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New approach for calculating nuclear binding energies of nickel isotopes $^{57-78}_{28}Ni$ by using the Shell Model

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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 the nuclear binding energies of nickel isotopes $^{57-78}_{28}Ni$. This formula is related only to the mass number of these isotopes and the number of valence nucleons outside the closed core $^{56}_{28}Ni$. When calculating the standard deviation of the experimental data from the theory, we found that our value is better than the value calculated by the Semi-Empirical Mass Formula; it is also better than that calculated by the Integrated Model and calculated by the Modified Integrated Model. This indicates that our inferred formula is better than the most important formulas previously used to calculate nuclear binding energies for our studied nuclei.

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

1. Introduction

One of the most important purposes of nuclear physics is to provide nuclear models that explain the properties and behavior of atomic nuclei. One of the most important nuclear properties is that the density of the nucleus is almost constant, so the size of the 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 the nuclear binding energies of the nuclei were calculated using the Semi-Empirical Mass Formula (SEMF), which is known as the Bethe-Weizsäcke formula [3]. In 2011, a new formula was developed to calculate the values of the nuclear binding energies, which was deduced by Nader Ghahramany and his group [4]. This relation 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 formula is called the Integrated Nuclear Model (INM). Hezekiah K. Cherop and Kapil M. Khanna [5] developed this formula in 2020, and it is called the Modified Integrated Nuclear Model (MINM).

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

On the other hand, the Shell Model developed by Mayer and Jensen was proposed in 1948[6] on the assumption that each nucleon in any nucleus moves independently in a median potential resulting from the rest of the nucleons, which is called the valance field, expressing a "central field.". This field, in addition to potential resulting from the mutual effects between each of the two nucleons of the nucleons, is called the residual potential. 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, predictive power of excited states for nuclei remote from the doubly magic nuclei, and their magnetic moments, but it did not give good value for the nuclear binding energies for most of the nuclei especially far from the stability line. Therefore, in this study, we found a new formula to calculate the values of nuclear binding energy in the function of the mass number and the number of valence nucleons when they are in the ground state, depending on the basic assumptions of the Shell Model and the selection of suitable potentials. We calculated the values of the nuclear binding energies by this new approach of all the isotopes of nickel odd (even - odd) and even (even - even), whose valence nucleons are located between the two magic numbers, $28 < N \leq 50$.

2. 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 the average interaction with the other nucleons in a nucleus. This independent motion can be qualitatively understood from a combination of the weakness of the 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 [7], i.e.:

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

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.:

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

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

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

where $\hat{H}^{(0)}$ is the zero Hamiltonian, a sum of single-particle Hamiltonians that expresses the 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 very large, 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 the many-nucleon system considered, and assumes the existence of a closed core is the closest doubly magic nucleus to the studied nucleus. Therefore, the study is limited to valence nucleons (the nucleons that lie outside the closed core) instead of being between all nucleons.

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

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

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

where $E(CORE) = -BE(CORE)$ is the nuclear binding energy of the closed core, $\bar{\varepsilon}$ the average nuclear binding energy of valance nucleons, and $\hat{n}$is the particle number operator. Now will describe how each term of this equation was calculated.

2.1. Average nuclear binding energy of valance nucleons $\bar{\varepsilon}$

We can obtain the value of average binding energy for each valence nucleon in the ground state by best fitting for the experimental single-particle energies [9]. The valence nucleons in our study fall within the pfgshell, outside the closed core $^{56}_{28}Ni$, which have the following valence levels, respectively [10]:

$$1p_{3/2} = -10.25MeV, 0f_{5/2} = -9.48MeV, 1p_{1/2} = -9.14MeV, 0g_{9/2} = -6.55MeV$$

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

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

where a and b constants that take the following values:

$$a = \text{-}10.94MeV, b = 0.2323MeV$$

2.2. Mean Field Potential

It is the central potential produced by all valence nucleons so that each nucleon of the valence nucleons 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]:

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

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 the mean-field considered, and $G > 0$ is an isovector paring strength, which is given in terms of mass number as follows $G = \frac{20}{A}$[9, 12].

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

$$E_v(N) = -\frac{1}{4}G(N-v)(2\Omega - N - v + 2) \quad (7)$$

where v 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, Nindicates the number of nucleons in the ground state (which represents the number of valence nucleons in our study), and Ω indicates the maximum number of paired pairs that a given level fits into nucleons; it is given by $\Omega = \frac{1}{2}(2j+1)$.

