Particle-hole symmetry parameters for nuclei

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Two parameters, \( \nu \) and \( \zeta \), motivated by particle-hole symmetry are introduced. These parameters are determined using the number of proton (or neutron) particles and holes counted from neighboring shell closures. The new parameters can be used to evaluate particle-hole and proton-neutron symmetries of adopted \( B(E2) \) values, which indicate that both symmetries are approximate for \( A \gtrsim 100 \). The combined symmetries motivate empirical fits of binding energies and the energy ratio \( E(4^+_1)/E(2^+_1) \). A global binding energy fit consisting of a traditional liquid droplet and one new shell term, comprised of a function of \( \nu \) and \( \zeta \), reproduces the experimental binding energies of 2353 nuclei with an r.m.s. standard deviation of 1.55 MeV.

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I. INTRODUCTION

Electron-hole symmetry has been used to model half-filled semiconductor systems, e.g. [1, 2]. This symmetry is often used as a simplification by treating the lack of an electron below the Fermi surface and particle above it, similarly [3]. In this paper, particle-hole symmetry is invoked to generate parameters for protons and neutrons. These parameters have various possible uses for the modeling features related to shell structure.

Shell structure in nuclei is analogous to atomic shell structure which is the basis for the layout of the periodic table [4]. Nuclear shell structure was first seen in the large number of stable nuclei with a given magic number [5], that are now known to be 2, 8, 20, 28, 50, 82, (126) for neutrons or protons. Experimentally measured energies of excited states [6], transition rates [7], and other related properties associated with the shape of a nucleus, indicate shell structure as has been shown more than 60 years ago in Refs. [8-10].

The Interacting Boson Model (IBM) [11], which treats pairs of valence protons and neutrons as bosons, sets a excellent foundation for modeling shell structure. There are several IBM based formalisms, that are correlated to shell structure. These contain operators exhibiting various symmetries and are superior to simply counting the number of protons (Z) or neutrons (N), see e.g. [12] or [13]. A strength of the IBM is that it provides the ability to classify nuclei based properties like the low lying states [14]. A new parameterization motivated by particle-hole symmetry is introduced in the following section that is seemingly comparable to two bodies of work that exist within the framework set by the IBM.

The first is the promiscuity factor \( (P) \) has proven to be arguably one of the best examples of an IBM based parameter used to model experimental observation. It is defined as \( P = \frac{N_p N_n}{N_{p+N_n}} \), where \( N_p \) and \( N_n \) are counted as the numbers of particles or holes for protons or neutrons depending on if the shell is less than or more than half full, respectively [15]. \( P \) serves as a measure of the average number of proton-neutron interactions per valence nucleon.

The ratio of excited states \( R_{4/2} = E(4^+_1)/E(2^+_1) \) in even-even nuclei is seen to vary depending on the shape of the nucleus. Small values of \( R_{4/2} \) occur for closed shell, spherical nuclei, and the larger values occur for well deformed nuclei in mid-shell regions. The \( P \) factor has been shown to correspond to small values for \( R_{4/2} \) near closed shells when \( P \) is small, and \( R_{4/2} \) increases at around \( P \approx 3 - 4 \) corresponding to the onset of deformation [16].

Shell structure can also be seen in experimental binding energies where nuclei with a closed shell are often more tightly bound together than are neighboring nuclei with no closures. Furthermore, nuclei with closed shells of both protons and neutrons are even more tightly bound than those with just one shell closure. The \( P \) factor is insufficient in describing this because it is unable to distinguish between singly and doubly magic nuclei.

Van Isacker has been able to reproduce shell seen in binding energies by introducing two IBM based terms proportional to \( (N_p + N_n) \) and \( (N_p + N_n)^2 \) [16]. The resulting fits consisting of just eight adjustable parameters were able reproduce experimental binding energies with a root mean squared standard deviation \( \sigma \) of 1.4 MeV. After modifying the location of three shell closures a fit with \( \sigma = 1.2 \) MeV can be made.

