A new formula to calculate nuclear binding energies for some nuclei around the closed core

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Abstract

Depending on the basic assumptions of the Shell Model and by using suitable potentials, we found a new formula to calculate nuclear binding energies for some nuclei around the closed core, which are $^{49-58}_{20}Ca$, $^{57-78}_{28}Ni$ and $^{101-132}_{50}Sn$.

This formula is related to the mass number and number of valence nucleons outside the closed core. We found the value of standard deviation is better than that calculated by the Semi-Empirical Mass Formula, it is also better than that estimated by the Integrated Nuclear Model, and better estimated by the Modified Nuclear Integrated Model. This indicates that our inferred formula is better than the most important formulas, which were used to calculate nuclear binding energies for studied nuclei.

Keywords: Nuclear Binding Energy, Shell Model, Valence Nucleons, Closed Core.

1. Introduction

One of the purposes of nuclear physics is to provide nuclear models, which explain the properties and behavior of atomic nuclei. the most important of these nuclear properties is the density of the nucleus which is almost constant, so the size of nuclei is proportional to their mass number [1].

We find that the same applies to liquids, so one of the first nuclear models was the Liquid Drop Model (LDM), which was presented by Carl Friedrich Von Weizsacker in 1935 and Bohr established its basic hypotheses [2].

Depending on this model, the values of nuclear binding energies is calculated using the Semi-Empirical Mass Formula (SEMF), which is known as the Bethe-Weizsäcke formula. [3] . In 2011, a new model called the Integrated Nuclear Model (INM) was introduced to calculate the nuclear binding energies, which were deduced by Nader Ghahramany and his group [4]. This model is based on the theory of Quantum Chromodynamics, where nuclear matter is treated as a plasma composed of a soup of quarks and gluons.

This model was developed in 2020 by Hezekiah K. Cherop and Kapil M. Khanna and it is called the Modified Integrated Nuclear Model (MINM) [5].

In these types of nuclear models, nucleons are not dealt with separately, it is considered as a static system. Therefore, these models succeeded in calculating some properties of nuclei, such as the average nuclear binding energy for each nucleon, as they failed to calculate other nuclear properties such as excited states and magnetic moments.

On the other hand, the Shell Model(SM) developed by Mayer and Jensen was proposed in 1948 [6], on the assumption this model, each nucleon in any nucleus moves independently in a median potential resulting from the rest of the nucleons which is called valance field, expressing a "central field" . This field adds to a potential resulting from the mutual effects between every two nucleons of the nucleons, called residual interaction. According to this model, nucleons are located on separate energy levels called single-particle levels, which are determined by solving the Schrödinger equation by choosing an appropriate potential. This model succeeded in calculating many nuclear properties, such as predicting magic numbers, spin-parity, excited states, and their magnetic moments, but it did not give a good value for nuclear binding energies for most nuclei especially far from the stability line.

2. Methods

In this study, we found a new formula to calculate values of nuclear binding energy in terms of mass number and number of valence nucleons in the ground state depending on basic assumptions of the Shell Model and selection of suitable potentials. We apply this new approach to calculate Thirty-two odd- isotopes and Thirty-two even -

even isotopes, whose valence nucleons are located outside the closed cores $^{48}_{20}Ca_{28}$, $^{56}_{28}Ni$ and $^{100}_{50}Sn$.

The LAB fit program was used to obtain the value of average binding energy for each valence nucleon in the ground state by best fitting for experimental single-particle energies, and the MATLAB program was used to perform the rest of the calculations and analyze the data.

3. Nuclear Shell Model

The basic assumption of the nuclear shell model is that to a first approximation, each nucleon moves independently in a potential that represents average interaction with other nucleons in a nucleus. This independent motion can be understood qualitatively from a combination of the weakness of long-range nuclear attraction and the Pauli exclusion principle.

