Microscopic study of deformation systematics in some isotones in the A ≈ 100 mass region

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Abstract. Variation after projection (VAP) calculations in conjunction with Hartree-Bogoliubov (HB) ansatz have been carried out for N=60, 62 isotones in the mass region A=100. In this framework, the yrast spectra with J\textsuperscript{\pi} ≥ 10\textsuperscript{2}, B(E2) transition probabilities, quadrupole deformation parameter and occupation numbers for various shell model orbits have been obtained. The results of calculations indicate that the simultaneous increase in polarization of p\textsubscript{1/2}, p\textsubscript{3/2} and f\textsubscript{5/2} proton sub-shells is a significant factor into the development of the deformation in neutron rich isotones in the mass region A=100.

1. Introduction
Since an important discovery made, in early seventies, about the occurrence of large deformation in the Zr and Mo nuclei around the mass number A≈ 100 by Cheifetz et al.[1], a lot of experimental work has been done now to prove the existence of deformation in some other nuclei also lying in the mass region A≈ 100.

It has been shown in the past that, in the neutron–rich even-even Zr nuclei, the deformation parameters increase gradually from β\textsubscript{2}~0.1 at N= 56, to β\textsubscript{2}~0.2 at N=58, to β\textsubscript{2}~0.4 at N = 64[2, 3]. Sometime back, it was also reported that nuclei around A=100 (36 ≤ Z ≤ 45 and 54 ≤ N ≤ 65) have well deformed shapes [4, 5]. On the basis of the experimental data deduced in the even-even nuclei around A≈ 100, it has been found that the deformation is large and sudden between N = 58 and N = 60 in Sr, Zr and Mo isotopes [6, 7] whereas this deformation becomes gradual at N > 60 in Ru and Pd isotopes [8, 9]

In order to examine the development of onset of deformation in the nuclei around mass number A≈ 100, various theoretical calculations including Shell Model theories and Mean Field theories have also been applied in the past. The Shell Model theories applied by Federman and Pittel [10-14] have explained the development of deformation in Zr and Mo isotopes in terms of n-p interaction operating between the SOP orbits- (1g\textsubscript{9/2})\textsubscript{π} and (1g\textsubscript{7/2})\textsubscript{υ} orbits. The Mean Field theorists [15- 17] have explained the development of large deformations in Zr isotopes in terms of the sudden occupation of low-K components of high-j orbits at the Fermi surface.

Now the question arises, if there are some other factors also, in the perspective of theoretical calculations, that are responsible for the development of deformation in the nuclei around A≈ 100?

In order to know and explain the causes that are responsible for bringing in sizeable collectivity / deformation in the nuclei around mass A≈ 100, we have performed Variation–After–Projection (VAP) calculations in conjunction with the Hartree-Bogoliubov(HB) ansatz for N = 60 and N = 62 isotones using the trial wave functions resulting from the pairing- plus-quadrupole-quadrupole model
of the two-body interactions(PQ) operating in a valence space spanned by $3s_{1/2}, 2p_{1/2}, 2p_{3/2}, 2d_{3/2}, 2d_{5/2}, 1f_{5/2}, 1g_{7/2}, 1g_{9/2}$ and $1h_{11/2}$ orbits for protons and neutrons outside the $^{56}$Ni core.

2. Calculational details

2.1. The one and two-body parts of the Hamiltonian

In our calculations presented here, the single particle energies(S.P.E.’s) of the valence orbits, that we have taken, are (in MeV) : $(3s_{1/2}) = 9.90$, $(2p_{1/2}) = 1.08$, $(2p_{3/2}) = 0.0$, $(2d_{3/2}) = 11.40$, $(2d_{5/2}) = 8.90$, $(1f_{5/2}) = 0.78$, $(1g_{7/2}) = 11.90$, $(1g_{9/2}) = 3.50$ and $(1h_{11/2}) = 12.90$. The energy values of single particle orbits for $2p-1f-1g$ levels are the same as employed for $^{56}$Ni core plus one nucleon. The energies of higher single particle valence orbits are the same as used by Vergados and Kuo [18] relative to $1g_{9/2}$ valence orbit. The two body effective interaction that has been employed is of PQ type. The parameters of PQ part of the two body interaction are also the same as used by Sharma et al. [19].

The procedure for obtaining the axially symmetric HB intrinsic states has been discussed in Ref.[20].

3. Deformation systematics of $N=60, 62$ Isotones.

3.1. Discussion of $E_2^+$ and intrinsic quadrupole moments in $N=60$ and $N=62$ isotones

It is well known from Grodzin’s relation[21] that $E_2^+$ of a nucleus bears an inverse correlation with the intrinsic quadrupole moment which means that if $E_2^+$ of a nucleus is small, its quadrupole moment should be large and vice-versa. In order to prove this relation, we have made calculations of ratio $RQ$ ($\langle <Q^2>_{HB}/<Q^2>_{Max} \rangle$) of intrinsic quadrupole moment to maximum quadrupole moment for $N=60$ and $N=62$ isotones and the results are presented in Table1. From Table 1, it is found that the value of $E_2^+$ is increasing from 0.144 for $^{96}$Sr to 0.512 for $^{106}$Pd for $N=60$ isotones whereas the value of $RQ$ for these isotones is decreasing from 0.66 for $^{96}$Sr to 0.50 for $^{106}$Pd, which proves the Grodzin’s relation. Hence there is a decrease of quadrupole collectivity vs Z as one goes from $Z=38$ ($^{96}$Sr) to Z= 46 ($^{106}$Pd). Similar results are also found in case of $N=62$ isotones and Grodzin’s relation is again proved here.