In this work shell corrections for \( R_{4/2} \) and binding energies will be introduced which make use of particle-hole symmetry. Section [17] discusses observations of particle-hole symmetry in nuclei. In Sections [18] and [19], the two new particle-hole symmetry parameters are defined and alternative representations are discussed. Section [20] explores the extent to which particle-hole and proton-neutron symmetries exist in \( B(E2) \) values. Section [21] makes use of the combined symmetries to provide empirical fits of binding energies and \( R_{4/2} \). The final section contains a brief summary.
II. PARTICLE-HOLE SYMMETRY IN NUCLEI

Particle-hole symmetry in nuclei is not exact. Furthermore it does not come out inherently when using the number of protons and neutrons because all nuclear shells, even adjacent shells, differ in length. The inherent exactness of this symmetry, or lack thereof, cannot be fixed, however the lengths of shells can be accounted for. The degree to which particle-hole symmetry exists can be demonstrated looking at experimentally measured quantities like the energy of the $2^+_1$ state.

Nuclei with at least one shell closure can be seen to have larger $2^+_1$ energies. The $2^+_1$ energies are further enhanced if the nucleus is doubly magic. This phenomena is demonstrated in the top panel of Fig. 1 which shows energy of the $2^+_1$ state for five chains of isotones. Particle-hole symmetry is invoked in order to simplify this figure.

Particle-hole symmetry has been used in nuclear structure before. Heyde et al. used it to group adjacent nuclei which have the same number of valence protons or neutrons [17]. Intruder spin and intruder analog states were introduced as a tool to help one understand collective structure built on the low lying $0^+_1$ intruder state near closed shells.

Particle-hole conjugation has been used by Bell [18] in the context of the shell model and extended further by Müller-Arke [19]. Davis et al. have employed a measure of the deviation from particle-hole conjugation symmetry of the form:

$$\rho = \frac{|E_{pp} - E_{hh}|}{E_{pp} + E_{hh}},$$

(1)

to compare F-spin multiplets [20]. Here $E_{pp}$ corresponds to the energy of an excited state in a nucleus with valence protons and neutrons, and $E_{hh}$ corresponds to nuclei with proton and neutron holes. The finding was that pairs of $E(2^+_1)$ and $E(4^+_1)$ states in an F-spin multiplet deviate from one another on the order of $10 - 20\%$ [20].

Shell model calculations by Volya may provide insight on the reason that this is not a perfect symmetry. In that work three body interactions are believed to cause a small $\approx 10\%$ lack of particle-hole symmetry for an $f_{7/2}$ shell [21].

The observation of a relatively small lack of particle-hole symmetry motivates the creation of particle-hole parameters with which model shell phenomena can be fit, modeled and predicted.

III. PARTICLE-HOLE SYMMETRY PARAMETERS

The number of valence nucleons has been long known to be related to collectivity and other nuclear properties. The new parameterization begins with some definitions that are introduced in the well known proton-neutron version of the IBM often referred to as the IBM-2 [22].
Bosons comprised of the number of pairs of valence proton and neutron are used [23]. The corresponding parameters:

\[ N_\pi = \frac{1}{2}(Z - Z_{\text{min}}), \text{ and } N_\nu = \frac{1}{2}(N - N_{\text{min}}), \]

(2)

which depend on magic numbers below or at the respective \( Z \) or \( N \) values, denoted \( Z_{\text{min}} \) and \( N_{\text{min}} \).

Valence bosons holes can be similarly defined as:

\[ \bar{N}_\pi = \frac{1}{2}(Z_{\text{max}} - Z), \text{ and } \bar{N}_\nu = \frac{1}{2}(N_{\text{max}} - N), \]

(3)

which also depend on the magic numbers at the end of a shell. Inherently asymmetric particle-hole parameters, motivated by Eq. (1), are defined for neutrons and protons, separately as:

\[ \nu = \frac{N_\nu - \bar{N}_\nu}{N_\nu + \bar{N}_\nu}, \]

(4)

and

\[ \zeta = \frac{N_\pi - \bar{N}_\pi}{N_\pi + \bar{N}_\pi}. \]

(5)

Particle-hole symmetry can be restored when the absolute value or even powers of these parameters are used.

The resulting parameters create a straight line with extrema at shell closures. More specifically, these parameters have a value of negative one at the beginning of a shell, positive one when at the end and cross through zero in the middle.