In a non-relativistic approximation, nuclear properties are described by the Schrodinger equation for A nucleons, i.e. [7].

$$\hat{H}\left|\Psi\right\rangle = E\left|\Psi\right\rangle \qquad (1)$$

where Ψ is an A-body wave function, and $\hat{H}$ contains nucleon kinetic energy operators and interactions between nucleons of a two-body, and a three-body character, in the present study we will consider only the two-body interaction, i.e

$$\hat{H} = \sum_{i=1}^{A}\left(-\frac{\hbar^2}{2m}\Delta_i\right) + \sum_{i<j=1}^{A}W(i,j) \qquad (2)$$

We can re-write the Hamiltonian (2), adding and subtracting a one-body potential of the form $\sum_{i=1}^{A}U(i)$ as [7]

$$\hat{H} = \sum_{i=1}^{A}\begin{bmatrix} [-\frac{\hbar^2}{2m}\Delta_i + U(i)] + \\ \sum_{i<j=1}^{A}W(i,j) - \sum_{i=1}^{A}U(i) \end{bmatrix} = \hat{H}^{(0)} + \hat{H}^{(1)} \qquad (3)$$

Where $\hat{H}^{(0)}$ is zero Hamiltonian and it is a sum of single-particle Hamiltonians, and expresses average potential of all nucleons. $\hat{H}^{(1)} = \sum_{i<j=1}^{A}W(i,j) - \sum_{i=1}^{A}U(i) \equiv V$ is called a residual interaction.

It is clear that when the number of nucleons is large, the Hamiltonian matrix becomes a huge, so we use an approximating valence space or model space [8], which consists of all single-particle orbitals actively involved in the generation of configurations of a many-nucleon system considered, and assumes the existence of a closed core is the closest doubly magic nucleus to studied nucleus, therefore the nucleus studied is limited to valence nucleons (nucleons that lie outside closed core) instead of being between all nucleons.

The reason for defining a core is that the computational effort increases very rapidly with an increasing number of single-particle orbitals included in the valence space.

We can re-write the Hamiltonian (3) according to Valance Space as [8]

$$\hat{H} = E(CORE) + \overline{\varepsilon}(\hat{n})\hat{n} + \sum_{i=1}^{A}U(i) + \hat{H}^{(1)} \qquad (4)$$

Where $E(CORE) = -BE(CORE)$ is the nuclear binding energy of the closed core, $\overline{\varepsilon}$ the average nuclear binding energy of valance nucleons, and $\hat{n}$ is the particle number operator, U is a mean - field potential and $\hat{H}^{(1)}$ is a residual interaction.

Now we will describe how each term in the last equation was calculated.

3.1. Average nuclear binding energy per nucleon of valance nucleons $\overline{\varepsilon}$

We can obtain the value of average binding energy for each valence nucleon in the ground state by best fitting for experimental single-particle energies [9].

The valence nucleons fall within pfg shell, and outside the closed core $^{48}_{20}Ca_{28}$, which has the following energy levels, respectively [10]

$1p_{3/2} = -5.15\,MeV$,

$1p_{1/2} = -3.12\,MeV$,

$0f_{5/2} = -1.20\,MeV$,

$0g_{9/2} = +0.45\,MeV$

And the valence nucleons fall within pfg shell, and outside the closed core $^{56}_{28}Ni$, which has the following energy levels, respectively

$1p_{3/2} = -10.25\,MeV$,

$0f_{5/2} = -9.48\,MeV$,

$1p_{1/2} = -9.14\,MeV$,

$0g_{9/2} = -6.55\,MeV$

In addition, the valence nucleons fall within dgs shell, and outside the closed core $^{100}_{50}Sn$, which has the following energy levels, respectively

$1d_{5/2} = -11.15\,MeV$,

$0g_{7/2} = -11.07\,MeV$,

$2s_{1/2} = -9.60\,MeV$,

$1d_{3/2} = -9.50\,MeV$,

$0h_{11/2} = -8.60\,MeV$

By performing best fitting (using the LAB fit program), we got the best form of the equation which represents the average energy of single particle energy in valence levels in terms of the number of valence nucleons, which takes the following form

$$\overline{\varepsilon}(\hat{n}) = a + b\,\hat{n} \quad (MeV) \qquad (5)$$

Where a and b constants that take the values $a = -4.47\,MeV$,$b = 0.272\,MeV$ for Calcium isotopes, and take the values

$a = -10.94\,MeV$, $b = 0.2323\,MeV$ for Nickel isotopes, Where that take the values $a = -11.73\,MeV$, $b = 0.1128\,MeV$ for Tin isotopes.

