Quantised orbital alignment and Identical High-K Bands in A=180 region

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The origin of the identical gamma-ray energies (IB) observed in the K=33/2⁺ and K=16⁺ bands in 177Lu and 178Hf respectively is investigated using deformed Hartree-Fock and Angular Momentum Projection technique. We find that quantised orbital (rather than spin) alignment of protons in the m=1/2⁺ inert orbit leads to identical energy spectra. A K=16⁺ band with identical spectrum is predicted in 176Yb at 4.48 Mev of excitation.

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The fascinating phenomena of Identical Band (IB) was first observed in the superdeformed (SD) bands of neighbouring even-even (152Dy) and odd-even (151Tb) nuclei during 1990 [1,2]. The γ-ray energies of the SD bands of 152Dy and 151Tb were found to be identical within 0.01% . Soon this phenomena was identified in the normally deformed even-even and odd-A rare-earth nuclei . The recent observation [3] of this identity in the bands based on high-K isomeric states in the neighbouring nuclei (177Hf and 177Lu) is interesting. The transition energies observed for a few states in the K=33/2⁺ (T1/2=902s) band in 177Lu, have exactly the same value as of the K=16⁺ (T1/2=31y) band in 178Hf. These high-K states occurring at a few MeV of excitation having four-five unpaired nucleons are isomeric and have intermediate deformation β= 0.28 . Compared to SD states the configurations of high-K states are fairly well known and hence study of IB in high-K states can enhance our understanding of the phenomena.

Explanation of this phenomena has been tried in various models [2,4-6]. These models invoke the phenomena of pairing, quantised spin alignment, pseudo-spin symmetry, supersymmetry etc. in nuclei. Quantised spin alignment leading to identical superdeformed bands was reported by Stephens et-al [4]. Cheng-Li Wu et-al [5] have conjectured that the quantised spin alignment may be model dependent. However the mechanism of identical high-K bands have not been identified. Using a quantum many body method based on deformed Hartree-Fock and angular momentum projection we find that identical high-K bands in 178Hf and 177Lu occur due to quantised orbital alignment of protons in the inert orbit. The relative orbital alignment between the J+1/2 states in the K=33/2⁺ band in 177Lu and J states in K=16⁺ bands of 178Hf and 176Yb are exactly 1/2h. The relative spin alignment between these states are negligible.

The model used by us is based on a quantum many-body method which has been quite successful in explaining the high-spin spectroscopy in A=180 region [7,13] and light mass region [8] also. It is based on deformed Hartree-Fock model for the intrinsic states and Angular Momentum Projection (or J projection, for short) for the physical states based on these intrinsic states.

FIG. 1: The prolate Hartree-Fock single-particle orbits for protons and neutrons are shown for 176Yb. Solid and dashed lines correspond to the positive and negative parity orbits, respectively. The length of these lines indicate the magnitude of the z-projection (m) of the angular momentum. Stars guide the eye to the Fermi level. The inert m=1/2⁺ proton orbit is just below the m=9/2⁻ Fermi level and the deformed m=1/2⁺ proton orbit is third from the bottom.

In deformed (axial) Hartree-Fock and angular momentum projection (PHF) technique [for details see [8,9] and references there in] we start with a model space and an effective interaction. The model space is presently limited to one major shell for protons and neutrons lying outside the 132Sn core. Reasonable spherical single particle energies [10] and surface-delta interaction (strength has been taken to be 0.3 MeV for pp, nn and pn interactions respectively) are used in our calculation. The 3s1/2, 2d3/2, 2d5/2, 1g7/2, 1h9/2 and 1h9/2 proton states have energies 3.654, 3.288 , 0.731, 0.0, 1.705 and 7.1 MeV, and the 3p1/2, 3p3/2, 2f5/2, 2f7/2, 1h9/2 and 1i13/2 neutron states have energies 4.462, 2.974, 3.432, 0.0, 0.686 and 1.487 MeV respectively. The prolate HF calculation for the valence nucleons lying outside the 132Sn core is performed for both the nuclei. The time reversal symmetry
preserved for the even-even $^{178}\text{Hf}$ nuclei for the K=0+ configuration is broken slightly in the odd-A case $^{177}\text{Lu}$ (where the ±m orbits are no more degenerate). However, for the high-K states it has been shown [11] that this symmetry is badly broken. The set of prolate deformed HF orbits (with well defined m-quantum numbers) shown in Fig.1 for $^{178}\text{Hf}$ forms the deformed single particle basis for the valence protons and neutrons. This basis is enriched compared to the Nilsson basis as the pp,nn and pn correlations are built in by the inclusion of residual interaction in a self-consistent manner through the HF iteration procedure. Occupation of the lowest HF orbits by the active neutrons and protons forms the ground band (K=0) intrinsic configuration with a well defined K quantum number. This intrinsic HF wavefunction $|\Phi_K\rangle$ is a superposition of states of good angular momenta which are projected using the angular momentum projection operator:

