A characteristic feature of transitional nuclei is the softness of nuclear surface. In an odd-mass transitional nucleus the unpaired particle exerts forces on the rest of the system which may lead to changes in shape depending on the j-orbital occupied by the extra particle. Thus one may expect different shapes of the doubly even core to be associated with the different orbitals occupied by the odd-particle. The odd proton nuclei \(^{121,123}\) with 53 protons and 68, 70 neutrons, respectively, are expected to show several features characteristic of a soft rotor. Theoretical calculations in \(^{121,123}\) [1-5] predict the prolate-oblate energy difference \((V_{po})\) to be small, and hence these nuclei should be sensitive to the shape polarizing effects of the valence quasiparticles. As a consequence of these effects and the softness of the nuclear cores, shape-coexistence phenomena are expected to occur [6-10]. Experimental results in \(^{121,123}\) (chapter III) also indicate coexistence of both oblate and prolate shapes in these nuclei.

The observed band structures in \(^{121,123}\) can be understood and explained in terms of the particle-rotor model [11,12] which describes the structure of the odd-A nucleus in terms of coupling of the motion of the last unpaired nucleon to the motion of the underlying even-even core consisting of the remaining nucleons. The calculations of the band structures of \(^{121,123}\) presented in this chapter are based on a version of the particle-rotor-model in which the experimental excitation energies of the neighbouring \((A-1)\) cores can be fed directly as input parameters [13,14]. The calculations have been carried out with axially symmetric Nilsson potential with both prolate and oblate deformations.
The parameters of the model have been chosen from earlier theoretical work [16] and experimental odd-even mass differences [17]. Only the Coriolis attenuation factor has been treated as adjustable parameter. The theoretically calculated band structures are compared with the experimental results. These calculations show very good agreement with the experimental data and provide interpretation of the various observed band structures in $^{121,123}$I.

4.1 Particle-rotor model

The particle-rotor model originally formulated by Bohr and Mottelson [11] and Kerman [12], is used extensively in the analysis of spectra of deformed as well as transitional odd-A nuclei. For simplicity one considers an axially symmetric even-even core, with only rotational degrees of freedom, and the odd nucleon coupled to the core through a deformed field. Under the adiabatic assumption the Hamiltonian $H_c$, which describes the slow motion of the core can be separated from the much faster particle motion, and the Hamiltonian of the odd-A system is expressed as

$$H = H_c + H_p$$

$$= H_c + \frac{P^2}{2m} + V(\beta, \gamma; r, l, s)$$

where

$H_c = \text{Hamiltonian of the core}$

$H_p = \text{Hamiltonian of the particle}$

The parameters $\beta$ and $\gamma$ specifying the shape of the deformed potential $V$ are just average values and not dynamical variables since the particle motion is much faster compared to that of the core [18].
Using the Nilsson potential, the Hamiltonian of the particle is written as [19]

$$H_p = \frac{p^2}{2m} + V(r) + C \cdot l \cdot s + D \cdot l \cdot l$$  \hspace{1cm} (2)

where $V(r) = \sum_{k=1}^{3} \frac{\omega_k^2 x_k^2}{r}$

Here $p$ and $m$ are the momentum and mass of the particle while $r$ is its position, and $l$ and $s$ are orbital and spin angular momenta. $C$ and $D$ are parameters adjusted to reproduce shell model levels when the deformation vanishes.

We take

$$\omega_1^2 = \frac{\omega_2^2}{2} \equiv \frac{\omega_0^2}{2} \left(1 + \frac{2}{3} \delta \right)$$

$$\omega_3^2 \equiv \omega_0^2 \left(1 - \frac{4}{3} \delta \right)$$

Thus $\delta$ gives the degree of deformation; $V(r)$ becoming spherically symmetric when $\delta = 0$. On noting that

$$r^2 Y_{20}(\theta, \phi) = \frac{1}{4} \sqrt{\frac{5}{\pi}} (3x_3^2 - r^2),$$  \hspace{1cm} (3)

one finds that

$$V(r) = \frac{1}{3} m \omega_0^2 \beta \left[1 - 2 \beta Y_{20}(\theta, \phi) \right],$$  \hspace{1cm} (4)