3.2. Mean Field Potential U

This potential is central; it is produced by all valence nucleons, so that each nucleon of valence space is moving independently in this central potential resulting from the rest of all the nucleons. This potential can take different forms, such as the Harmonic Oscillator, Woods-Saxon potential, and Paring potential.

Assuming that the valence nucleons are all in the ground state and are paired with each other, the most appropriate potential to describe this system is the Paring potential, which takes the following form [11]

$$V_{PAIR} = -G \sum_{\rho} A_{\rho}^{+} A_{\rho} \qquad (6)$$

Where $A_{\rho}^{+} = \sum_{i=1}^{p} A_{\rho}^{+}(i)$ and $A_{\rho} = \sum_{i=1}^{p} A_{\rho}(i)$ is pair creation operators and ρ is the number of j-orbits in mean-field potential considered, and $G > 0$ is a isovector paring strength, which is giving in terms of mass number as follows $G = \dfrac{20}{A}$ [9, 12].

Depending on Paring potential, Paring energy is given by the following equation when all the nucleons are in the ground state as [8]

$$E_{\nu}(N) = -\frac{1}{4}G(N-\nu)(2\Omega - N - \nu + 2) \qquad (7)$$

Where ν is the Seniority quantum number, which is the number of nucleons not pairwise coupled to angular momentum zero, in short, the number of unpaired nucleons, N indicates the number of nucleons in the ground state (which represents a number of valence nucleons), and Ω indicates the maximum number of paired pairs that given level fits into nucleons, it is given by $\Omega = \dfrac{1}{2}(2j + 1)$.

When Increase the number of neutrons N over the number of protons Z in nucleus it causes decreases their stability and thus decreases their total nuclear binding energy, so we will add another term to mean field potential that results from the Symmetry Effect, which takes the following equation [4]

$$V_{sym} = \sum_{1,2} \frac{t_1 t_2}{A} V_1 \qquad V_1 \approx 100\,(MeV) \qquad (8)$$

Where t_1 and t_2 Isospin for two nucleon interaction.

Depending on previous Symmetry potential, the energy from this potential is given by following equation

$$E_{Asy} = (N - Z)\frac{V_1}{A} \qquad (9)$$

In our study, the amount $(N - Z)$ represents a number of valence nucleons outside the closed core.

$\hat{H}^{(1)}$ 3.3. Residual Interaction

The effect of residual interaction only occurs between valence nucleons, and its contribution to total Hamiltonian is small compared to mean field potential, so it is treated as a perturbation, and this interaction takes different forms. In this study, we choose the Surface Delta Interaction (SDI) because it is easy to deal with, and it is a separable potential, which allows for obtaining an analytical solution to the Schrödinger equation. This form of interaction was postulated in 1966 by Moszkowski et.al. [14]. This is based on the Pauli principle, which forbids collisions occur at full levels and allows collisions to occur mainly at valance levels. This interaction was developed by Glaudesmans [15], and is called the Modified Surface Delta Interaction (MSDI). The matrix element of residual interaction for one of the interacting valence-nucleon pairs is

$$\left\langle j_a j_b, JT \left| V_{MSDI} \right| j_c j_d, JT \right\rangle_{JT} =$$

$$\frac{A_T}{2(2J+1)} \left[\frac{(2j_a+1)(2j_b+1)}{(2j_c+1)(2j_d+1)} \frac{1}{(1+\delta_{ab})(1+\delta_{cd})} \right]^{\frac{1}{2}}$$

$$\{(-1)^{\ell_a + \ell_c + j_b + j_d}(j_b -\tfrac{1}{2} j_a \tfrac{1}{2}|J\,0)$$

$$(j_d -\tfrac{1}{2} j_c \tfrac{1}{2}|J\,0)[1-(-1)^{\ell_c + \ell_d + J + T}]$$

$$-(j_b \tfrac{1}{2} j_a \tfrac{1}{2}|J\,1)(j_d \tfrac{1}{2} j_c \tfrac{1}{2}|J\,1)[1+(-1)^{T}]\}$$