A comparison of the \( E(2^+_1) \) as a function of the promiscuity factor and the absolute value of the new proton parameter are also provided in Fig. 1. The \( P \)-factor is shown here to be poorly correlated with the excitation energy for nuclei with one shell or more closures because \( P = 0 \). Comparable values of \(|\zeta|\) correspond to similar \( E(2^+_1) \) values for a given chain of isotones. This observation is evidence for particle-hole symmetry. Furthermore, there is also a separation of the nuclei with a closed shell of neutrons with \(|\nu|=1\), compared to those which are mid-shell with \( \nu=0 \). The energies \( 2^+_1 \) of nuclei with the same value of \(|\nu|\) for a given isotone are generally within 10\% of each other, and groups of nuclei with a constant value of \(|\nu|\) and the same value of \(|\zeta|\) are typically within 20\% of one another.

\section{IV. ALTERNATIVE REPRESENTATIONS}

F-spin is a scheme within the IBM that can also be used to generate \( \nu \) and \( \zeta \). This also involves a classification of variables based on functions of the number of valence protons and neutrons.

Two quantities related to the total number of valence bosons:

\[ N_T = N_\pi + N_\nu \]

(6)

and the third projection of the F-spin:

\[ F_Z = \frac{1}{2}(N_\pi - N_\nu), \]

(7)

which commute with one another [13]. The resulting \( F_Z \) multiplets consist of nuclei which vary by an alpha particle. The \( F_Z \) parameter has been shown to allow for the prediction of various properties, from masses e.g. [20], to spectroscopic factors e.g. [21].

There are also hole equivalents to \( F_Z \) and \( N_T \):

\[ \bar{N}_T = \bar{N}_\pi + \bar{N}_\nu, \text{ and } F_{\bar{Z}} = \frac{1}{2}(\bar{N}_\pi - \bar{N}_\nu), \]

(8)

with \( F_{\bar{Z}} = -F_Z \), if the protons and neutrons are in the same shell. A combination of these, and a few other related parameters have been used to describe energy levels in the ground state band of even-even nuclei [24].

The particle-hole parameters can be defined in terms of these F-spin related variables as:

\[ \nu = \frac{N_T - \bar{N}_T - 2F_Z + 2\bar{F}_Z}{N_T + N_T - 2F_Z - 2\bar{F}_Z} \]

(9)

and

\[ \zeta = \frac{N_T - \bar{N}_T + 2F_Z - 2\bar{F}_Z}{N_T + N_T + 2F_Z + 2\bar{F}_Z}. \]

(10)

The particle-hole parameters can also be generalized to include nuclei with odd numbers of nucleons. This can be done by defining them in terms of proton and neutron numbers and the neighboring magic numbers, instead of using valence bosons, using:

\[ \nu = \frac{2N - N_{\text{max}} - N_{\text{min}}}{N_{\text{max}} - N_{\text{min}}} \]

(11)

and

\[ \zeta = \frac{2Z - Z_{\text{max}} - Z_{\text{min}}}{Z_{\text{max}} - Z_{\text{min}}}. \]

(12)

where again the maximum and minimum values are defined by the nearest magic numbers.

Because the lack of experimental evidence of shell closures above \( Z = 82 \) and \( N = 126 \), a theoretical calculation was used to predict the next major shell closure. The use of the magic number 196 for neutrons results from a Nilsson level calculation based on parameters from [20]. In the calculation a substantial gap in the spherical levels was determined to exist at 184. A gap roughly two times larger was found at 196, which indicates that the 184 gap, which has been suggested elsewhere in the literature e.g. [27], should be treated as a sub-shell closure and for this reason the value with the larger gap at 196 is used. The proton gap at 126 also results from the calculation and is comparable to the observed neutron shell closure at the same number. Therefore, for protons, \( Z_{\text{min/max}} = [2, 8, 20, 28, 50, 82, 126] \) has been used and for neutrons, \( N_{\text{min/max}} = [2, 8, 20, 28, 50, 82, 126, 196] \).
V. TEST OF PARTICLE-HOLE AND PROTON-NEUTRON SYMMETRIES

Some features of nuclei in neighboring shells can be inferred from the bottom panel of Fig. 1. Take for example, the N=28 shell which corresponds to $|\nu|=1$. Based on the observations from the figure, it may be expected that any isotones with $\zeta = 0$ should have a $E(2^+)$ of around 1.25 MeV and for $|\zeta|=1$ this energy should be approximately 4 MeV. $^{52}\text{Cr}$ is one case, of an N=28 isotope with $\zeta = 0$, which has $E(2^+_1) = 1.4$ MeV. There are two $|\zeta|=1$ cases $^{48}\text{Ca}$ and $^{56}\text{Ni}$, with $2^+_1$ energies at 3.8 and 2.7 MeV, respectively.