$$P^M_K = \frac{2I + 1}{8\pi^2} \int d\Omega D^M_{IK}*(\Omega) R(\Omega) \tag{1}$$

The angular-momentum-projected normalised states are given by

$$\Psi^M_K = \frac{P^M_K |\Phi\rangle}{\sqrt{\langle\Phi | P^M_K |\Phi\rangle}} \tag{2}$$

The energy of the states are obtained from the hamiltonian overlap given by,

$$\langle \Psi^I_{K_2} | H | \Psi^I_{K_1} \rangle = \frac{2I + 1}{2} \left( N^I_{K_1 K_2} N^I_{K_2 K_1} \right)^{1/2}$$

$$\times \int d\theta \sin \theta d\phi d\phi_2 \langle \phi_2 | \phi_1 \rangle |H\rangle e^{-i\theta J_\nu} |\phi_1\rangle \tag{3}$$

with $N^I_{K K}$ = $\langle \Phi | P^I_K |\Phi\rangle$. $N^I_{K K}$ essentially represents the intensity of angularmomentum I in a K configuration. Interestingly $N^I_{K K}$ for the I=16,17,18... states of K=16+ band in $^{178}\text{Hf}$ is found to be identical respectively with those of the I=33/2,35/2,37/2... states of the K=33/2+ band in $^{177}\text{Lu}$. Using these projected states the expectation values of various tensor operators including E2,M1, $J$ and $\bar{L}$ are evaluated. Evaluation of the matrix elements of the operator J for the projected states provide the information about the nature of alignment of the protons (neutrons) in individual orbits for the J (or I) states. Similarly calculation of $\langle JJ \mid L_z \mid JJ \rangle$ and $\langle JJ \mid S_z \mid JJ \rangle$ provide the spin and orbital alignments of nucleons in various shell model orbits in a K configuration (see Fig.3). This provides a microscopic explanation of the identical high-K bands.

Dracoulis et-al [3] have identified the IB in K=33/2+ band in $^{177}\text{Lu}$ and K=16+ in $^{178}\text{Hf}$ at excitation of 2.771 and 2.447 MeV respectively. The excitation energies of these high-K IB in these nuclei agree fairly well with our calculated values of 3.252 and 2.255 respectively. The K=16+ and the K=33/2+ isomers are obtained by particle hole excitations over the ground state have the following intrinsic structures. K=16+ in $^{178}\text{Hf}$ - $(7/2^{-} + 7/2^{+})^p$ and $(7/2^{-} + 9/2^{+})^n$. K=33/2+ in $^{177}\text{Lu}$ - $(7/2^{+} + 9/2^{-} + 1/2^{-})^{n_{even}}$ and $(7/2^{-} + 9/2^{+})^{n_{odd}}$. J projection ( AMP for short) from these high-K structures give rise to the identical high-K bands (see Table-1 and Fig.2). The $\gamma$-ray transition energies of the high-K states are found to be identical within 10-20 keV. The absolute values of the theoretical (before mixing) $\gamma$-ray energies are overestimated compared to the experiment. Band mixing improves the agreement considerably (see Table). Similar High-K IB in neighbouring ($^{179}\text{Lu}$,$^{180}\text{Hf}$) and ($^{181}\text{Lu}$,$^{182}\text{Hf}$) nuclei are predicted.[12]

Let us analyse the microscopic structure of the intrinsic HF configurations of the high-K isomers. The two high-K structures differ in occupation of proton in the m=1/2 orbit. Hence the role of this unpaired proton in the natural parity orbit (m=1/2+) in K=33/2+ of $^{177}\text{Lu}$ becomes important in understanding the IB. Let us examine the HF wave function of this orbit.