$$+B_T\left[2T(T+1)-3\right]\delta_{ac}\delta_{bd}$$

$$(10)$$

Where A_T, B_T is two constants represents a strength interaction of MSDI, $(j -\tfrac{1}{2} j \tfrac{1}{2}|J\,0)$ indicates to Clebsch-Gordan coefficients, and j is angular momentum of nucleon, and J is total angular momentum of two nucleon interaction, and T refers to total isospin produced by isospin coupling of two interacting nucleons. When valence nucleons are in ground state, the formula(10) turns out to be

$$\left\langle j_a\, j_b, JT \left| V_{MSDI} \right| j_a\, j_b, JT \right\rangle_{JT} =$$

$$-A_T \frac{(2j_a+1)(2j_b+1)}{2(2J+1)(1+\delta_{ab})}$$

$$\left\{ \left[(j_a \tfrac{1}{2} j_b -\tfrac{1}{2} | J0) \right]^2 [1-(-1)^{\ell_a+\ell_b+J+T}] + \right. \tag{11}$$

$$\left[(j_b \tfrac{1}{2} j_a \tfrac{1}{2} | J1) \right]^2$$

$$[1+(-1)^T]\Big\} + B_T \left[2T(T+1)-3 \right]$$

When two valence nucleons fall within same level, the previous formula becomes as follows

$$\left\langle j^2, J1 \left| V_{MSDI} \right| j^2, J1 \right\rangle_{JT=1} =$$

$$A_T \frac{(2j+1)^2}{2(2J+1)} (j-\tfrac{1}{2} j \tfrac{1}{2} | J0)^2 + B_T \tag{12}$$

If valence nucleons are pairwise coupled to angular momentum zero, the previous formula becomes after parameter Ω is substituted as follows

$$\left\langle j^2, 01 \left| V_{MSDI} \right| j^2, 01 \right\rangle_{J=0T=1} =$$

$$\frac{1}{2} A_T (2j+1) + B_T = A_T \Omega + B \tag{13}$$

We benefit from following transformation[8]

$$(j\, m\, j\, m' | 00) = (-1)^{j-m} \hat{j}^{-1} \delta_{m,-m'} \tag{14}$$

The value of MSDI strengths can be obtained by fitting with experimental values, it is also approximated in terms of mass number as follows $A_T \approx B_T \approx \dfrac{25}{A} MeV$ [16], so we can rewrite the formula(13) as

$$H^{(1)} \equiv \left\langle j^2, 01 \left| V_{MSDI} \right| j^2, 01 \right\rangle_{J=0T=1}$$

$$= \frac{25}{A} (\Omega+1) \tag{15}$$

The previous formula can also be written in terms of isovector paring strength as

$$H^{(1)} \equiv \left\langle j^2, 01 \left| V_{MSDI} \right| j^2, 01 \right\rangle_{J=0T=1} =$$

$$1.25G(\Omega+1) \tag{16}$$

4. Results

The nuclear binding energies were calculated for some nuclei around the closed core that valance nucleons lie outside the closed cores $^{48}_{20}Ca_{28}$, $^{56}_{28}Ni$ and $^{100}_{50}Sn$.

Thirty-two of them are odd-nuclei and Thirty-two are even - even nuclei depending on the new formula (4), and that is after compensating the equation (5), (7), (9), and (16) in them, and making some calculation to take the following form

$$E = -BE =$$

$$E(CORE) + C_1 n^2 + C_2 n + C_3 \tag{17}$$

where

$$E(CORE[^{48}_{20}Ca_{28}]) = -416.001\,(MeV),\ E(CORE[^{100}_{50}Sn]) = -825.298\,(MeV)$$

and $E(CORE[^{56}_{28}Ni]) = -483.98811\,(MeV)$ [17], C_1, C_2

and C_3 takes the following values

$$C_1 = b + \frac{1}{4}G,\ \ C_2 = a - \frac{1}{2}G(\Omega+11),$$

$$C_3 = \frac{G}{4}\{v(2\Omega-v+2)+5(\Omega+1)\} \tag{18}$$

When nucleons located in ground state, the seniority quantum number takes $v=0$ for even - even nuclei and the value $v=1$ for odd nuclei [8].