Similarly, the transition probabilities of some particle-hole symmetric nuclei included in Table I. These are intended to demonstrate the extent to which this symmetry exists in the adopted $B(E2: 0^+_1 \rightarrow 2^+_1)$ values from Ref. [7]. Each row contains a four-fold multiplet with the same $|\nu|$ and $|\zeta|$. A demonstration of two sample multiplets are given in Fig. 2. In other words, the rows contain pairs of isotones and isotopes at the same distance from the respective shell closures. The coefficient of variation ($c_{B(E2)}$) can be used to compare $B(E2)$ values among the particle-hole symmetric nuclei. It is defined as:

$$c_{B(E2)} = \frac{\sigma_{B(E2)}}{\bar{B}(E2)},$$

where $\bar{B}(E2)$ is the mean transition probability and $\sigma_{B(E2)}$ is the standard deviation about that mean. The coefficient of variation metric demonstrates that on average the symmetry holds up to $c_{B(E2)} = 10\%$ for the nuclei in this region.

An additional proton-neutron symmetry may exist as well, as has been argued for many years, see e.g. [29]. This can be tested by examining the $B(E2)$ values for two groups of four-fold multiplets where $|\nu|$ and $|\zeta|$ are swapped such as the two multiplets shown in Fig. 2. Table 1 contains thirteen such octets with combined particle-hole and proton-neutron symmetric nuclei. These octets have on average $c_{B(E2)} = 11\%$.

The resulting octets can be used predict unmeasured observables in a similar manner as other near neighbor comparison techniques, such as Garvey-Kelson relations [29]. In this case, the mean $B(E2)$ value for a multiplet could be used to predict the remaining unmeasured $B(E2)$ values. For example, there is one octet shown in Table I with three known adopted $B(E2)$ values for $^{112,120,144}\text{Sn}$. These could be used to predict that $^{112}\text{Sm}$ will have $B(E2) \approx 0.235 e^2b^2$.

Alternatively, chains of nuclei can also be fit using some combination of polynomial expansions in $\nu$ and/or $\zeta$, in a manner similar to the Isobaric Mass Multiplet Equation (IMME) [30]. However, instead of using multiple coefficients to fit a dozen or so nuclei, as is done with the IMME, an attempt is made to provide global fits with the minimum number of fit coefficients using the new parameterization.

VI. GLOBAL FITS BASED ON $\nu$ AND $\zeta$

The approximate proton-neutron symmetry as seen in transition rates can be used to justify a global fit consisting of the same leading powers of $\nu$ and $\zeta$. Further, combinations of even powers of these parameters invokes particle-hole symmetry. One combination that satisfies these two criteria is of the form $(\nu^4 + c\nu^2\zeta^2 + \zeta^4)$, where $c$ is a constant. In the following subsections this combination accounts for shell corrections.

A. $4^+_1/2^+_1$ Ratios

The top panel of Fig. 3 shows some noticeable periodicity for the $R_{4/2}$ values which come to a maximum value...
The difference $\Delta R_{4/2} = R_{4/2, \text{exp.}} - R_{4/2, \text{fit}}$ is shown in the bottom panel of Fig. 3 can be used to probe where there are irregularities which can be used as an indicator of sub-shell structure.

The $R_{4/2}$ metric provides insight on cases such as the N=32 sub-shell closure that corresponds to a low $2^+_1$ excitation seen experimentally for titanium and chromium 54. This sub-shell closure corresponds to a low $4^+_1$ state in titanium, but not in chromium as can be inferred from Fig. 3 where $^{54}\text{Ti}$ deviates from the trend but $^{50}\text{Cr}$ does not. Furthermore, $\Delta R_{4/2}$ can be used to demonstrate that the $R_{4/2}$ for nuclei including $^{30}\text{Ne}$, $^{32}\text{Mg}$, $^{32}\text{S}$, $^{38,50}\text{Ca}$, $^{54}\text{Ti}$, $^{66}\text{Ni}$, $^{72}\text{Kr}$, $^{88}\text{Sr}$, and $^{96,98}\text{Zr}$ deviate substantially from the globally fit trends. In some cases this may suggest that further measurements are needed.