Table 1. The experimental values of excitation energy of the $E_2^+$ state in MeV, ratio $RQ$ ($= \langle <Q^2>_{HB}/<Q^2>_{Max} \rangle$) for $N=60$ isotones ($^{98}$Sr, $^{100}$Zr, $^{102}$Mo, $^{104}$Ru & $^{106}$Pd) and $N=62$ isotones ($^{100}$Sr, $^{102}$Zr, $^{104}$Mo, $^{106}$Ru, $^{108}$Pd) obtained with PQ interactions. The quadrupole moments have been computed in units of $b^2$ where $b=\hbar/m_0$ is the oscillator parameter.

| For $N=60$ isotones | For $N=62$ isotones |
|---------------------|---------------------|
| Nuclei | $E_2^+$ | $\langle <Q^2>_{HB} \rangle$ | $\langle <Q^2>_{Max} \rangle$ | $RQ$ | Nuclei | $E_2^+$ | $\langle <Q^2>_{HB} \rangle$ | $\langle <Q^2>_{Max} \rangle$ | $RQ$ |
| $^{98}$Sr | 0.144$^a$ | 81.73 | 122.84 | 0.66 | $^{100}$Sr | 0.129$^b$ | 80.43 | 121.08 | 0.70 |
| $^{100}$Zr | 0.212$^b$ | 87.51 | 128.02 | 0.68 | $^{102}$Zr | 0.151$^c$ | 89.45 | 126.36 | 0.70 |
| $^{102}$Mo | 0.295$^d$ | 93.21 | 130.91 | 0.71 | $^{104}$Mo | 0.192$^e$ | 93.17 | 129.97 | 0.66 |
| $^{104}$Ru | 0.358$^d$ | 77.50 | 134.94 | 0.57 | $^{106}$Ru | 0.270$^f$ | 82.23 | 133.36 | 0.61 |
| $^{106}$Pd | 0.512$^g$ | 69.77 | 138.31 | 0.50 | $^{108}$Pd | 0.433$^h$ | 73.35 | 136.41 | 0.53 |

$^a$Data taken from Ref. [22]  $^b$Data taken from Ref. [23]  $^c$Data taken from Ref. [24]
$^d$Data taken from Ref. [25]  $^e$Data taken from Ref. [26]  $^f$Data taken from Ref. [27]
$^g$Data taken from Ref. [28]  $^h$Data taken from Ref. [29]

3.2. Discussion of sub-shell occupation numbers and polarization

In order to examine the causes that are responsible for the development of deformation in $N=60$ and $N=62$ isotones in the perspective of Shell Model theory and Means Field theory, as discussed above in
In section 1, we have made calculations of sub-shell occupation numbers of the valence orbits and presented them in Figure 1. From Figure 1, it is noted that \((g_{7/2})_\pi\) remains almost constant at its value of 2 and 3 units for \(N=60\) and \(N=62\) isotones respectively whereas \((g_{9/2})_\pi\) goes on increasing, thereby, indicating that the deformation is increasing in the isotones with \(Z > 42\), which is contrary to what is observed experimentally. Hence, Shell model theory, as propounded by Federman and Pittel, is not reproduced by our results. It is again noted from Figure 1 that the value of \((h_{11/2})_\nu\) orbit, the low-\(K\) components of high-\(j\) orbit in our case, suffers a sudden decrease at \(Z = 44\) and could be thought responsible for the decrease in deformation in \(N=60\) and \(N=62\) isotones beyond \(Z = 42\), thereby, reproducing the causes explained for development of deformation in the Mean Field theory.

In order to find some other factors/causes that are responsible for development of deformation in \(N=60\) and \(N=62\) isotones, we have calculated the polarization factor from the results of sub shell occupation numbers using the formula

\[
Polarization = \frac{(2j+1) - \text{sub shell occupation number}}{(2j+1)}
\]

The calculated results of polarization factor for \(N=60\) and \(N=62\) isotones are presented in Figure 2. From Figure 2, it is found that the simultaneous increase in polarization of \((p_{1/2})_\pi\), \((p_{3/2})_\pi\) and \((f_{5/2})_\pi\) orbits is responsible for development of deformation in the nuclei with \(Z \leq 42\) (\(^{98,100}\)Sr, \(^{100,102}\)Zr and \(^{102,104}\)Mo) whereas simultaneous decrease in polarization of \((p_{1/2})_\pi\), \((p_{3/2})_\pi\) and \((f_{5/2})_\pi\) orbits at \(Z = 44\) is responsible for decrease in deformation for nuclei with \(Z > 42\) (\(^{104,106}\)Ru and \(^{106,108}\)Pd).

