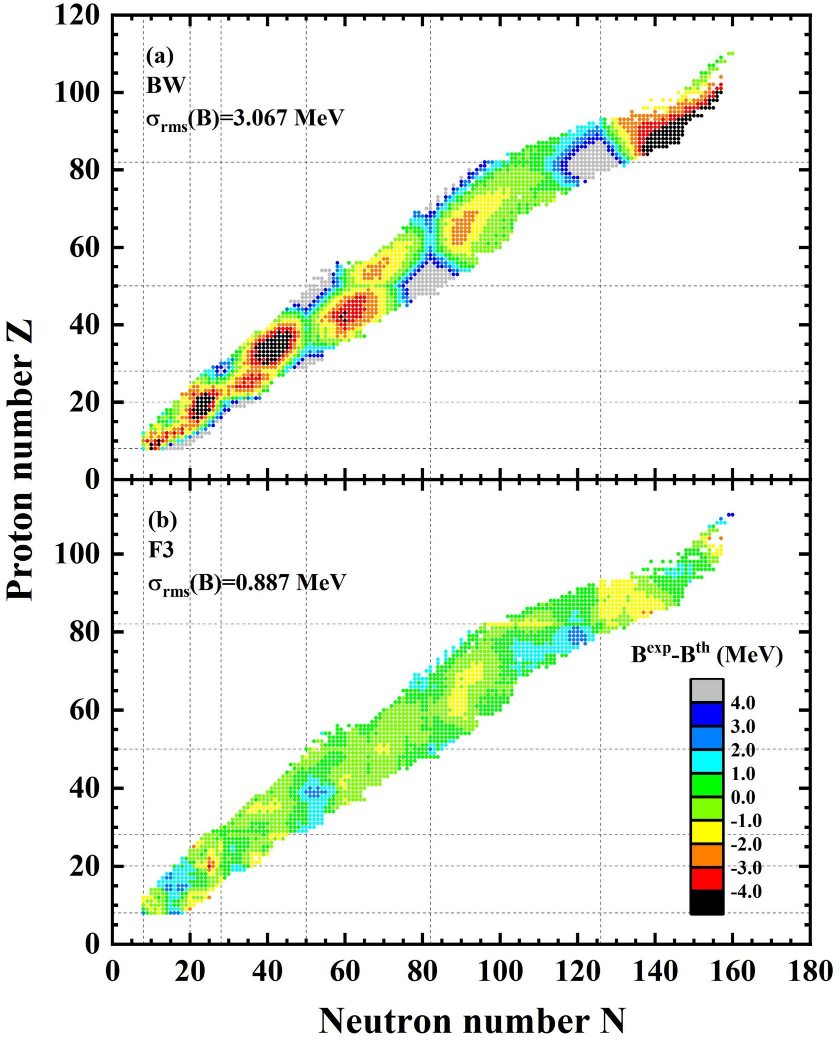

Fig.4 Binding energy differences between the experimental data with the BW and F3 predictions.

▲ Compared to BW, the F3 significantly improves the description of nuclear binding energies, especially for light nuclei, superheavy nuclei, and nuclei near the magic number (including single and double magic number nuclei).

Data set	Percentage decrease compared to BW	$\sigma_{rms}(B)$
$Z, N \geq 8$	**71.09 %**	**0.887 MeV**
$A \geq 60$	**72.38 %**	**0.838 MeV**
magic number nuclei	**78.57 %**	**1.605 MeV**

