Correction to Relativistic Mean Field binding energy and $N_p N_n$ scheme

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Abstract

The differences between the experimental and Relativistic Mean Field binding energies have been calculated for a large number of even-even nuclei from $A = 50$ to 220. Excluding certain mass regions, the differences, after suitable corrections for particular isotope chains, are found to be proportional to the Casten factor $P$, chosen as a measure of n-p interaction strength in a nucleus. Results for even-Z odd-N nuclei are also seen to follow the same relation, if the odd-even mass difference is taken into account following the semiempirical formula. This indicates that the n-p interaction is the major contributor to the difference between the calculated and the experimental binding energies.

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It is well known that simplified parametrization of various nuclear quantities are obtained as functions of $N_p N_n$, the product of effective number of valance particles (or holes) \cite{1}. Essentially this simple product is seen to represent integrated n-p interaction strength and to bear smooth relationships with the observables. The correlations beyond mean field results are due principally to residual two body interaction. In a mean field calculation, the residual interaction between similar nucleons is described by the pairing force. However, the calculations usually ignore the residual n-p interaction.
For a chain of isotopes, the difference between the experimental and the calculated binding energies may be a measure of the integrated strength of n-p interaction in a particular nucleus and vary smoothly with certain simple functions of \(N_p\) and \(N_n\).

Various quantities such as deformation and \(B(E2)\) values \([2, 3, 4]\), rotational moments of inertia in low spin states in the rare earth region \([5]\), ground band energy systematics \([6]\), core cluster decomposition in the rare earth region \([7]\), and properties of excited states \([8, 9]\) have been found to follow certain simple trends when expressed as a function of the product of \(N_p\) and \(N_n\) or certain simple functions of the above two quantities. In the present work, we attempt to show that binding energy corrections to Relativistic Mean Field (RMF) calculations can also be expressed in a similar fashion.

However, not all the difference between the experimental and the theoretical binding energies can be ascribed to the effect of n-p interaction. To extract this effect, we have selected the isotope for each \(Z\) with magic neutron number \(i.e.\) isotopes with no valence n-p pairs. In these nuclei, we expect the effect of n-p interaction to be small and the difference between the experimental and calculated binding energies to be due to all the other effects combined. The difference between theory and experiment in the change in the binding energy from the isotope with \(N_n = 0\) for a particular \(Z\) is taken as a measure of the contribution of \(N_p, N_n\) interaction and expressed as \(\Delta_{\nu\pi}\). Thus we write

\[
\Delta_{\nu\pi}(Z, N) = A(B_{th}(Z, N) - B_{ex}(Z, N) + B_{corr}(Z))
\]

where, \(B_{th}\) and \(B_{ex}\) are respectively the theoretically calculated and experimentally measured binding energies per nucleon and, \(A = Z + N\), the mass number. We have defined \(B_{corr}(Z) = B_{ex}(Z, N_0) - B_{th}(Z, N_0)\), \(N_0\) being a magic number. Depending on the neutron core, the quantity \(B_{corr}(Z)\) may have more than one value. For example, for Cd isotopes with \(N \geq 66\), one has to use the experimental and theoretical binding energy values for the isotope with \(N = 82\) while for the lighter isotopes, one uses the values for \(N = 50\). Obviously \(\Delta_{\nu\pi}(Z, N)\) vanishes for magic \(N\). The experimental binding energy values are from Ref. [10].

There exist different variations of the Lagrangian density as well as a number of different parametrization in RMF. The Lagrangian density FSU Gold [11], which involves self-coupling of the vector-isoscalar meson as well as
coupling between the vector-isoscalar meson and the vector-isovector meson, was earlier employed in our study of proton radioactivity\cite{12}, alpha radioactivity in heavy and superheavy nuclei\cite{13, 14}, and cluster radioactivity\cite{15}. In Ref \cite{14}, spectroscopic factors and $\Delta_{\nu\pi}$ values in actinides were seen to follow a certain pattern. In that region the only appropriate major doubly closed shell nucleus is $^{208}\text{Pb}$ and it was necessary to employ subshell closures. In the present work we look for a more robust systematics in $\Delta_{\nu\pi}$, valid in a large mass region and dependent only on the known major shells. The FSU Gold Lagrangian density seems very appropriate for a large mass region \textit{viz.} medium mass to superheavy nuclei. We have solved the equations in co-ordinate space. The strength of the zero range pairing force is taken as 300 MeV-fm for both protons and neutrons. We have also checked our conclusions using the density NL3\cite{16} which gives very similar results. Unless otherwise mentioned, the results refer to the calculations with FSU Gold.

