Theoretical Study on Rotational Bands and Shape Coexistence of $^{183,185,187}$Tl in the Particle Triaxial-Rotor Model

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Abstract

By taking the particle triaxial-rotor model with variable moment of inertia, we investigate the energy spectra, the deformations and the single particle configurations of the nuclei $^{183,185,187}$Tl systemically. The calculated energy spectra agree with experimental data quite well. The obtained results indicate that the aligned bands observed in $^{183,185,187}$Tl originate from the $[530]_{1}^{\frac{1}{2}}$, $[532]_{2}^{\frac{3}{2}}$, $[660]_{1}^{\frac{1}{2}}$ proton configuration coupled to a prolate deformed core, respectively. Whereas, the negative parity bands built upon the $[\frac{9}{2}^{-}]$ isomeric states in $^{183,185,187}$Tl are formed by a proton with the $[505]_{9}^{\frac{9}{2}^{-}}$ configuration coupled to a core with triaxial oblate deformation, and the positive parity band on the $[\frac{13}{2}^{+}]$ isomeric state in $^{187}$Tl is generated by a proton with configuration $[606]_{13}^{\frac{13}{2}^{+}}$ coupled to a triaxial oblate core.

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1 Introduction

It has been known that nuclei in the $Z = 82$ region are rich in shape coexistence. In particular, the important deformation driving orbitals has been assigned as the $h_{9/2}$ and $i_{13/2}$ proton shells \[^{1,2}\]. In odd-mass Tl isotopes (with $Z = 81$), one-particle–two-hole (1p-2h) intruder states and shape coexistence have been discovered through the observation of low-lying $9/2^-$ isomeric states \[^{3}\]. The structure of these isomeric states was confirmed to be decided by the odd proton occupying the $h_{9/2}$ intruder orbital \[^{4,5}\]. Later, the rotational bands associated with both oblate ($\pi h_{9/2}$, $\pi i_{13/2}$) and prolate ($\pi h_{9/2}$, $\pi i_{13/2}$, $\pi f_{7/2}$) structures have been observed in lighter isotopes \[^{185,187}\]Tl \[^{6}\]. The band-head of the 1p-2h oblate $\pi h_{9/2}$ intruder band has been observed to lie lowest in energy near $N=108$. In contrast, the band-head of the prolate intruder band based on the $i_{13/2}$ structure has been predicted to decrease continuously in excitation energy as the neutron number decreases beyond the neutron mid-shell. This prolate structure is presumably formed by coupling the odd $i_{13/2}$ proton to the prolate Hg core with 4p-6h structure \[^{6}\]. Recently, a rotational-like yrast cascade was established in \[^{183}\]Tl and assigned to associate with the prolate $i_{13/2}$ structure \[^{7}\]. Furthermore the band-head energy of its yrast band was later determined \[^{8}\].

Besides the coexistence of prolate and oblate shapes mentioned above, the signature splitting observed in the [505]9/2$^-$ band in \[^{187}\]Tl which is significantly larger than that observed in its heavier odd-mass isotopes with $A \geq 191$ suggests that there may exist triaxial deformation \[^{1,6}\] and the discrepancy between the calculated equilibrium energy and the experimental data of the band-head energy of the [606]13/2$^+$ band in \[^{187}\]Tl hints that there may also involve triaxial deformation \[^{6}\]. However, no concrete investigations on the triaxiality in \[^{185,187}\]Tl have been reported up to now. Furthermore, there does not exist, at present, a systematic theoretical investigation on the structure of \[^{183}\]Tl. In addition, whether the [532]3/2$^-$ ($h_{9/2}$) state in \[^{185,187}\]Tl can be distinguished from the [530]1/2$^-$ ($f_{7/2}$) state (the band originated from such a configuration has not yet been observed in \[^{185}\]Tl) has not yet been determined definitely \[^{6}\].