Since Ω indicates the maximum number of pairs of nucleons that each level of shell accommodates, so in our case it takes certain values as follows

$$\Omega\begin{cases} 1\ \ for\ A=67\to68,\ A=119\to120 \\ 2\ \ for\ A=49\to52,\ 57\to60,\ 115\to118 \\ 3\ \ for\ A=53\to58,\ 61\to66,\ 109\to114 \\ 4\ \ for\ A=101\to108 \\ 5\ \ for\ A=69\to77 \\ 12\ for\ A=121\to132 \end{cases} \tag{19}$$

The value of isovector paring strength G can be obtained in terms of mass number, then parameter C_1, C_2 and C_3 will be

$$C_1 = b + \frac{5}{A},\ \ C_2 = a - \frac{10}{A}(\Omega+11),$$

$$C_3 = \frac{5}{A}\{v(2\Omega-v+2)+5(\Omega+1)\} \tag{20}$$

When we calculate standard deviation for nuclear binding energy between our model and experimental values by using standard deviation equation

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left[BE_{SM}^i - BE_{exp.}^i \right]^2} \tag{21}$$

We found the standard deviation for studied nuclei are $\sigma = 2.7451(MeV)$ for Calcium isotopes, $\sigma = 6.5758(MeV)$ for Nickel isotopes, and $\sigma = 0.0445(MeV)$ for Tin isotopes.

5. Discussion

To confirm our results, we calculated the values of binding energies of the studied nuclei using the most important used formula by calculated the value of the standard deviation, and compared it with our value.

When we calculate nuclear binding energies using SEMF, which is the most popular formula for finding nuclear binding energies, which is given as [3]

$$BE = a_V A - a_S A^{2/3} -$$

$$a_C \frac{Z^2}{A^{1/3}} - a_{AS} \frac{(A-2Z)^2}{A} \pm \delta \qquad (22)$$

Where $a_V, a_S, a_C, a_{AS}, a_p$ are the coefficients of SEMF, which takes many sets of values. We choose the most common and used ones, which are [18]

$a_V = 15.78(MeV)$, $a_S = 18.34(MeV)$,

$a_C = 0.71(MeV)$, $a_{Sym} = 23.21(MeV)$,

$$a_p = \begin{cases} 12(MeV) & for \quad even-even \\ 0 & for \quad odd-even \end{cases}$$

We found the standard deviation value for studied nuclei by SEMF are $\sigma = 14.3743(MeV)$ for Calcium isotopes, $\sigma = 11.7440(MeV)$ for Nickel isotopes, and $\sigma = 0.1366(MeV)$ for Tin isotopes.

When we calculated nuclear binding energies using INM, which are given by the following formula [4]

$$BE(A,Z) =$$

$$\left[3A - \left(\frac{(N^2 - Z^2) + \delta(N-Z)}{Z} \right) + 3^2 \right] \frac{m_u c^2}{100}, \quad (23)$$

$for \ A > 5$

Where $m_u c^2 = 330(MeV)$ is the nucleon mass, and δ is related to stability of nuclei against beta decays and takes the following two values

$$\delta(N-Z) \begin{cases} 0 & for \quad N \neq Z \\ 1 & for \quad N = Z \end{cases}$$

We found the standard deviation value for studied nuclei by INM are $\sigma = 62.8029(MeV)$ for Calcium isotopes, $\sigma = 54.5307(MeV)$ for Nickel isotopes, and $\sigma = 0.6083(MeV)$ for Tin isotopes.

When we calculated nuclear binding energies using MINM, which are given as formula [5]

$$BE(A,Z) =$$

$$\left[3A - \left(\frac{(N^2 - Z^2) + \delta(N-Z)}{\sqrt{NZ}} \right) + \lambda \right] \qquad (24)$$

$$\frac{m_u c^2}{100}, \quad for \ A > 5$$

Where the parameter λ take the constant value $\lambda = 9$ for $Z \leq 30$, and take the value $0.4Z$ for $Z = 31$ to $Z = 59$.