Results and discussion

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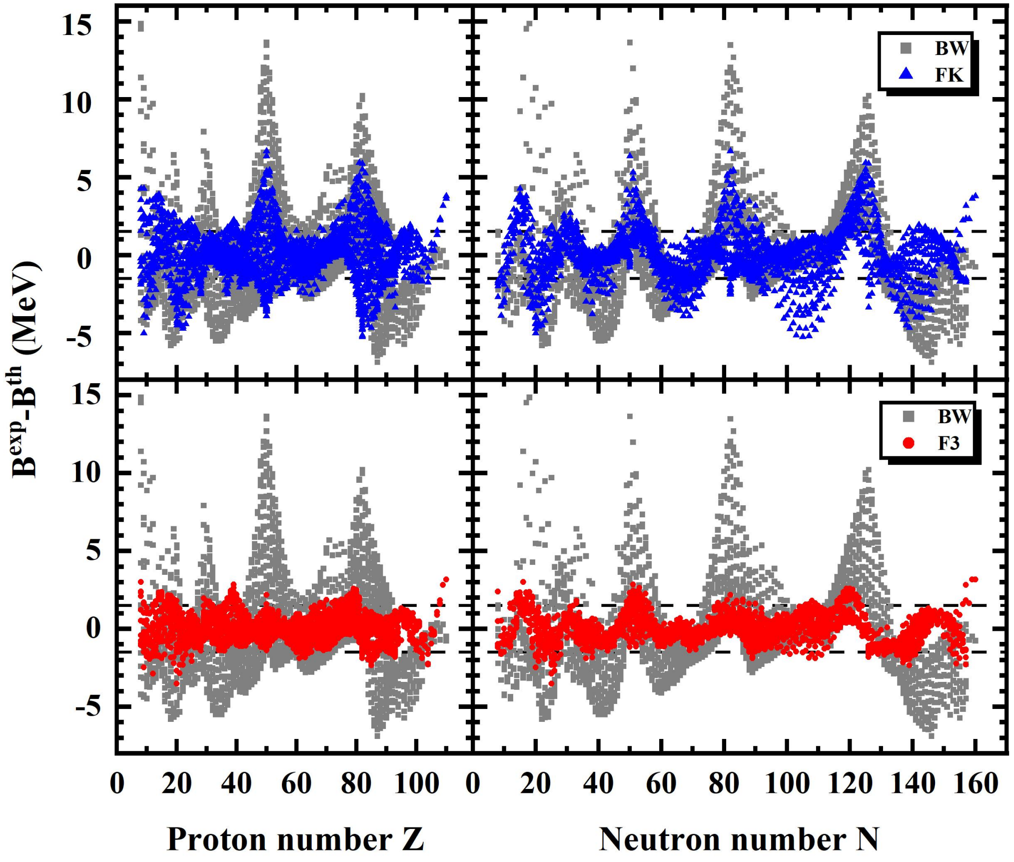

Fig. 5 Differences between the experimental nuclear binding energies and the predictions with BW, FK, and F3 for the 2457 selected nuclei with $Z \geq 8$, $N \geq 8$ versus nuclei number.

▲ The predictive ability of the nuclear binding energy formula can be improved by considering the relevant physical terms.

▲ F3 improves the description of the binding energy of nuclei near the magic numbers by introducing linear and exponential terms related to v_p and v_n.

▲ The percentage of nuclei for which the predictions of BW, FK and F3 deviate from the experimental data within 1.5 MeV is **43.71%**, **70.20%**, and **91.90%**, respectively.

04 Summary and perspectives

Summary

★ The new formula is proposed by introducing microscopic correction terms related to v_p and v_n. The rms deviation of the predicted results from the experimental binding energies is **0.887 MeV**.

★ Compared to Bethe-Weizsäcker (BW) formula, the new empirical formula significantly improves the description of nuclear binding energies, especially for light nuclei, superheavy nuclei, and nuclei near the magic number.

★ The percentage of nuclei for which the predictions of the new formula deviate from the experimental data within 1.5 MeV is **91.90%**.

Perspectives

In the future, the nuclear mass predictions from this work can be applied to the simulation of *r*-process to study its influence on the abundance and evolution of *r*-process.

Thank You!

Appendix

BW:

$$B = a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{sym}(N-Z)^2 A^{-1} + a_p \delta A^{-1/2}, \tag{1}$$

FK:

$$\begin{aligned} B =& a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{sym}(N-Z)^2 A^{-1} + a_p \delta A^{-1/2} \\ &+ a_{xc} Z^{4/3} A^{-1/3} + a_w |N-Z| A^{-1} + a_{st}(N-Z)^2 A^{-4/3} + a_r A^{1/3} + \alpha_m P + \beta_m P^2, \end{aligned} \tag{2}$$

FK*:

$$\begin{aligned} B =& a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{sym}(N-Z)^2 A^{-1} + a_p \delta A^{-1/2} \\ &+ a_{xc} Z^{4/3} A^{-1/3} + a_w |N-Z| A^{-1} + a_{st}(N-Z)^2 A^{-4/3} + a_r A^{1/3}, \end{aligned} \tag{3}$$

Appendix

F1:

$$
\begin{aligned}
B =& a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + a_{sym}(N-Z)^2 A^{-1} + a_p \delta A^{-1/2} \\
& + a_{xc} Z^{4/3} A^{-1/3} + a_w |N-Z| A^{-1} + a_{st}(N-Z)^2 A^{-4/3} + a_r A^{1/3} \\
& + \alpha_m P + \beta_m P^2 + c_m(\nu_p + \nu_n),
\end{aligned} \tag{4}
$$