where $\beta = \frac{4}{3} \sqrt{\frac{1}{3} \pi \delta}$, the deformation parameter introduced by A.Bohr [11]

let $\rho^2 = \frac{m \omega_0}{\hbar} \beta^2$

Then

$$H_{\hbar \omega_0} = \frac{1}{2} \left(-\nabla^2 + \rho^2 \right) - \frac{\hbar^2}{m \omega_0} \sum_{k=1}^{3} \frac{\partial^2}{\partial x_k^2}$$

$$+ \beta^2 Y_{20}(\theta, \phi) - 2 \cdot l \cdot s - \mu \cdot l \cdot l$$  \hspace{1cm} (5)
where \( \kappa = \frac{C}{2\hbar \omega_0} \), \( \mu = \frac{2D}{C} \),

\[ \hbar \omega_0 = 41A^{1/3} \text{ MeV} \]

and \( \omega_0 = \omega_0 (1 - \frac{4}{3} \delta - \frac{16}{27} \delta^3)^{1/6} \)

where \( \omega_0^2, \omega_0^2, \omega_0^3 = \text{const} = \frac{\delta}{\omega_0} \).

Now we have to look into two other aspects of the Hamiltonian for the odd-A system, namely the effect of the pairing interaction, and the rotational motion of the core on the motion of the unpaired odd nucleon.

The pairing correlation is included in the calculations by using standard BCS (Bardeen, Cooper and Schreiber) transformation to the quasi-particle picture \([20, 21, 22]\). This transformation leads from the particle picture described by \( a^\dagger_\mu \) and \( a_\mu \) (particle creation and destruction operators) to the new, quasi-particle picture: described by the operators \( \alpha^\dagger_\mu \) and \( \alpha_\mu \),

\[
\alpha^\dagger_\mu = U^\dagger \alpha^\dagger_\mu - V a_\mu
\]

(6)

\[
\alpha_\mu = U a_\mu - V^\dagger \alpha^\dagger_\mu
\]

(7)

where \( \mu \) and \( \bar{\mu} \) represent a conjugate pair of states, \( \bar{\mu} \) being the time-reversed partner of \( \mu \). In our calculation for a deformed system \( \mu > 0 \) means \( m > 0 \). It can be easily seen that the \( \alpha_\mu \)'s are also fermion operators and they satisfy their usual anticommutation relations. They are known as the quasi-particle operators. The amplitude, \( V_\mu \) gives the occupancy of the orbitals \((\mu, \bar{\mu})\) in the ground state wavefunction \( |\text{BCS}\rangle \) and consequently, \( U_\mu = (1 - V^2_\mu)^{1/2} \) gives a measure of the non-occupancy of the orbitals \((\mu, \bar{\mu})\). It is much easier to work with these transformed operators since the trial wavefunction \( |\text{BCS}\rangle \) is a vacuum with respect to these operators, i.e

\[
\alpha_\mu |\text{BCS}\rangle = 0 \text{ for all } \mu,
\]

(8)

where \( |\text{BCS}\rangle = \prod_{\mu > 0} (U^\dagger_\mu + V a^\dagger_\mu a_\mu) |0\rangle \)
It is evident from the definition that the $|\text{BCS}\rangle$ is a superposition of different numbers of pairs, i.e., it no longer has a sharp particle number. This is actually a great disadvantage of the application of BCS theory in nuclear physics. In solid state physics, where $N = 10^{23}$, the violation of particle number has no influence on any physical quantity. So in a nuclear system, the variation of energy to determine $U$ and $V$ of the trial wave function is constrained by the subsidiary condition that the expectation value of particle number should have the desired value $N$

$$<\text{BCS}|\hat{N}|\text{BCS}\rangle = 2 \sum_{\mu>0} \mu^2 = N$$

(10)

This can be achieved by adding the term $-\lambda \hat{N}$ to the variational Hamiltonian

$$H' = H - \lambda \hat{N}$$

(11)

The Lagrange multiplier $\lambda$ is fixed by the above condition and is called the chemical potential or the Fermi energy because it represents the change of energy $E = <\text{BCS}|H|\text{BCS}\rangle$ for a corresponding change in the particle number

$$\lambda = \frac{dE}{dN}$$

For this reason $|\text{BCS}\rangle$ may be regarded as an average of the wave functions of a few neighbouring nuclei with particle numbers $N, N-2, N+2, \ldots$ For large $N$, the spread $<\text{BCS}|(\hat{N} - N)^2|\text{BCS}\rangle$ in particle number is small and contribution of the nucleus under study is predominant.