4. Yrast Spectra

To check the reliability of applied framework, it is important to calculate other observable quantities such as excitation energy spectra and \(B(E2)\) transition probabilities. We have calculated, through a
projection calculation, the excitation energy spectra in the N=60 and 62 isotones. From the results of calculations on yrast spectra for N=60 and N=62 isotones presented in Figures 3(a-e) and 4(a-e), it is found that the low-lying yrast states are very well reproduced and the overall agreement can be considered to be satisfactory which proves the reliability of HB wave function.

Figure 3 [a-e]. The comparison of the observed (exp.) and theoretical (th.) low-lying yrast spectra of N=60 Isotones (98Sr, 100Zr, 102Mo, 104Ru & 106Pd).

Figure 4 [a-e]. The comparison of the observed (exp.) and theoretical (th.) low-lying yrast spectra of N=62 Isotones (100Sr, 102Zr, 104Mo, 106Ru & 108Pd).
5. Systematics of calculated values of E2 transition probabilities in N=60 and N=62 isotones

The reliability and goodness of the HB wave-function is also examined by calculating the B(E2) values. In Table 2, the calculated values of E2 transition probabilities between the states $E^J_i$ and $E^J_f$ are presented. The calculated values are expressed in parametric form in terms of the proton ($e_p$) and neutron ($e_n$) effective charges, such that $e_p = 1 + e_{\text{eff}}$ and $e_n = e_{\text{eff}}$, and have been obtained through a rigorous projection calculation. The B(E2; $J_i^+ \rightarrow J_f^+$) values have been calculated in units of $e^2 b_n^2$ (where $b_n$ stands for barn, 1 barn = $10^{-28}$ m$^2$). The results indicate that by choosing $e_{\text{eff}} = 0.00$ to 0.23, a good agreement with the observed values for B(E2; 0$^+ \rightarrow 2^+$) transition probabilities is obtained for N = 60 and N = 62 isotones.

Table 2. The reduced transition probabilities for E2 transitions for the yrast levels in the N=60 and N=62 isotones. Here $e_p$($e_n$) denotes the effective charge for protons(neutrons). The entries presented in the third column correspond to the reduced matrix elements of the quadrupole operator between yrast states [Ref.17]. The reduced matrix elements have been expressed in a form that brings out their explicit dependence on the effective charges. The entries presented in the fourth column correspond to the effective charges indicated in the first column.

| Nucleus (e$^p$,e$^n$) | Transition | $|<J^+_f \rightarrow J^+_i>|^2_{\text{R}}$ | B(E2 ; $J^+_i \rightarrow J^+_f$) | Theory | (Expt.) |
|----------------------|------------|----------------------------------|----------------------------------|--------|--------|
| $^{98}$Sr             | 0$^+ \rightarrow 2^+$ | $0.80e_p + 0.95e_n$ | 1.32 | 1.28(39)* |
| $^{100}$Zr            | 0$^+ \rightarrow 2^+$ | $0.94e_p + 0.94e_n$ | 1.11 | 1.11(6)* |
| $^{102}$Mo            | 0$^+ \rightarrow 2^+$ | $1.02e_p + 0.98e_n$ | 1.04 | 0.96(31)* |
| $^{104}$Ru            | 0$^+ \rightarrow 2^+$ | $0.75e_p + 0.79e_n$ | 0.82 | 0.82(12)* |
| $^{106}$Pd            | 0$^+ \rightarrow 2^+$ | $0.63e_p + 0.75e_n$ | 0.65 | 0.66(35)* |

*Expt. Data taken from Ref.[8]  
*Expt. Data taken from Ref.[9]  
*Expt. Data taken from Ref.[30]
6. Quadrupole deformations ($\beta_2$) in N=60, 62 isotones

We have also calculated values for deformation parameter ($\beta_2$) for N=60 isotones and N=62 isotones. The deformation parameter $\beta_2$ is related to B(E2↑) by the formula suggested by Raman et al [31] as

$$\beta_2 = (4\pi / 3Z R_0^2 \left[ B(E2↑) / e^2 \right]^{1/2},$$

where $R_0$ is usually taken to be 1.2 A$^{1/3}$ fm and B(E2↑) is in units of e$^2$b$^2$.

The deformation parameter $\beta_2$ has been calculated by using the calculated B(E2↑) values given in Table 2. From the calculations, we find that $\beta_2$ values for N = 60 isotones (106Sr, 107Zr, 102Mo, 106Ru and 106Pd) are 0.408(6), 0.355(10), 0.311(5), 0.271(20) and 0.229(6) respectively. Similarly, the calculated $\beta_2$ values for N = 62 isotones (106Sr, 107Zr, 105Mo, 106Ru and 106Pd) are 0.427(44), 0.362(11), 0.257(34) and 0.243(6) respectively. From the comparison of the data, we find that there is a good agreement of $\beta_2$ values for the N=60, 62 isotones.

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