On the theoretical side, it has been well established that the total energy surface calculation is quite successful in studying the equilibrium shape of a nucleus and shape coexistence (see for example Refs. \[^{9,10,11}\]). In addition, the projected shell model \[^{12}\] and particle triaxial-rotor model \[^{13,14,15}\] are also suitable to study triaxial deformation and configuration mixing \[^{16,17}\]. However, the triaxial deformation in the light odd-$A$ Tl-isotopes has not yet been studied. Because of its simplicity, we take the particle
triaxial-rotor model with variable moment of inertia of the core to analyze the structure and deformation of the energy bands in $^{183,185,187}\text{Tl}$ systemically and to identify their microscopic configuration.

The paper is organized as follows. After this introduction, we describe briefly the formalism of the particle triaxial-rotor model in Section II. In Section III, we describe our calculation and obtained results. In Section IV, we give a summary and brief remark.

2 Particle Triaxial-Rotor Model

In the particle rotor model, the Hamiltonian of an odd-$A$ nucleus is usually written as

$$\hat{H} = \hat{H}_{\text{core}} + \hat{H}_{\text{s.p.}} + \hat{H}_{\text{pair}} .$$  \hspace{1cm} (1)

In the case of triaxial deformation, the Hamiltonian of the even-even core is given as

$$\hat{H}_{\text{core}} = \sum_{i=1}^{3} \frac{\hbar^2 R_i^2}{2\Im_i} = \sum_{i=1}^{3} \frac{\hbar^2 (I_i - j_i)^2}{2\Im_i},$$  \hspace{1cm} (2)

where $R$, $I$ and $j$ are the angular momentum of the core, the nucleus and the single particle, respectively. The three rotational moments of inertia are assumed to be connected by a relation of hydrodynamical type

$$\Im_\kappa = \frac{4}{3} \Im_0(I) \sin^2\left(\frac{2\pi}{3}\kappa\right),$$  \hspace{1cm} (3)

with

$$\Im_0(I) = \Im_0\sqrt{1 + bI(I + 1)}$$  \hspace{1cm} (4)

being the variable moment of inertia \cite{13} of the core to replace the original constant $\Im_0$ to improve the calculation. In present calculation, we take $b = 0.013$ as the same as that in Refs. \cite{19,20,21}.

$\hat{H}_{\text{s.p.}}$ describes the Hamiltonian of the unpaired single particle. In the triaxial deformed field of the even-even core, $\hat{H}_{\text{s.p.}}$ is given by

$$\hat{H}_{\text{s.p.}} = -\frac{\hbar^2}{2m} \nabla^2 + \frac{1}{2m\omega_0^2}\{1 - 2\beta[Y_{20}\cos\gamma + \frac{1}{\sqrt{2}}(Y_{22} + Y_{2-2})\sin\gamma]\}
-\kappa\hbar\omega_0\{2l \cdot s + \mu(l^2 - < l_N >^2)\},$$  \hspace{1cm} (5)

where $\kappa$ and $\mu$ are Nilsson parameters, $Y_{2q}$ is the rank-2 spherical harmonic function.
\[ \hat{H}_{\text{pair}} \] is the Hamiltonian to represent the pairing correlation which can be treated in the Bardeen-Cooper-Schrieffer (BCS) formalism.

The single-particle wavefunction can be expressed as

\[ |\nu\rangle = \sum_{Nlj\Omega} C_{Nlj\Omega}^{(\nu)} |Nlj\Omega\rangle, \tag{6} \]

where \( \nu \) is the sequence number of the single-particle orbitals, \( |Nlj\Omega\rangle \) represents the corresponding Nilsson state, \( C_{Nlj\Omega}^{(\nu)} \) is the coefficient to identify the configuration mixing. Diagonalizing the single-particle Hamiltonian in the basis \( |Nlj\Omega\rangle \), we can obtain the \( C_{Nlj\Omega}^{(\nu)} \) and the single-particle eigenvalue \( \varepsilon_{\nu} \). The corresponding quasi-particle energy can then be determined by \( E_{\nu} = \sqrt{(\varepsilon_{\nu} - \lambda)^2 + \Delta^2} \), with \( \lambda \) and \( \Delta \) being the Fermi energy and the energy gap, respectively.