In Fig. 1, we plot the results of a large number of even-even nuclei, lying between mass 50 and mass 220 as shown in Table 1. The results have been plotted only for the nuclei whose experimental binding energies are available. Certain isotope chains, \textit{e.g.} the chains of isotopes for $Z = 64 - 70$ and $88 \leq Z \leq 92$, do not follow the pattern that we have observed in the nuclei of Table 1 and have been discussed later. Values of $\Delta_{\nu\pi}$ could not be calculated for certain nuclei as experimental binding energies for the isotopes with $N_n = 0$ are not available and have been treated separately. In the left hand plot of Fig. 1, we have plotted the quantity $\Delta_{\nu\pi}$ as a function of number of $N - N_{\text{core}}$, where $N$ is the number of neutrons and $N_{\text{core}}$ is the nearest closed neutron shell. It is difficult to see a pattern for the different mass regions, or even, within a mass region. However, we find that the points lie very close to a straight line if plotted as a function of the Casten factor, $P = N_pN_n/(N_p + N_n)$ which has been widely used as a measure of the integrated n-p interaction strength. In fact the quantity may be expressed as simply proportional to $P$. One can fit a straight line

$$\Delta_{\nu\pi} = aP$$

with $a = -2.148 \pm 0.029$ with rms deviation 1.15 MeV. The fitting does not include the values for nuclei with $P = 0$ which are defined to be zero. The fitted line has been shown in the right panel of Fig. 1. In a few cases, to improve the results, certain shell closures, which are not apparent, are chosen. For example, in lower $Z$ nuclei among those represented by ‘C’, proton shell
closure is 38, and not 20 or 28. However, in most situations, the choice of the magic number is self-evident.

The theoretical values may be corrected using the fitted straight line in eqn. (2) enormously improving the agreement between the calculated and experimental binding energy values. It is worth noting that that the present mean field calculation does not take deformation into account and is expected to underpredict the binding energy far away from the closed shell. However, with this correction from eqn. (2), it is possible to obtain an agreement comparable to or even better than the values calculated using a deformed mean field approach.

It is possible to extend our calculation to situation where the experimental binding energy for the isotope with magic neutron number is not known. The nuclei, with the proton and neutron magic numbers chosen to calculate \( N_p \) and \( N_n \) given in parentheses, \(^{112-120}\text{Pd}(50,82), ^{110-116}\text{Te}(50,50), ^{112-118}\text{Xe}(50,50), ^{114-120}\text{Ba}(50,50)\) have been studied. We also include all the nuclei with \( N \geq 106 \) and \( Z = 70-78 \), all with the same magic core (82,126), whose experimental binding energies are known i.e. \(^{176,178}\text{Yb}, ^{178-184}\text{Hf}, ^{180-190}\text{W}, ^{182-196}\text{Os}, \) and \(^{184-200}\text{Pt}\).