We found the standard deviation value for studied nuclei by MINM are $\sigma = 33.2596(MeV)$ for Calcium isotopes, $\sigma = 31.2226(MeV)$ for Nickel isotopes, and $\sigma = 0.4394(MeV)$ for Tin isotopes.

Therefore, the value of standard deviation in our model is better than calculated by SEMF, it is also better than calculated by INM and better than calculated by MINM.

This indicates that our inferred formula is better than the most important formulas, which is previously used to calculate nuclear binding energies for studied nuclei.

The binding energies of our model (in black circle), SEMF (in blue inverse triangle), INM (in green diamond), and MINM (in pink square) compared to experimental values (in red star) are shown in figure (1) for Calcium isotopes, figure (2) for Nickel isotopes, and Figure (3) for Tin isotopes.

Also, we calculated a value $\Delta BE = |BE_{(the)} - BE_{(exp.)}|(MeV)$,which represents the difference between calculated binding energies per nucleon and experimental binding energies per nucleon for each studied nuclei.

The $\Delta BE(MeV)$ value in our model are shown in figure (4) for Calcium isotopes, figure (5) for Nickel isotopes, and figure (6) for Tin isotopes, SEMF is shown in a blue inverse triangle, INM is shown in a green diamond, and MINM is shown in the pink square.

4. Conclusion

Depending on the basic assumptions of the Shell Model and by using suitable potentials, we found a new simple formula to calculate nuclear binding energy for some nuclei around the closed core in terms of mass number and number of valence nucleons. We calculated by this formula, the nuclear binding energies of sixty-four nuclei for Calcium isotopes $^{49-58}_{20}Ca$, Nickel isotopes $^{57-78}_{28}Ni$, and Tin isotopes $^{101-132}_{50}Sn$, thirty-two are odd- nuclei and thirty-two are even-even nuclei, which valence nucleons are located outside the closed core, $^{48}_{20}Ca_{28}$, $^{56}_{28}Ni$ and $^{100}_{50}Sn$.