B. Binding Energies

Semi-empirical binding energy formulas involve the treatment of the nucleus as a charged droplet of nuclear matter 32. Typically, semi-empirical formulas lack considerations for shell structure. The semi-empirical formula from Myers and Swiatecki 33 is used as a starting point for a binding energy fit. The form of the Coulomb, pairing and symmetry energy terms have been modified and the shell term is generated using Eqs. (11) and (12).

A five term fit used to model “macroscopic” binding energy contributions which is of the form:

$$B_{\text{mac., fit}} = (a_v A + a_s A^{2/3})(1 + \kappa T_Z(T_Z + 1)A^{-2})$$

$$+ (a_c Z(Z - 1) + \Delta)A^{-1/3},$$

where $A = N + Z$ is the total number of nucleons and $T_Z = (N - Z)/2$ is the isospin projection. The coefficient $a_v$ corresponds to the volume term, $a_s$ is the surface term, $\kappa$ is the asymmetry scaling, $a_c$ is the Coulomb contribution and $\Delta$ is the pairing contribution which is $\Delta = +a_p$ if the nucleus is even-even, $\Delta = -a_p$ if odd-odd, and $\Delta = 0$ otherwise. The use of a pairing term proportional to $A^{-1/3}$ provides a minor improvement globally on the order of 20 keV compared to the more common $A^{-1/2}$ dependence. The $Z(Z - 1)$ expansion results from the semi-classical treatment of the protons which doesn’t allow for self-repulsion. The expansion of the form $T_Z(T_Z + X)$ is consistent with experimental observations for $N \approx Z$ nuclei 34, with deviations from $X = 1$ likely resulting from changes in level density near the Fermi surface as discussed in Ref. 35. A sixth shell term roughly accounts for these effects.

To allow for better understanding of the shell term, the macroscopic binding energy fit can be removed from the experimental binding energies leaving just the “experimental microscopic” contribution:

$$B_{\text{mic., exp.}} = B_{\text{exp.}} - B_{\text{mac., fit}}.$$
FIG. 3: (Color on-line) The top panel contains the experimental $R_{4/2}$ values from \([6]\). The middle panel shows the two parameter fit to the $R_{4/2}$ using Eq. (14). The bottom panel shows the difference between the top and middle panels. Please note that the range shown on the bottom panel is $2/3$ the range of the panels above.

which is comparable to the use of semi-empirical microscopic masses in Ref. \([36]\). The periodicity of the microscopic binding energy components has long been known, see e.g. \([33]\), and can be seen in the top panel of Fig. 4. These variations are typically thought of as result of deformation effects, the related level density near the Fermi surface and pairing effects.

The "microscopic" binding energy component can be modeled by a function that is large if one shell is closed and about four times larger if both shells are closed. The combination $(\nu^2 + \zeta^2)^2 = \nu^4 + 2\nu^2\zeta^2 + \zeta^4$ satisfies this requirement because the sum of $\nu^4$ and $\zeta^4$ is twice as large for a doubly magic nucleus as it is for a singly magic nucleus. Adding in a cross term of $2\nu^2\zeta^2$ causes the value at with two shell closures to be the desired value. This

FIG. 4: (Color on-line) The top panel contains the experimental "microscopic" binding energy component determined using Eq. (16) along with modified data from \([38]\) where the electron binding energy contribution has been removed. The middle panel has the theoretical shell contribution fit using Eq. (17) and the Fit I coefficients in Table III. The bottom panel is the difference between the experimental and theoretical values. Please note that the range shown on the bottom panel is $1/3$ the range of the panels above.
TABLE III: Binding Energy Coefficients and Standard Deviation.

| Fit   | $a_v$   | $a_s$   | $\kappa$ | $a_c$ | $a_p$ | $a_{shell}$ | $\sigma$ |
|-------|---------|---------|----------|-------|-------|-------------|-----------|
|       | (MeV)   | (MeV)   | (MeV)    | (MeV) | (MeV) | (MeV)       | (MeV)     |
| I     | 15.91   | -18.63  | -7.26    | -0.7203 | 5.13 | 2.68       | 1.71      |
| II    | 15.79   | -18.12  | -7.18    | -0.7147 | 5.49 | 0          | 2.65      |
| III   | 15.88   | -18.53  | -7.25    | -0.7184 | 0   | 2.70       | 1.88      |
| IA    | 15.91   | -18.65  | -7.26    | -0.7197 | 5.00 | 2.91       | 1.55      |

sets the form of the shell correction as:

$$B_{mic, fit} = a_{shell}(\nu^4 + 2\nu^2\zeta^2 + \zeta^4), \quad (17)$$

which is fit using one new coefficient $a_{shell}$. The structure of this function is demonstrated in the middle panel of Fig. 4.