Increasing the number of neutrons$N$over the number of protons$Z$in the nucleus, it decreases their stability. It thus decreases their total nuclear binding energy, so we will add another term to mean field potential (Paring potential) that results from the Symmetry Effect, which takes the following equation [13]:

$$V_{sym} = \sum_{1,2}\frac{t_1.t_2}{A}V_1V_1 \approx 100(MeV) \quad (8)$$

where $t_1$and t_2 are the isospin for two nucleon interactions. Depending on the previous Symmetry potential, the energy from this potential is given by the following equation:

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

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

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

The effect of the residual interaction is only between valence nucleons, and its contribution to the total Hamiltonian is small compared to the mean field potential, so it is treated as a perturbation, and this interaction takes different forms. In this study, we chose the Surface Delta Interaction (SDI) because it is easy to deal with and has a separable potential, which allows 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 is forbidden when collisions occur at the full levels and allows collisions to occur mainly at the valance levels. This interaction was developed by Glaudesmans [15], and is called Modified Surface Delta Interaction (MSDI). The matrix element of residual interaction for one of the interacting valence-nucleon pairs is as follows:

$$\begin{aligned}&\langle j_a j_b, JT|V_{\text{MSDI}}|j_c j_d, JT\rangle_{JT}\\ &= \frac{A_T}{2(2J+1)}\Big[\frac{(2j_a+1)(2j_b+1)(2j_c+1)(2j_d+1)}{(1+\delta_{ab})(1+\delta_{cd})}\Big]^{\frac{1}{2}}\{(-1)^{\ell_a+\ell_c+j_b+j_a}(j_b -\frac{1}{2}j_a\frac{1}{2}|J0)\\ &(j_d -\frac{1}{2}j_c\frac{1}{2}|J0)[1-(-1)^{\ell_c+\ell_d+J+T}] - (j_b\frac{1}{2}j_a\frac{1}{2}|J1)(j_d\frac{1}{2}j_c\frac{1}{2}|J1)[1\\ &\qquad + (-1)^T]\}\\ &\qquad + B_T[2T(T+1)-3]\delta_{ac}\delta_{bd} \quad (10)\end{aligned}$$

where A_T,B_T is two constants represent the strength interaction of MSDI. The symbol $(j -\frac{1}{2}j\frac{1}{2}|J0)$ indicates to Clebsch-Gordan coefficients, and j is

the angular momentum of the nucleon, and J is the total angular momentum of two nucleon interaction, and the symbol T refers to total isospin produced by the isospin coupling of the two interacting nucleons. When the valence nucleons are in the ground state, the formula (10) turns out to be:

$$\langle j_a j_b, JT|V_{MSDI}|j_a j_b, JT\rangle_{JT} = -A_T \frac{(2j_a+1)(2j_b+1)}{2(2J+1)(1+\delta_{ab})}\{\left[(j_a \frac{1}{2} j_b - \frac{1}{2}|J0)\right]^2 [1 - (-1)^{\ell_a+\ell_b+J+T}] + \left[(j_b \frac{1}{2} j_a \frac{1}{2}|J1)\right]^2 [1+(-1)^T]\} + B_T[2T(T+1)-3] \quad (11)$$

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

$$\langle j^2, J1|V_{MSDI}|j^2, J1\rangle_{JT=1} = A_T \frac{(2j+1)^2}{2(2J+1)}(j - \frac{1}{2} j \frac{1}{2}|J0)^2 + B_T \quad (12)$$

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

$$\langle j^2, 01|V_{MSDI}|j^2, 01\rangle_{J=0T=1} = \frac{1}{2}A_T(2j+1) + B_T = A_T\Omega + B \quad (13)$$

We have benefited from the following transformation [8]:

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

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

$$H^{(1)} \equiv \langle j^2, 01|V_{MSDI}|j^2, 01\rangle_{J=0T=1} = \frac{25}{A}(\Omega+1) \quad (15)$$

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

$$H^{(1)} \equiv \langle j^2, 01|V_{MSDI}|j^2, 01\rangle_{J=0T=1} = 1.25G(\Omega+1) \quad (16)$$

3. Calculations and Results

The nuclear binding energies were calculated for the twenty-two nuclei of nickel isotopes that lie outside the closed core $^{56}_{28}Ni$, related to the following mass numbers $A = 57 - 78$. Eleven nuclei of them are odd (even - odd), and eleven nuclei are even (even - even) depending on the new formula (4), and that is after compensating the equations (5), (7), (9) and (16) in them, and making some reforms to take the following form:

$$E = -BE = E(CORE) + C_1 n^2 + C_2 n + C_3 \quad (17)$$

where $E(CORE) = -BE(^{56}_{28}Ni) = -483.98811(MeV)$ [17] , C_1,C_2 and C_3 takes the following values.