### Table I: The $\gamma$ ray energies (E=$E_{1}\oplus E_{j-1}$) of the high-K bands are compared with experiment(EXP). The agreement improves after band mixing (BM). IB for $^{179}\text{Yb}$ is predicted.

| $^{179}\text{Hf}$ | PHF | BM | EXP | $^{178}\text{Lu}$ | PHF | BM | EXP |
|-----------------|-----|-----|-----|-----------------|-----|-----|-----|
| K=16+ $I(\hbar)$ |     |     |     | K=16+ $I(\hbar)$ |     |     |     |
| E$_{\gamma}$ keV | E$_{\gamma}$ keV | E$_{\gamma}$ keV | keV | keV | keV |
| 17 | 579 | 419 | 357 | 35/2 | 591 | 443 | 357 | 17 | 580 |
| 18 | 464 | 378 | 37/2 | 624 | 487 | 377 | 18 | 613 |
| 20 | 657 | 565 | 41/2 | 689 | 566 | 20 | 679 |
| 21 | 712 | 582 | 43/2 | 721 | 602 | 21 | 712 |
| 22 | 744 | 617 | 45/2 | 752 | 637 | 22 | 744 |
| 23 | 775 | 652 | 47/2 | 783 | 669 | 23 | 775 |
| 24 | 806 | 685 | 49/2 | 814 | 701 | 24 | 806 |
| 25 | 836 | 716 | 51/2 | 843 | 732 | 25 | 835 |
| 26 | 865 | 747 | 53/2 | 871 | 762 | 26 | 865 |
| 27 | 893 | 777 | 55/2 | 898 | 791 | 27 | 892 |
| 28 | 919 | 806 | 57/2 | 923 | 818 | 28 | 919 |
| 29 | 943 | 834 | 59/2 | 945 | 847 | 29 | 946 |
| 30 | 966 | 860 | 61/2 | 965 | 875 | 30 | 970 |

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### The Role of the natural parity HF inert orbit m=1/2+:

The HF wave function (-388, 35/2, $\pm$362, 2d$_{3/2}$, +438, 2d$_{5/2}$, -508, 1g$_{7/2}$) of this orbit indicate considerable mixing from all the four shell model states with d$_{5/2}$ dominance. The mixing is such that the quadrupole deformation of this orbit is negligible (i.e. -0.009 b$^2$, where b is the harmonic oscillator length parameter). Hence occupation or non occupation of this orbit does not change the deformation and the moment of inertia significantly. So the transition energies of the high-K band in $^{178}\text{Yb}$ where
the inert orbit is empty should also be identical to the $K=16^+$ band of $^{178}Hf$ and $K=33/2^+$ band of $^{177}Lu$. In fact (see fig.2) we find that the spectrum of the $K=16^+$ structure in $^{176}Yb$ is identical with the $K=16^+$ band of $^{178}Hf$ and $K=33/2^+$ band of $^{177}Lu$. But if a deformed $m=1/2^+$ orbit is occupied (as in case of $K=33/2^+_{def}$ of $^{177}Lu$ in fig.2) the spectra is not identical to the $K=16^+$ band in $^{178}Hf$. It is because this $m=1/2^+$ proton HF orbit (3rd from the bottom of Fig.1) is not inert and contributes to deformation (i.e quadrupole moment of this deformed orbit is 1.341 b$^2$). It appears that the pair of protons in the well mixed $m=1/2^+$ natural parity inert orbit remain as spectator in $^{178}Hf$. In $^{177}Lu$ the lone proton aligns its angular momentum with $^{176}Yb$ as the rotating core. Experimental observation of this $K=16^+$ band in $^{170}Yb$ predicted to be at about 4.48 MeV of excitation in our calculation is essential to confirm the above proposition. It is clear that occupation or non occupation of this orbit matters little to the energy spectra. Thus this orbit really acts as an inert orbit (as evident from its contribution to quadrupole moment) and leads to identical band.