The corresponding best fit coefficients are given in Table III listed as Fit I. The fit was determined by first performing a $\chi^2$ minimization using OriginPro 9.0 [37] followed by a standard deviation minimization. The six terms generate a fit that has a value of $\sigma = 1.71$ MeV for 2353 nuclei in the range $N > 8$ and $Z > 8$ found in the 2012 Atomic Mass Evaluation [38] with the electron binding energy contribution removed using Eqn. (A4) from Ref. [39]. The difference $\Delta B = B_{exp.} - B_{fit}$, where $B_{fit} = B_{mac, fit} + B_{mic, fit}$, shown in the bottom panel of Fig. 4 indicates where the fit is less accurate.

To compare the importance of shell and pairing effects on the binding energy, fits were also performed in which either the shell or pairing coefficients were set equal to zero and the remaining five terms were adjusted. For Fit II with $a_{shell} = 0$, the best fit results in a standard deviation of $\sigma = 2.65$ MeV as opposed to Fit III with $a_p = 0$, the best fit results $\sigma = 1.88$ MeV. This result indicates that the pairing gap, which is often included in semi-empirical mass formulas, is far less important for modeling binding energies than the shell term. The coefficients corresponding to these fits have also been included in Table III.

Additional improvement can be made to the binding energy fit if the N,Z=20 shell closures are replaced by N,Z=14 and the Z=114 is used in place of Z=126 as has been suggested by Dieperink and Van Isacker [40]. These changes in magic numbers require only a slight modification of some of the fit coefficients, to create the new best fit with a standard deviation of $\sigma = 1.55$ MeV. The corresponding coefficients are included in Table III as Fit IA, where the A denotes the use of alternative shells.

VII. SUMMARY

The $\nu$ and $\zeta$ parameters have been introduced which are preferable to simply using $N$ and $Z$, in providing a basic model of shell effects, because they make all shells comparable. The parameters can be used to predict observables based on the behavior of nuclei at comparable locations in the same shell or in adjacent shells. Particle-hole and proton-neutron symmetries can be easily explored using these parameters. Relatively good ($\approx 10\%$) agreement has been shown for the $B(E2)$ values of $A \geq 100$ nuclei within the four and eight-fold symmetric groupings. Whereas a similar evaluation of the $B(E2)$ values for lower mass octets, between 28 $\leq N,Z \leq 50$, have on average $c_{B(E2)} \approx 25\%$. This is the result of substantial sub-shell structure in lower mass nuclei. In this region the $N = 40$, and $Z = 40$ sub-shell closures are problematic because they occur immediately next to the expected mid-shell position at $N = 39$ and $Z = 39$. Further testing and prediction of other nuclear properties is planned for the future.

As opposed to focusing on multiple parameter fits, even powers of these parameters have been combined to model global features of binding energies and $R_{4/2}$ over the chart of the nuclides. After fixing the respective $\nu^2\zeta^2$ cross terms, only one fit parameter is required.

Overall, the $P$ factor is the preferable variable to use with $R_{4/2}$, as opposed to Eq. (14), because of its proven success and relative ease of use. It should be noted, however, that $P$ cannot provide a sufficient simple description of the constitute $E(2^+_1)$ and $E(4^+_1)$, $B(E2)$ values or binding energies because it doesn’t distinguish between singly and doubly magic nuclei. Fits using $F_Z$ or other related quantities which do make the appropriate distinction, often require multiple fit coefficients, see e.g. [20] or [25].

For binding energies, the inclusion of a single, relatively simple, shell term has reduced the standard deviation of the fit by more than 1 MeV. The new shell term has been observed to play a substantially more critical role in the given binding energy fits than the commonly included pairing term does.

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