A little algebra, given in several standard text books [20,21] yields some important relations. For monopole pairing, the pairing gap parameter $\Delta$ is defined as

$$\Delta = G \sum_{\mu>0} U_{\mu} V_{\mu}$$

(12)

where $G$ is the (positive) pairing strength. The $U$ and $V$ coefficients are given by
The energy of a quasi-particle is given by

$$E_\mu = \sqrt{\left( \frac{\epsilon_\mu - \lambda}{\epsilon_\mu - \lambda + \Delta^2} \right)^2}$$ (15)

In the limit of vanishing pairing correlations ($U_\mu$, $V_\mu = 0$), the quasi-particles are either particles ($\epsilon_\mu > \lambda$) or holes ($\epsilon_\mu < \lambda$).

The calculation of matrix elements of the particle operators between quasi-particle states needs some attention. These matrix elements can be obtained by transforming the particle operators ($a^\dagger$, $a$) to quasi-particle operators ($a'^\dagger$, $a'$). Thus a one particle operator $F$ expressed in the form

$$F = \sum_{\nu_1 \nu_2} \langle \nu_2 | F | \nu_1 \rangle a'^\dagger(\nu_2) a(\nu_1)$$ (16)

can be shown to have matrix elements given by

$$\langle n = 1, \nu_1 | F | n = 1, \nu_2 \rangle = (U_1 U_2 + CV_1 V_2) \langle \nu_2 | F | \nu_1 \rangle$$ (17)

and,

$$\langle n = 2, \nu_1 \nu_2 | F | n = 0 \rangle = (V_1 U_2 - CU_1 V_2) \langle \nu_2 | F | \nu_1 \rangle$$ (18)

where $|n = 1, \nu_1\rangle$ and $|n = 2, \nu_1 \nu_2\rangle$ represent one and two quasi-particle states given by

$$|n = 1, \nu\rangle = a'^\dagger(\nu) |n = 0\rangle$$

$$|n = 2, \nu_1 \nu_2\rangle = a'^\dagger(\nu_2) a'^\dagger(\nu_1) |n = 0\rangle$$, respectively.

The phase factor $C$ is determined by the transformation of the operator $F$ under particle-hole conjugation, which is a combination of time reversal and Hermitian conjugation.
\[
\langle \vec{v}_1 | F | \vec{v}_2 \rangle = -C \langle \vec{v}_2 | F | \vec{v}_1 \rangle
\]  \hspace{1cm} (19)
and
\[
\langle \vec{v}_1 | F | \vec{v}_2 \rangle = C \langle \vec{v}_2 | F | \vec{v}_1 \rangle
\]  \hspace{1cm} (20)

### 4.2 Actual Hamiltonian used

We use the following Hamiltonian for our calculations:

\[
H = H^0_{qp} + c \ R_j + E_c(R)
\]  \hspace{1cm} (21)

The first term is the Hamiltonian of a single quasiparticle and is given by

\[
H^0_{qp} = \sum_K E_K \ \alpha_K^\dagger \alpha_K
\]  \hspace{1cm} (22)

with

\[
E_K = \sqrt{(\epsilon_K - \lambda)^2 + \Delta^2}
\]  \hspace{1cm} (23)

The \( \epsilon_K \) is the energy of a single particle moving in a standard axially symmetric Nilsson potential. The pairing gap and the Fermi level are represented by \( \Delta \) and \( \lambda \), respectively.