Since the neutron configuration is same for both $K=16^+$ and $K=33/2^+$ bands, the role of neutrons must be identical in these two bands. It is found that the amount of J carried by the neutrons in various shell model orbits included in the model space are identical for both these bands. Except for the $1g_{7/2}$ and $2d_{5/2}$ protons the contribution to angular momentum from the rest of the protons and neutrons in various other orbits are same for both the nuclei.

As emphasized before the two high-K configurations differ in the occupation of protons in the inert orbit $m=1/2^+$. Hence the angular momentum carried by protons in these natural parity orbits needs microscopic analysis to pin point the underlying reason for identical energy spacing. In Figure 3 both the orbital and spin angular momenta contributions from individual proton orbits are shown. As evident from the figure the spin contributions from various proton orbits are same for $^{178}Hf$, $^{177}Lu$ and $^{176}Yb$ but the orbital contribution from orbits (other than $3s_{1/2}$) are not identical. We sum these contributions from different orbits both for orbital and spin parts and substract the contribution of $^{178}Hf$ from $^{177}Lu$ (as shown in upper most panel of Fig. 4). One finds that the relative orbital alignment is quantised ($L_{def}=1/2\hbar$). The relative spin alignment ($S_{def}$) is almost zero for the identical bands. Similar plots for the case of $K=33/2^+_{def}$ in $^{177}Lu$ shown in the lower panel of the Fig.4 . As is evident the orbital contribution slowly increases for the deformed case and saturates to $1\hbar$ at higher spin. Although spin contribution is non-zero it remains constant (and hence quantised ) for all J. Infact quantised spin alignment of $1/2\hbar$ have been reported for the identical superdeformed bands by Stephens et-al.[4] But we find the spin alignment to be negligible in these two high-K IBs.

The PHF calculation well reproduces the lowlying band structures in $^{178}Hf$ and $^{177}Lu$ nuclei. High-spin states in several bands are also predicted. Our calculation reproduces the identical high-K bands in these nuclei. The $K=16^+$ band, predicted in $^{176}Yb$, is found to be identical with the K=16$^+$ band (of $^{178}Hf$) and K=33/2$^+$ band (of $^{177}Lu$). This identity suggests that $^{176}Yb$ acts as a core in the high-K isomers of $^{177}Lu$ and $^{178}Hf$ with the rest of the protons being spectator. We find that quantised orbital alignment of protons in the

\begin{figure}
\begin{center}
\includegraphics{figure2.png}
\end{center}
\caption{The energy spacings of two K=33/2$^+$ bands (one with deformed m=1/2$^+$ proton orbit and the other with an inert m=1/2$^+$ orbit) in $^{177}Lu$ are compared with those of K=16$^+$ (in $^{178}Hf$). The K=33/2$^+$ inert band is identical to K=16$^+$ band in $^{178}Hf$ and $^{176}Yb$.}
\end{figure}

\begin{figure}
\begin{center}
\includegraphics{figure3.png}
\end{center}
\caption{The orbital and spin alignment from various proton orbits are compared with K=16$^+$ (in $^{178}Hf$, $^{176}Yb$) and K=33/2$^+$ bands (in $^{177}Lu$).}
\end{figure}
FIG. 4: The proton orbital and spin alignments in $^{177}$Lu (K=33/2$^+$) relative to $^{178}$Hf (K=16$^+$) are given for the inert case (upper panel) as well as deformed case (lower panel). As evident the orbital angular momentum is quantised for the inert case (i.e identical bands) and not so for the deformed case (non-identical bands).

$m=1/2$ natural parity inert orbit leads to identical high-$K$ bands in neighbouring nuclei. Thus the inert orbit near the Fermi level leads to quantised "orbital alignment" of nucleons in this orbit. The deformed configuration mixing leads to the inertness of the m=1/2 proton orbit, the occupation/non-occupation of which does not affect the energy spectra. The variation in the nature of orbital/spin alignments in the identical bands starting from normal deformed to superdeformed nuclei need further investigation.

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