We found the standard deviation between calculated nuclear binding energies by our model is better than the standard deviation calculated by SEMF, it is also better than the value by INM, and by MINM. This indicates that our formula is better than the most important formulas used to calculate nuclear binding energies for studied nuclei. We expect an improvement in the values of the nuclear binding energies of studied nuclei compared to the experimental values when adding another term to mean field potential related to the deformation of a nucleus, especially when the number of valence nucleons increases significantly outside the closed core, as in the case of the last three isotopes $^{130-132}_{50}Sn$. We believe the results obtained from our model are not only simple to understand but also more physical and relatively closer to the experimental data than other models. Other characteristics of nuclei, such as calculating the excitation energy of these nuclei are being studied in the framework of our model.
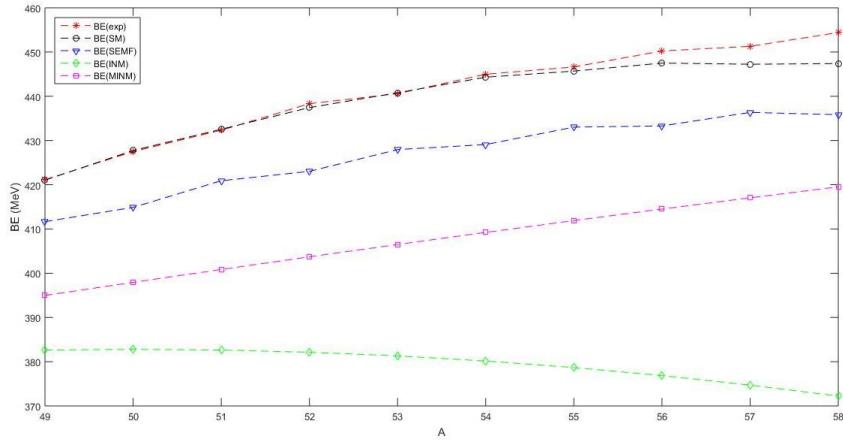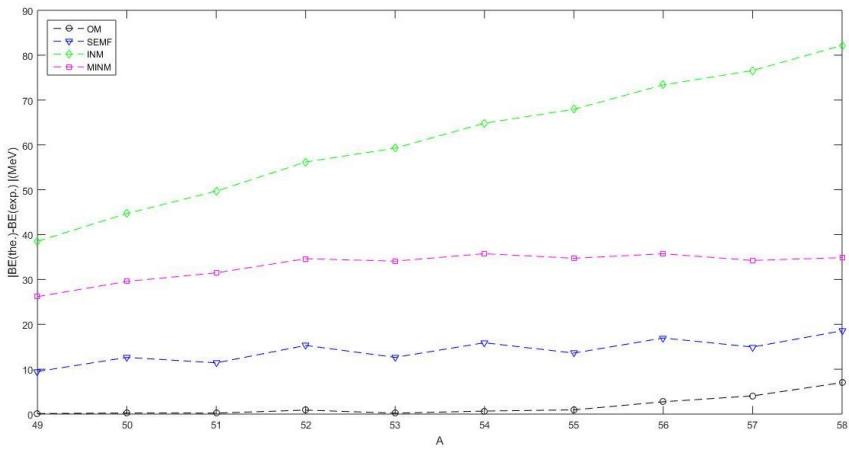
Figure 1. nuclear binding energies calculated in our model of Tin isotopes $^{49-58}_{20}Ca$ (in black circle), SEMF (in blue inverse triangle), INM(in green diamond) and MINM(in pink square) compared to experimental values (in red star).
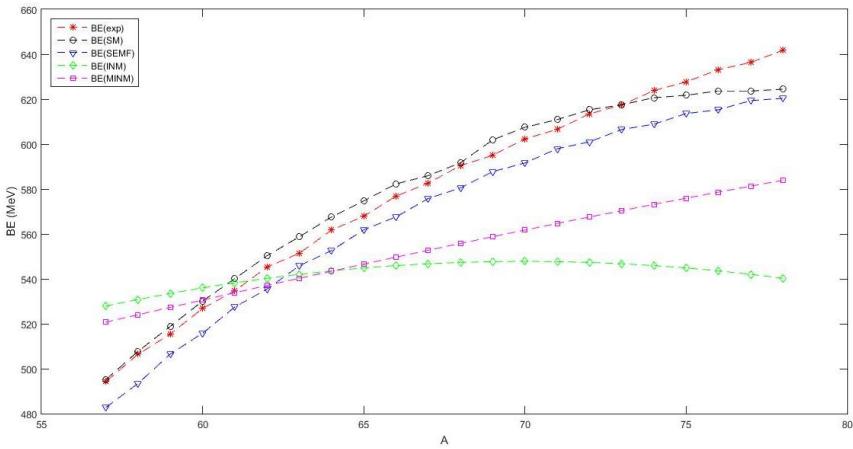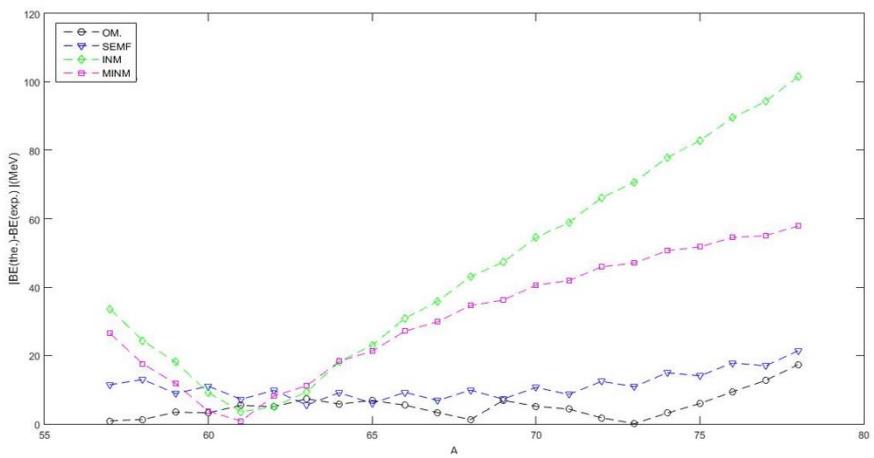

