Valence particles and the correction to relativistic mean field binding energy

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Abstract.
The differences between the experimental and the theoretically calculated binding energies in Relativistic Mean Field (RMF) approach have been calculated for a large number of odd-Z nuclei from $A = 47$ to 229. Neutron-proton (n-p) interaction is expected to be the major contributor to this difference. This difference, excluding certain mass regions and taking other effects as well as the odd-even mass difference into account, may be linearly parametrized by the Casten factor, a recognized measure of the n-p interaction in the nucleus. The results follow the same pattern as in the case of even-Z nuclei observed earlier.

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1. Introduction

The effective numbers of valence particles (or holes) are often found to be useful in the parametrization of various nuclear quantities\textsuperscript{[1]}. The product of numbers of valence protons ($N_p$) and neutrons ($N_n$), or similar functions of $N_p$ and $N_n$, represent the integrated n-p interaction strength and hence have been found to bear smooth relationships with certain observables such as deformation and B(E2) values\textsuperscript{[2, 3, 4]}, properties of excited states \textsuperscript{[5, 6]}, rotational moments of inertia and ground band energy systematics\textsuperscript{[7, 8]}, spectroscopic factors \textsuperscript{[9, 10]} etc. In Ref. \textsuperscript{[9]}, spectroscopic factors and the contribution of the n-p interaction to binding energy in actinides were seen to follow a certain pattern. In actinides, the only appropriate major doubly closed shell nucleus is $^{208}$Pb and it was necessary to employ subshell closures. In another communication \textsuperscript{[11]}, we obtained a more robust systematic behaviour in the latter quantity in even-proton nuclei, valid in a large mass region and dependent only on the known major shell closures. In the present work, we extend our study to odd-proton nuclei.

As was pointed out in \textsuperscript{[11]}, the correlations beyond mean field results are due principally to residual two body interaction. In mean field calculations, while the residual interaction between similar nucleons is taken care of by the introduction of $T = 1$ pairing, the residual n-p interaction is often ignored. The difference between the experimental and the calculated binding energies, suitably corrected for effects not related to the n-p interaction including odd-even mass difference, may vary smoothly as a function of the integrated strength of the n-p interaction. This difference, thus, may be expected to scale as the Casten factor $P = N_pN_n/(N_p + N_n)$, \textsuperscript{[12]} a widely used measure of the n-p interaction strength.

2. Calculation and Results

Following the method in \textsuperscript{[11]}, the effect of the n-p interaction in the difference between the experimental and the theoretical binding energies has been extracted by assuming that, in a nucleus with magic neutron number, this difference is due to the combined effects other than the n-p interaction. As $N_n$ is zero in these particular nuclei, the effect of the n-p interaction is expected to be small. 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 the n-p 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. The quantity $\Delta_{\nu\pi}(Z, N)$ is defined to be zero in magic $N$ nuclei. The experimental binding energy values are from Ref. \textsuperscript{[13]}. This difference also incorporates the odd-even mass difference in odd-$N$ nuclei.
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The choice of appropriate Lagrangian density is not unique as there are different variations of the Lagrangian density as well different parametrizations for them in RMF. In Ref. [11], we employed two such densities FSU Gold[14] and NL3[15] and obtained nearly identical behaviour. Accordingly, most of the results presented here use only the former one. This density involves self-coupling of the vector-isoscalar meson as well as coupling between the vector-isoscalar meson and the vector-isovector meson. The FSU Gold Lagrangian density seems very appropriate for a large mass region 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.

Table 1. The magic proton and neutron numbers used to calculate \( N_p \) and \( N_n \) for nuclei in different mass regions.

| Z-range | N-range | Core(Z, N) |
|---------|---------|------------|
| 21 - 23 | 26 - 34 | 20, 28     |
| 25 - 37 | 30 - 40 | 38, 40     |
| 35, 37  | 42 - 50 | 38, 50     |
| 43 - 55 | 50 - 65 | 50, 50     |
| 49 - 63 | 66 - 96 | 50, 82     |
| 71 - 87 | 104-142 | 82, 126    |

In figure 1, we plot the results for a large number of odd-even nuclei, lying between mass 47 (\( Z = 21 \)) and mass 229 (\( Z = 87 \)) as shown in table 1. The results have been plotted only for the nuclei whose experimental binding energies are available. The mass regions of table 1 are nearly identical with the corresponding ones in Ref. [11]. The experimental binding energy values in closed neutron shell nuclei between \( Z = 49 \) and \( Z = 55 \) (with \( N = 50 \) as magic number), and \( Z = 71 \) and \( Z = 79 \) (with \( N = 126 \) as magic number) are not known. Following [11], we have assumed the \( B_{\text{corr}}(Z) \) values to
be identical for $N = 50$ and 82 for the nuclei with $Z = 49 – 55$ and $N = 51 – 65$. For the nuclei with $Z = 71 – 79$, we have calculated the $B_{\text{corr}}(Z)$ values from the straight line in Ref. [11] obtained for even-even nuclei in this mass region. A total of 278 nuclei have been included in our calculation.