F2:

$$
\begin{aligned}
B =& a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + \delta_{np} a_p A^{-1/3} + a_{xc} Z^{4/3} A^{-1/3} + a_r A^{1/3} \\
& + a_{sym} I^2 A f_s + \alpha_m P + \beta_m P^2 + c_m(\nu_p + \nu_n) + e_{m1} e^{e_{m2}(\nu_p^2 + \nu_n^2)},
\end{aligned} \tag{5}
$$

F3:

$$
\begin{aligned}
B =& a_v A + a_s A^{2/3} + a_c Z^2 A^{-1/3} + \delta_{np} a_p A^{-1/3} + a_{xc} Z^{4/3} A^{-1/3} + a_r A^{1/3} \\
& + a_{sym} I^2 A f_s + \alpha_m P + \beta_m P^2 + c_m(\nu_p + \nu_n) + e_{m1} \delta_{shell} e^{e_{m2}(\nu_p^2 + \nu_n^2)}.
\end{aligned} \tag{6}
$$

Appendix

The Z, N, and A represent the proton, neutron, and mass numbers, respectively. Three extra physical quantities I, δ and P related to nuclear isospin, pairing and shell effects, which are

$$I = (N - Z)/A, \quad \delta = [(-1)^Z + (-1)^N]/2, \quad P = \nu_p \nu_n/(\nu_p + \nu_n). \tag{7}$$

According to Ref [1], we give the following defintion

$$\delta_{np} = \begin{cases} \frac{17(2-|I|-I^2)}{16} & \text{even} - \text{even nuclei} \\ |I| - I^2 & \text{odd} - \text{odd nuclei} \\ 1 - |I| & \text{even} - \text{odd nuclei with } N > Z \\ 1 - |I| & \text{odd} - \text{even nuclei with } N < Z \\ 1 & \text{even} - \text{odd nuclei with } N < Z \\ 1 & \text{odd} - \text{even nuclei with } N > Z \end{cases}, \tag{8}$$

$$f_s = 1 + \kappa((I - \frac{0.4A}{A+200})^2 - I^4)A^{1/3} \tag{9}$$

$$a_{sym} = c_{sym}(1 - \frac{k}{A^{1/3}} + \xi \frac{2 - |I|}{2 + |I|A}) \tag{10}$$

δ_{shell} values for different regions are also given with

$$\delta_{shell} = \begin{cases} -1 & 8 \leqslant Z \leqslant 24 \text{ and } 8 \leqslant N \leqslant 24 \\ 0 & 24 < Z \leqslant 39 \text{ and } 8 \leqslant N \leqslant 66 \\ 0 & 8 \leqslant Z \leqslant 24 \text{ and } 24 < N \leqslant 66 \\ 1 & \text{else} \end{cases} \tag{11}$$

TABLE I: Free parameters and $\sigma_{\rm rms}(B)$ values of the BW, FK, F1, F2, and F3 formula. And it use the unit in MeV.

	BW	FK	FK*	F1	F2	F3
a_v	15.5414	16.4920	16.1707	16.3845	15.9108	16.7043
a_s	−16.9443	−25.5618	−23.5820	−24.7172	−19.5107	−26.3000
a_c	−0.7033	−0.7614	−0.7408	−0.7611	−0.7404	−0.7615
$a_{sym}(c_{sym})$	−23.0214	−32.5777	−31.7110	−31.8596	−33.1442	−35.3636
a_p	12.4998	11.0409	11.9953	11.1655	6.0387	5.9751
a_{xc}		1.6997	1.4587	1.8009	1.2311	1.4405
a_w		−61.7229	−57.7605	−44.4585		
a_{st}		61.1172	57.5972	55.2362		
a_r		13.3315	10.0163	11.2350	−2.1600	14.1287
α_m		−2.0293		−1.1379	−1.0369	−1.0877
β_m		0.1595		0.1979	0.1052	0.1615
c_m				−0.3665	0.0318	−0.2343
e_{m1}					7.3839	5.4713
e_{m2}					−0.0103	−0.0444
k					1.9017	2.0829
ξ					1.0950	1.2216
κ_s					0.2417	0.2491
$\sigma_{\rm rms}(B)$	3.0667	1.6254	2.4183	1.2496	1.1112	0.8865