The \( B_{\text{corr}} \) values for the above chains may be estimated in two ways. It may be taken from a different shell closure where the experimental data is available. For example, the binding energies for Te, Xe and Ba nuclei with \( N = 50 \) are obviously not available as they lie beyond the proton drip line. However, the \( B_{\text{corr}} \) values for these nuclei with \( N = 82 \) have already been calculated in the present work and we use the same values for the nuclei mentioned above. In Pd nuclei, the value obtained from \( N = 50 \) cannot be used for the \( N = 82 \) shell closure and is actually calculated in the following approach. In nuclei with \( Z = 70-78 \), the experimental binding energy is not available for \( N = 126 \). The binding energy for \(^{152}\text{Yb}\) is known, but the Yb isotopes in its vicinity do not share the simple trend of eqn. (2). In nuclei with \( Z = 46 \) and \( 74-78 \) we have estimated \( B_{\text{corr}} \) from the differences between the theoretical and experimental binding energies in isotopes with \( N_n \neq 0 \) by using eqn. (2) with the fitted value for \( a \). For \( Z = 70 \) and 72, the number of available \( \Delta_{\nu\pi} \) values are rather small to extract \( B_{\text{corr}} \) meaningfully. However, we find that the values of \( B_{\text{corr}} \) obtained for \( Z = 74-78 \) along with that obtained from the theoretical and experimental binding energy values of \(^{206}\text{Hg}\) lie on a straight line. We have obtained the values for \( Z = 70 \) and \( Z = 72 \) from the fitted line. The values of \( B_{\text{corr}} \) used for \( Z = 70-80 \) have been shown in Fig. 2. The \( \Delta_{\nu\pi} \) values for the above nuclei have been plotted.
against \( P \) in Fig. 3. Once again, one can see the excellent agreement between the extracted values of \( \Delta_{\nu\pi} \) and the straight line of eqn. (2) also shown in the figure, plotted with the previously fitted value of \( a \).

To check whether this remarkable correlation is a property of the particular Lagrangian density alone, we have chosen another Lagrangian density, NL3 and studied the nuclei for which results have been plotted in Fig. 1. The results, shown in Fig. 4 show a very similar trend though with slightly different slope \( (a = -2.609 \pm 0.044) \) and a slightly higher rms deviation of 1.68 MeV. We have also compared our results with those of a deformed RMF calculation by Lalazissis et al. [17] for Nd and Sm isotopes. We find that the agreement in binding energies and two nucleon separation energies using the present approach is comparable to or better than that observed in the deformed calculation.

The excellent results for even-even isotopes have prompted us to study even-\( Z \) odd-\( N \) isotopes. This has the added advantage that the \( B_{\text{corr}}(Z) \) values are already known from the study of the even-even chains. We have studied the odd \( N \) even \( Z \) isotopes within the ranges given in Table I. Additionally, we calculate \( \Delta_{\nu\pi} \) values for the ranges of isotopes discussed earlier where the binding energy values for the isotope with magic neutron number are not known and \( B_{\text{corr}}(Z) \) values have been estimated. In no case we have modified the \( B_{\text{corr}}(Z) \) values for odd isotopes. In our calculation, we neglect the fact that, the unpaired neutron actually occupies a particular single particle state, and breaks the symmetry. However, it is known that the effect of this correction to the binding energy is small. The results, plotted in Fig. 5 again show a similar trend for even-odd isotopes. Keeping the odd-even mass difference term in the semiempirical mass formula in mind, we try to fit the results using a simple function of the form \( aP + d/A \), where \( A \) is the mass number of the isotope. A least square fitting procedure gives the values as \( a = -2.129 \pm 0.042 \) and \( d = 145.7 \pm 14.3 \) with a standard deviation of 1.09 MeV for 209 nuclei. There are two points of interest here. The coefficients for the Casten factor \( P \) for even-even and even-odd isotopes are identical within errors. Secondly, the value for \( d \) is nearly the same as the corresponding coefficient in semi-empirical mass formula, i.e. 140 MeV. In Fig. 6 the results for all the isotopes described so far, except the ones with \( P = 0 \), have been plotted. The results for the even-odd isotopes have been shifted by the amount \(-145.7/A\). A least square fit of the points using eqn. (2) leads to a value, \( a = -2.139 \pm 0.017 \), with rms deviation of 1.09 MeV for 443 nuclei and have also been shown. Fig. 6 clearly demonstrates that the \( n-p \) interaction
is the dominating factor in the correction to the RMF binding energy.