Similar to our observation for even $Z$ nuclei, we find that the points lie very close to a straight line if plotted as a function of the Casten factor. Thus, $\Delta_{\nu\pi}$ may be expressed as simply proportional to $P$. One can fit a straight line

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

with $a = -1.973 \pm 0.024$ MeV with rms deviation 1.126 MeV. The fitting is for 252 nuclei and does not include the values for nuclei with $P = 0$ which are defined to be zero. The fitted line has been shown in figure 1.

We next turn our attention to odd-odd nuclei. The $B_{\text{corr}}(Z)$ values are already known from the study of the odd-even chains. We have studied the odd-odd nuclei within the ranges given in table 1. In no case we have modified the $B_{\text{corr}}(Z)$ values for odd-$N$ isotopes. In our calculation, we ignore 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 and is included in the odd-even mass difference. The results again show a similar trend for odd-odd nuclei. Keeping the odd-even mass difference term in the semiempirical mass formula in mind, we fit the results using a simple function of the form

$$\Delta_{\nu\pi} = aP + \frac{d}{\sqrt{A}}$$

in terms of the Casten factor and the mass number of the nuclide. A least square fitting procedure gives the values as $a = -2.035 \pm 0.042$ MeV and $d = 10.48 \pm 1.30$ MeV with a standard deviation of 1.138 MeV for 245 nuclei. As in the case of even-$Z$ nuclei, we find that the coefficients for the Casten factor $P$ for odd-even and odd-odd nuclei are identical within errors. The value for $d$ is nearly the same as the corresponding coefficient in semi-empirical mass formula, i.e. 11 MeV. In figure 2 the results for all the nuclei described so far, except the ones with $P = 0$, have been plotted. The results for the odd-odd nuclei have been shifted by the amount $-10.48/\sqrt{A}$. A least square fit of the points using eqn. (2) leads to a value, $a = -2.003 \pm 0.017$, with rms deviation of 1.134 MeV and have also been shown in the form of a straight line. Figure 2 clearly demonstrates once again that the n-p interaction is the dominating factor in the correction to the RMF binding energy. The odd-even mass difference may also be expressed as inversely proportional to mass number, but we find that in this case, the former prescription fits the data better.

The results for even-$Z$ nuclei from Ref. [11] and for odd-$Z$ nuclei in the present work are clearly seen to follow the same linear pattern. In order to express all the values with a single relation, we have assumed the form in eqn (3). Least square fitting yields the values for the parameters as $a = -2.070 \pm 0.015$ MeV and, in odd-$N$ nuclei, $d = 12.05 \pm 0.70$ MeV with an average deviation of 1.132 MeV for 932 nuclei. The
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Figure 2. $\Delta_{\nu\pi}$ as a function of $P$ for odd-even and odd-odd nuclei. The values for odd-odd nuclei have been shifted as described in the text.

constant $d$ is taken to be zero in even-neutron isotopes. The results for nuclei with $P \neq 0$, after shifting the values for odd neutron nuclei taking the second term in eqn (3) into account, have been plotted in figure 3 where the straight line represents the equation $\Delta_{\nu\pi} = -2.070P$.

The corrections derived in the present procedure may be employed to improve the agreement between the calculated and experimental binding energy values. The present mean field calculation is a spherical one, and does not take deformation into account. It is expected to underpredict the binding energy far away from the closed shell. However, with the corrections, it is possible to obtain an agreement comparable to or even better than the values calculated using a deformed mean field approach. Thus the present approach may be very useful in predicting the mass of nuclei far from the stability valley.

As an example of comparison with RMF calculations which take deformation explicitly into account, we have chosen the Nd isotope chain and studied the two

Figure 3. $\Delta_{\nu\pi}$ as a function of $P$. See text for details.
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neutron separation energy values for even-even isotopes. The results are plotted in figure 4. Values obtained from both the FSU Gold and the NL3 spherical calculations have been corrected using the method described in the present work and Ref. [11]. The deformed NLSH results are from Lalazissis et al [17]. The deformed NL3 calculations use a deformed harmonic oscillator basis using gap parameters obtained from odd-even mass difference whenever available. In $^{130,150}$Nd, the values have been calculated using the empirical prescription $11.2/\sqrt{N(Z)}$. We find that the agreement using the present approach is comparable to or sometimes better than that observed in the deformed calculations.

![Figure 4](image.png)

Figure 4. Two neutron separation energy in Nd in various approaches. See text for details.

One obvious shortcoming in the present procedure is that the odd-even mass difference has been taken care of by a global relation while the actual quantity may be more appropriately described in a proper mean field procedure. It may be more appropriate to consider the effect of odd-even mass difference in a fully microscopic approach.

3. Summary

To summarize, the differences between the experimental and the theoretically calculated binding energies in RMF approach have been calculated for a large number of odd-Z nuclei from $A = 47$ to 229. The n-p interaction is expected to be the major contributor to the difference between the theoretical and the experimental binding energies in RMF. This difference, excluding certain mass regions and taking different effects into account, may be linearly parametrized by the Casten factor, a commonly used measure of n-p interaction. The trend is similar to the case of even-Z nuclei.

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