$$C_1 = b + \frac{1}{4}G, C_2 = a - \frac{1}{2}G(\Omega+11), C_3 = \frac{G}{4}\{\nu(2\Omega - \nu + 2) + 5(\Omega+1)\} \quad (18)$$

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

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

$$\Omega = \begin{cases} 2 for A = 57 \to 60 \\ 3 for A = 61 \to 66 \\ 1 for A = 67 \to 68 \\ 5 for A = 69 \to 77 \end{cases} \quad (19)$$

The value of the isovector paring strength G can be obtained by fitting with the experimental nuclear binding energies, and its value can also be obtained in terms of mass number, then the parameter C_1,C_2 and C_3 will be

$$C_1 = b + \frac{5}{A}, C_2 = a - \frac{10}{A}(\Omega+11), C_3 = \frac{5}{A}\{\nu(2\Omega - \nu + 2) + 5(\Omega+1)\} \quad (20)$$

Applying the formula (17) to the isotopes of nickel $^{57-78}_{28}Ni$ using the given parameters in the equation (20). We get the nuclear binding energies of these isotopes $B_{SM}(MeV)$ which are shown in Table 1 compared with the values of the experimental binding energies $B_{exp.}$[17]

Table 1: The nuclear binding energies of our calculated nickel isotopes $^{57-78}_{28}Ni$ compared with the experimental values.

Even-Odd- A				Even- Even-A			
A	$B_{SM}(MeV)$*	$B_{exp.}$	$\lvert B_{SM} - B_{exp}$	A	$B_{SM}(MeV)$*	$B_{exp.}$	$\lvert B_{SM} - B_{exp}\rvert$
57	495.1413	494.2430	0.8983	**58**	507.7906	506.4590	1.3316
59	518.8768	515.4580	3.4188	**60**	530.1215	526.8460	3.2755
61	540.1006	534.6660	5.4346	**62**	550.3045	545.2620	5.0425
63	558.7161	551.3840	7.3321	**64**	567.5853	561.7570	5.8283
65	574.7156	567.8550	6.8606	**66**	582.2862	576.8080	5.4782
67	585.9282	582.6150	3.3132	**68**	591.6767	590.4080	1.2687
69	601.8838	594.9940	6.8898	**70**	607.4813	602.3000	5.1813
71	610.8979	606.5640	4.3339	**72**	615.2606	613.4550	1.8056
73	617.4978	617.4090	0.0888	**74**	620.6498	623.8280	3.1782
75	621.7280	627.6890	5.9610	**76**	623.6908	633.1240	9.4332
77	623.6284	636.3330	12.7046	**78**	624.4213	641.7870	17.3657

*The values of our calculated nuclear binding energy (in black) compared to the experimental values (in red) are shown in Figure 1.

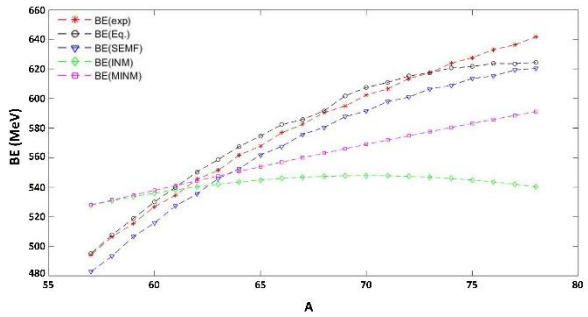

Figure 1: nuclear binding energies of our computed nickel isotopes $^{57-78}_{28}Ni$ (in black) and calculated using the Semi-Empirical Mass Formula (in blue), computed using the Integrated Model (in green) and computed using the Modified Integrated Model (in pink) compared to the experimental values (in red).

When we calculate the standard deviation between our nuclear binding energy values for the studied nuclei and the experimental values, we used the following standard deviation equation:

$$\sigma = \sqrt{\frac{1}{N}\sum_{i=1}^{N\Sigma}\left[\left[BE^{i}_{SM} - BE^{i}_{exp.}\right]^2\right]} \qquad (21)$$

We found that the standard deviation for the studied nuclei is $\sigma = 6.5758$ (MeV), where a value $\Delta B = |B_{eq.} - B_{exp}$ for each studied nuclei is shown (in black) in Figure 2.