The last term, \( E_c(R) \), represents the collective part of the Hamiltonian, whereas the middle term originally introduced by Neergard [22], describes the rotational dependence of the interaction between the core and the quasiparticle. The coefficient \( c \) is defined [13] in terms of the core moment of inertia corresponding to the lowest \( 2^+ \) state in the rotational band and another parameter \( \alpha \),

\[
c = (I - \alpha) / \tilde{\varepsilon}_2 = (I - \alpha)E_c(R=2)/3\hbar^2
\]  \hspace{1cm} (24)

(It may be noted that the symbol \( \alpha \) has been used here to define a
parameter, and that it is different from the operator $\alpha$ mentioned in section 4.1 above. The significance of the parameter $\alpha$ can easily be seen if the core is assumed to have constant moment of inertia. Remembering that

$$R = I - j$$

(25)

(where $I$ is the total angular momentum of the nucleus and $j$ is that of the quasiparticle),

$$H = H_{qp}^0 + c R j + E_c(R)$$

$$= H_{qp}^0 + \frac{(1-\alpha)}{2} (1-j) j + \frac{(1-j)^2}{2j^2}$$

$$= H_{qp}^0 + I_{\perp}^2 + \frac{1}{2i} + (2\alpha - 1) \frac{J_{\perp}^2}{2j^2} - \alpha \frac{1}{2}$$

(26)

Here $I_{\perp}$ and $J_{\perp}$ denote the components perpendicular to the symmetry axis. So, for a constant moment of inertia, $\alpha$ is identical to the usual Coriolis attenuation factor. Moreover, it can be seen from the expressions (24) and (26) that the introduction of the $c R j$ term in the Hamiltonian effectively reduces the recoil energy if there is attenuation of the Coriolis matrix elements. In the limit of very small attenuation ($\alpha \approx 1$), this interaction term loses its significance.

The basis states are taken in the form

$$|IMK\rangle = \left[\frac{(2I+1)}{8\pi}\right]^{1/2} \times \left[D_{MK}(j^2K^2)D_{M,K}^I\right]^{1/2} (27)$$

Here $\chi_K$ represent the Nilsson single particle states which can be expanded into eigenstates of $j^2$,

$$\chi_K = \sum_j c_{jK}^I |jK\rangle,$$

(28)
However, we have to transform the basis into a representation with sharp \( R \) and \( J \) to calculate the \( R \)-dependent terms in the Hamiltonian. The necessary transformation is given by

\[
\langle (n\!\!j)_{IM}|IMK\rangle = C_{K}^{j,j'}(\!\!j)_{K}^{R} R_{0} \left[ I + (-)^{R} \right]^{1/2} \tag{29}
\]

In this representation, the matrix elements of any arbitrary functions \( f(j) \) and \( f(R) \) are given by

\[
\langle K_f |f(j)|K'\rangle_{qp} = (U_{K}^{+} U_{K'}^{+} V_{K} V_{K'}) \langle K_f |f(j)|K'\rangle_{qp}, \tag{30a}
\]

and

\[
\langle IMK |f(R)|IM'K'\rangle = \delta_{II'} \delta_{R} \sum_{R,J} \langle R |f(R) |J\rangle \left[ C_{K}^{j,j'}(\!\!j)_{K}^{R} R_{0} \right]^{1/2} \left[ C_{K}^{J,J'}(\!\!j)_{K}^{R} R_{0} \right]^{1/2} \tag{30b}
\]

In the above expressions, the \( U_{K} \) and \( V_{K} \) are the usual Bogoliubov transformation co-efficients. Using the above expressions, it can be shown that in this representation, energies of the rotational band built on a Nilsson orbital \( \chi_{K} \) are given by

\[
E_{J} = E_{K} + 2 \sum_{j,R} \left| C_{K}^{j,j'}(\!\!j)_{K}^{R} R_{0} \right|^{2} \left| E_{c}(R) \right| \tag{31}
\]

When the moment of inertia of the core \( (I_{R}) \) changes with increasing spin \( R \), the expression (26) for the Hamiltonian of the system, is obviously modified. The contribution to the Coriolis force is then

\[
- \frac{I_{J}J_{J}}{I_{R}} + \frac{I_{J}J_{J}}{I_{R}} \frac{1-a}{3} = -\alpha_{\text{eff}} \frac{I_{J}J_{J}}{I_{R}} \tag{32}
\]

Where
\[ \alpha_{\text{eff}} = 1 - \frac{\mathcal{J} \mathcal{R}}{\mathcal{J}^2} \left[ 1 - \alpha \right] \] (33)

This shows that, in the present formalism, the Coriolis attenuation factor will, in general be a function of the angular momentum (I) of the excited state.