Finally we would like to make a brief comment on the nuclei in various mass regions not included in the above discussion, particularly the rare earth nuclei \( Z = 64 \sim 74, \ N = 78 \sim 104 \) and actinide nuclei \( Z = 88 \sim 92, \ N = 114 \sim 148 \). The \( \Delta_{\nu\pi} \) values for even-even nuclei in these regions follow a different trend as shown in Fig. 7. First of all, the dispersion in the values is larger than the case of lighter nuclei. More importantly, clearly there are two different trends in the values with the points beyond \( P = 5 \) showing a sharp downward tendency.

Subshell closures, such as \( Z = 38 \) or 64, often become important in the systematics of certain observables[1] [18]. As mentioned earlier, we also invoked a number of different subshell closures in our work on systematics of spectroscopic factors[14]. In the present work, we have already used \( Z = 38 \) as a closure. We note that among the nuclei mentioned in the preceding paragraph, the subshell closure \( Z = 64 \) brings the \( \Delta_{\nu\pi} \) values for nuclei with \( Z = 66, 68, 82 \leq N \leq 92 \), very close to the straight line in Fig. 6. However, a more detailed analysis is required to bring out the role of subshell closures in the binding energy corrections.

The differences between the experimental and the theoretically calculated binding energies in RMF approach have been calculated for a large number of even-even nuclei from \( A = 50 \) to 220. As the n-p interaction is the major contributor to the difference between the theoretical and the experimental binding energies in RMF, we have taken the Casten factor \( P \) as a measure of n-p interaction and found that excluding certain mass regions, the differences, after suitable corrections for particular isotope chains, are proportional to \( P \). Results for even-\( Z \) odd-\( N \) nuclei are also seen to follow the same relation, if the odd-even mass difference is taken into account.

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Table 1: Symbols used in Fig. 1 for nuclei in different mass regions and the magic proton and neutron numbers used to calculate \( N_p \) and \( N_n \) for them.

| Symbol | Z-range   | \( N \)-range | Core(\( Z, N \)) |
|--------|-----------|---------------|-----------------|
| A      | 22 - 24   | 26 - 34       | 20, 28          |
| B      | 26 - 36   | 30 - 40       | 38, 40          |
| C      | 34,36     | 42 - 50       | 38,50           |
| D      | 42        | 46 - 64       | 38, 50          |
| E      | 44        | 50 - 64       | 40, 50          |
| F      | 46 - 48   | 50 - 64       | 50, 50          |
| G      | 48, 52 - 62 | 66 - 98   | 50, 82          |
| H      | 80, 84-86 | 106-136       | 82, 126         |

Figure 1: \( \Delta \nu \pi \) as a function of \( N-N_{\text{core}} \) (left hand plot) and \( P = N_p N_n / (N_p + N_n) \) (righthand plot). Symbols used for nuclei in different mass regions are indicated in Table I.
Figure 2: $B_{\text{corr}}$ values for $Z = 70 - 80$. See text for details.

Figure 3: $\Delta_{\nu\pi}$ as a function of $P$ for the isotopes $Z = 46, N \geq 66; Z = 52 - 56, N \leq 64$; and $Z = 70 - 78, N \geq 106$ as described in the text.
Figure 4: $\Delta_{\nu\pi}$ as a function of $P$ for the nuclei of Fig. 1 for the density NL3.

Figure 5: $\Delta_{\nu\pi}$ as a function of $P$ for odd-even isotopes as described in the text.
Figure 6: $\Delta_{\nu\pi}$ as a function of $P$ for even-even and odd-even isotopes as described in the text.

Figure 7: $\Delta_{\nu\pi}$ as function of $P$ for the nuclei as indicated with the closed core given in parentheses. A: $Z = 30, 32, 42 \leq N \leq 50$ (38,50); B: $Z = 64, 78 \leq N \leq 98$ (50,82); C: $Z = 66 - 74, 82 \leq N \leq 104(82,82)$; D: $88 \leq Z \leq 92, 114 \leq N \leq 148(82,126)$