When calculating nuclear binding energies for the studied nuclei using the Semi-Empirical Mass Formula, which is the most popular formula for finding nuclear binding energies, which is given as follows [3]:

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

where $a_V, a_S, a_C, a_{AS}, \& a_p$ are the coefficients in the Semi-Empirical Mass Formula, which takes many sets of values; we chose the most common and used ones, which are [18]:

$$a_V = 15.78(MeV), a_S = 18.34(MeV), a_C, = 0.71(MeV), a_{Sym} = 23.21(MeV),$$
$$a_p = \begin{cases} 12(MeV) for even - even \\ 0 for odd - even \end{cases}$$

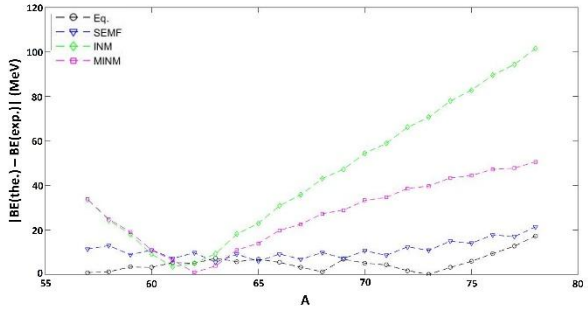

Figure 2: Values for our calculated nickel isotopes $^{57-78}_{28}Ni$ (in black), calculated using the Semi-Empirical Mass Formula (in blue), calculated using the Integrated Model (in green), and computed using the Modified Integrated Model (in pink).

The nuclear binding energies calculated by the Semi-Empirical Mass Formula are shown (in blue) in Figure 1. We found the standard deviation calculated using the Semi-Empirical Mass Formula for the nuclei we studied is$\sigma = 11.7440(MeV)$, where the value $\Delta B(MeV)$ of these nuclei is shown (in blue) in Figure 2.

When we calculate the nuclear binding energies of the studied nuclei using the Integrated Model, which is given by the following formula [4]:

$$BE(A,Z) = \left[3A - \left(\frac{(N^2 - Z^2) + \delta(N-Z)}{Z}\right) + 3^2\right]\frac{m_u c^2}{100}, for\ A > 5 \qquad (23)$$

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

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

where the nuclear binding energies of the studied nuclei calculated by the previous formula are shown (in green) in Figure 1. We found that the standard deviation value calculated for the studied nuclei by the Integrated Model formula is $\sigma = 54.5307\ (MeV)$, where the value $\Delta B(MeV)$ calculated with this formula is shown (in green) in Figure 2.

When we calculate the nuclear binding energies for the studied nuclei using Modified Integrated Model, which are given as follows [5]:

$$BE(A,Z) = \left[3A - \left(\frac{(N^2 - Z^2) + \delta(N-Z)}{\sqrt{NZ}}\right) + \lambda\right]\frac{m_u c^2}{100}, for\ A > 5 \qquad (24)$$

where the parameter λ is taken for $Z \leq 30$ the constant value $\lambda = 9$.

The nuclear binding energies of the studied nuclei calculated by the previous formula are shown (in pink) in Figure 1. We found that the standard deviation value calculated for the studied nuclei by the Modified Integrated Model formula is $\sigma = 31.2226\ (MeV)$, where the value $\Delta B\ (MeV)$ calculated with the last formula is shown (in pink) in Figure 2.

4. Conclusion

Depending on the basic assumptions of the Shell Model and using suitable potentials, we found a new simple formula to calculate the nuclear binding energy in the function of the mass number and the number of valence nucleons.

We calculated by this formula the nuclear binding energies of twenty-two nuclei of nickel isotopes, eleven of which are even-odd and eleven even-even nuclei whose valence nucleons are located outside the closed core $^{56}_{28}Ni$ which have a valence nucleon located between the two magic numbers $28 < N \leq 50$.

We found the standard deviation between our calculated nuclear binding energies and the experimental values is better than the value calculated by the Semi-Empirical Mass Formula, and it is also better than the value calculated by the Integrated Model and calculated by the Modified Integrated Model. This indicates that our deduced formula is better than the most important formulas previously used to calculate the nuclear binding energies of the studied isotopes of nickel.

We expect an improvement in the values of the nuclear binding energies of the studied nuclei compared to the experimental values when taking the residual interaction between all valence nucleons; we also expect an improvement in the values when adding another term to the mean field potential related to the deformation of the nucleus, especially when the number of valence nucleons increases significantly outside the closed core, as in the case of the last three isotopes $^{76,77,78}_{28}Ni$.

After determining the form of the equation for the average nuclear binding energy of valence nucleons, we suggest studying the possibility of applying the formula used in this study to other areas of nuclei. We also suggest studying the possibility of using this formula to calculate the excitation energy of the nuclei.

Data Availability

The datasets used and analyzed during the current study are available from the corresponding author upon reasonable request.

Conflict of Interest

The authors declare no conflict of interest.

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