4.3 Parameter choice

The Nilsson single-particle parameters \( \mu \) and \( \kappa \) are taken to be 0.48(0.54) and 0.07(0.056), respectively, for the \( N = 4(5) \) proton oscillator shell [23]. Earlier calculations [16] based on the Strutinsky shell correction method predict \( \beta = 0.20 \) and -0.15 for the prolate and oblate deformations, respectively, for both these nuclei. The present calculation has been carried out with these \( \beta \) values. The pairing gap parameter is estimated from the expression \( \Delta = 12/vA \) MeV. The Fermi level \( \lambda \) is chosen near the Nilsson orbital on which the ground state band is based. A fine adjustment in the Fermi level is made after initial energy diagonalization in order to achieve better agreement with relative bandhead energies. The average values of the yrast energies in neighbouring even Te and Xe nuclei are used as core energies, which are directly fed as input parameters. The Coriolis attenuation factor is adjusted to get the best fit to the level energies.

4.4 Comparison of theoretical results with experimental data

The theoretical level energies in \( {^{121,123}}I \) are shown in Figs.4.1-4.4 along with their corresponding experimental data. The energy levels in each isotope are classified into several bands (A,B,C,D,E) depending upon the dominant single particle orbitals on
which they are based and their equilibrium deformations. It is seen that
the present calculation is able to reproduce experimental band spectra
quite accurately and some of the relative bandhead energies. Detailed
comparisons are made below for each individual band members.

4.4.1 Bands based on oblate intrinsic orbital

**Band A**: The positive parity energy levels classified as band A in $^{121}$I
and $^{123}$I, are shown in Figs.4.1 and 4.2 respectively. The relevant
proton positive parity orbitals in this mass region are the $[413]^{5/2^+}$
and $[404]^{7/2^+}$ Nilsson states arising from the $\pi d_{5/2}$ and $\pi g_{7/2}$ orbitals.
The experimental E2/M1 ratios for the $\Delta I = 1$ intraband $\gamma$- transitions
have a negative sign [chapter-III ] indicating an equilibrium oblate
deformation for the intrinsic states on which these bands are based.
The present calculation with $\beta = -0.15$ nicely reproduces these bands in
both nuclei. Except for the $7/2^+$ states, the calculated energy values
are in good agreement with their experimental counterparts. The
calculated wavefunction shows that the ground state is almost a pure
proton $[413]^{5/2^+}$ state. The band A is however based on a
configuration with dominant contribution from the $[404]^{7/2^+}$ orbital.
With increasing angular momentum, the Coriolis perturbation increases.
As a result, the configuration becomes more mixed in nature with
contribution from the $[413]^{5/2^+}$ orbital also. It is found that the
calculation with prolate deformation cannot reproduce these band
members. So the present calculation lends supporting evidence to the
earlier findings [16,25,26] that the oblate deformation is energetically favourable for the $\pi d_{5/2}$ and the $\pi g_{7/2}$ orbitals.The
Coriolis attenuation factor needed to fit the experimental energy
levels ($\alpha=0.72$) lies within the range of values normally used in this
mass region.
Bands with oblate deformation

Fig. 4.1. Theoretical and experimental energy levels in $^{121}$ with oblate deformation.
Bands with oblate deformation

Fig. 4.2. Theoretical and experimental energy levels in 1231 with oblate deformation.
Band B: Another positive parity band (band B in figs 4.1 and 4.2) with ΔI=1(2) character is observed in $^{123}$I ($^{121}$I). The experimental energies of the band members in both nuclei are in very good agreement with those of a calculated band based on the [413]5/2$^+$ orbital. The experimental results in $^{123}$I show states of both signatures up to $\pi=\hbar 15/2^+$. However, in $^{121}$I only the states of one signature are observed, although the corresponding theoretical band shows a normal ΔI=1 nature. Since this band is very weakly populated, further experimental search for the missing signature partner in $^{121}$I would be necessary for a better understanding of the character of this band.