Figure 2. nuclear binding energies per nucleon calculated in our model of Nickel isotopes $^{57-78}_{28}Ni$ (in black circle), SEMF (in blue inverse triangle), INM (in green diamond) and MINM (in pink square) compared to experimental values (in red star).
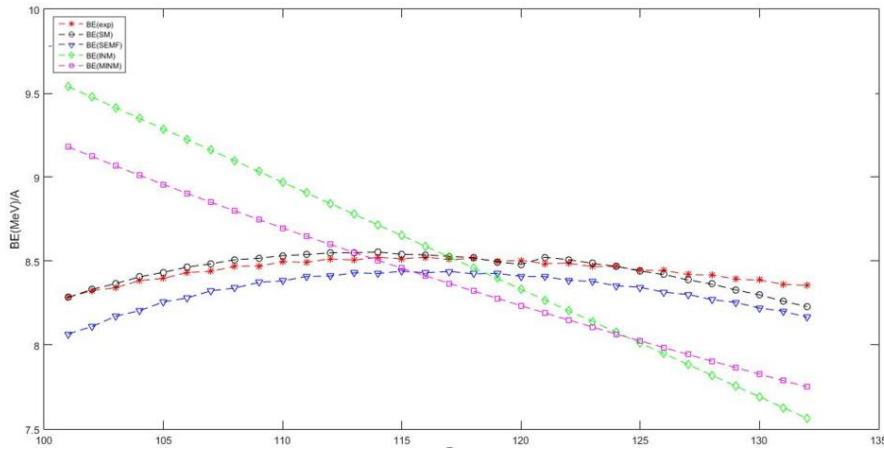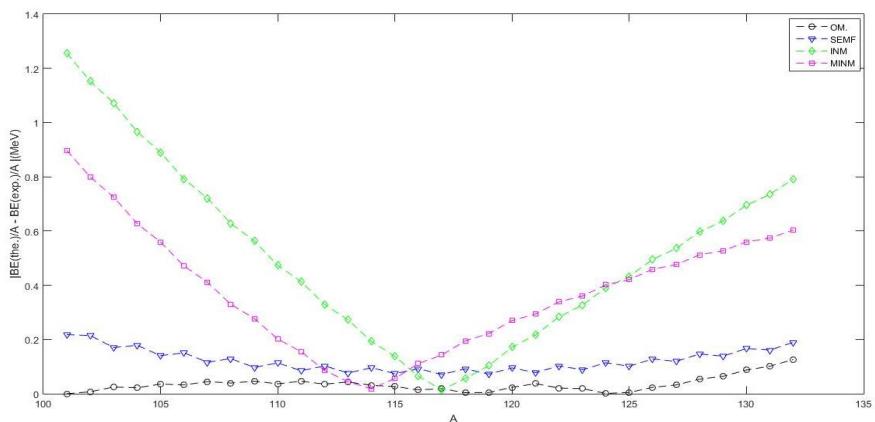

Figure 3. nuclear binding energies per nucleon calculated in our model of Tin isotopes $^{101-132}_{50}Sn$ (in black circle), SEMF (in blue inverse triangle), INM (in green diamond) and MINM (in pink square) compared to experimental values (in red star).

Figure 4. $\Delta BE(MeV)$ Values calculated using our model for Tin isotopes $^{49-58}_{20}Ca$ (in black circle), SEMF (in blue inverse triangle), INM (in green diamond), and MINM (in pink square).

Figure 5. $\Delta BE(MeV)$ Values calculated using our model for Tin isotopes $^{57-78}_{28}Ni$ (in black circle), SEMF (in blue inverse triangle), INM (in green diamond), and MINM (in pink square).

Figure 6. $\Delta BE(MeV)$ Values calculated using our model for Tin isotopes $^{101-132}_{50}Sn$ (in black circle), SEMF (in blue inverse triangle), INM (in green diamond), and MINM (in pink square).

List of abbreviations

SM: Shell Model.
SEMF: Semi-Empirical Mass Formula
INM: Integrated Nuclear Model.
MNIM: Modified Nuclear Integrated Model.
LDM: Liquid Drop Model.

SDI: Surface Delta Interaction.
MSDI: Modified Surface Delta Interaction.
OM: Our Model.

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