Band C: The calculation predicts the existence of a ΔI=1 negative parity band in both nuclei (Figs 4.1 and 4.2). The theoretical energies of the members of this band relative to the bandhead in $^{121}$I, based on the [505]11/2$^-$ orbital are in excellent agreement with those of an experimentally observed negative parity band. Good agreement is also achieved for the relative band head energies. The experimental E2/M1 ratios for the ΔI = 1 transitions in this band have a negative sign indicating that the band is associated with an oblate deformation. This is consistent with the present calculations with oblate deformation $\beta = -0.15$. Existence of a similar band in $^{123}$I is also predicted although this band has not been experimentally observed in this nucleus. It may be mentioned that this band is very weakly populated in $^{121}$I. It is also likely that in $^{123}$I it is not observed due to its relatively poorer intensity.

4.4.2 Bands based on prolate intrinsic orbital

Band D: This band of positive parity states based on a 9/2$^+$ state is experimentally observed in both $^{121}$I and $^{123}$I [Figs 4.3 & 4.4]. The
Bands with prolate deformation.

Fig. 4.3. Theoretical and experimental energy levels in \( ^{121}I \) with prolate deformation.
Fig. 4.4. Theoretical and experimental energy levels in \(^{123}I\) with prolate deformation.
characteristics of the levels of this band, and their decay modes are already discussed in chapter III. We notice that the levels of this band decay with $\Delta I=1$ cascade and $\Delta I=2$ cross-over transitions. The cross-over transitions have a stretched E2 character and the $\Delta I=1$ cascade transitions show a positive quadrupole to dipole mixing ratio indicating a positive deformation for this band. The $9/2^+$ band heads decay to the lowest $5/2^+$ and $7/2^+$ states in both nuclei. As mentioned earlier (chapter III) the lifetime of the $9/2^+$ band head shows the $9/2^+ \rightarrow 7/2^+$ (M1) and $9/2^+ \rightarrow 5/2^+$ (E2) transitions to be hindered with respect to the Weisskopf single particle estimates. These observations indicate that the $9/2^+$ band head is of different character from that of the lowest $5/2^+$ and $7/2^+$ states. In our calculations with prolate deformation ($\beta=0.20$), a band based on the $\left[404\right]9/2^+$ orbital is obtained in both isotopes. The excitation energies of the members of this band are in good agreement with those of the experimental bands in $^{121}\text{I}$ and $^{123}\text{I}$ (figs 4.3, 4.4).

**Band E**: The calculation with prolate deformation ($\beta=0.20$) also predicts the existence of a $\Delta I=2$ decoupled band in $^{121,123}\text{I}$, based on the $\left[550\right]1/2^-$ Nilsson state with admixtures from the nearby $\left[541\right]3/2^-$ and $\left[532\right]5/2^-$ Nilsson states arising out of the $\pi h_{11/2}$ orbital. A distinguishing feature of the calculated levels of this band is the large signature splitting obtained for this band. Only states of one signature, which are lower lying, are seen in the experiments, with $\Delta I=2$ sequence of states $11/2^-$, $15/2^-$, $19/2^-$... etc., connected by stretched E2 transitions. The $\Delta I=2$ character of this band is reproduced in this calculation, and although the absolute energy of the $11/2^-$ bandhead is not accurately reproduced, the energy level separations of the calculated $\Delta I=2$ levels are in excellent agreement with the experimental values.
4.4.3 Conclusion

The present work shows that the band structures observed in $^{121,123}$I nuclei can be nicely reproduced within the framework of the particle-rotor model, using only one adjustable parameter, i.e. the Coriolis attenuation factor. The fitted values of this parameter lie within a range which is considered to be normal for the weakly deformed nuclei. It is found that the calculation with either prolate or oblate deformation cannot reproduce the complete band structures in the experimental spectra. The bands based on the $\pi g_{7/2}$, $\pi d_{5/2}$ and large $\Omega$ $\pi h_{11/2}$ orbitals are reproduced in the present work with oblate deformation, $\beta = 0.15$, predicted in earlier theoretical study [16]. The bands based on the $\pi g_{9/2}$ and low $\Omega$ $\pi h_{11/2}$ orbitals are reproduced with prolate deformation $\beta = 0.20$, also predicted in the same study. The present work lends strong support to the suggestions of the earlier workers about the coexistence of prolate and oblate shapes in these nuclei.
REFERENCES