The total Hamiltonian in Eq. (1) can be diagonalized in the symmetrically strong coupling basis

\[ |IKM\nu\rangle = \sqrt{\frac{2I+1}{16\pi^2}} \left[ D_{MK}^I \alpha_\nu^+ |\tilde{0}\rangle + (-1)^{I-K} D_{M-K}^I \alpha_\nu^+ |\tilde{0}\rangle \right], \tag{7} \]

where \( \alpha_\nu^+ \) is creation operator of the single nucleon (in present case, proton) in the orbital \( |\nu\rangle \), \( D_{MK}^I \) is the rotational matrix.

### 3 Calculation and Results

In the present calculation to investigate the property of \(^{183,185,187}\)Tl, we take the \( \kappa \) and \( \mu \) in standard values \([22]\), i.e., 0.054, 0.690, respectively, and the pairing gap parameter as \( \Delta = 12/\sqrt{A} \). To improve the agreement between calculated results and experimental data, we introduce a Coriolis attenuation factor \( \xi \) and take value as that giving the best agreement between the calculated and experimental energy spectra. We found that, when \( \xi = 0.95 \), the calculated results agree best with the experimental data of \(^{183,185,187}\)Tl. In general principle, in order to describe the nuclear property more accurately and to make better agreement between calculated and experimental data, it is necessary to involve sufficient single-particle orbitals near the Fermi surface in the calculation. Then we take 13 orbitals near the Fermi surface to couple with the core for \(^{183}\)Tl, \(^{185}\)Tl, \(^{187}\)Tl, respectively. Practical calculation shows that the Fermi levels of the bands 6 (we denote the band labels here as the same as those for nucleus \(^{187}\)Tl in Ref. [6], so that the similar bands can be compared) of the nuclei lie between the 20th and the 21st single particle orbitals, and
the others lie between the 19th and the 20th. For the deformation parameters $\beta$ and $\gamma$ of $^{185,187}$Tl, we take those given in Ref.[6] as the trial initial values to fit. For the deformation parameters of $^{183}$Tl, since there does not exist any report to discuss them, we take the values of its neighbor nucleus $^{185}$Tl[6] as the trial initial ones. Then we accomplished a series diagonalization of the total Hamiltonian with various values of $\beta$ and $\gamma$ to make the calculation error $\chi^2 = \frac{1}{N} \sum_j (E_{cal}^j - E_{exp}^j)^2$ of the spectrum of a band (where $N$ is the number of levels in the band) smaller (in such a process, the band-head energy is fixed artificially with the definite angular momentum assigned in experiment. The best fit is, in fact, focused on the energy separations). Meanwhile, it should be noted that the parameter sector we used in the present work is the same as that taken in the book by Nilsson and Ragnarsson [23], where the value of $\beta$ can be positive or negative, the value of $\gamma$ varies from 0 to 30 degrees. The best fitted values of the $\beta$ and $\gamma$ are listed in Table 1, 2, 3 for nucleus $^{183}$Tl, $^{185}$Tl, $^{187}$Tl, respectively. At the same time, we obtain the total wavefunctions in terms of the single-particle orbitals which, as mentioned above, is fixed by diagonalizing the single particle Hamiltonian at each set of deformation parameters ($\beta$, $\gamma$). The calculated main components of the single-particle orbitals in terms of the Nilsson levels (in the case of best fitted deformation parameters) of nucleus $^{183}$Tl, $^{185}$Tl, $^{187}$Tl are also listed in Table 1, 2, 3, respectively. The resulting energy spectra for the nuclei $^{183,185,187}$Tl, as obtained from the best fit, are illustrated in Fig.1. From inspecting the results shown in Fig. 1, we observe a good agreement with the experimental data.

Because the experimentally observed rotational bands in $^{187}$Tl are richer and more characteristic than those in $^{183}$Tl and $^{185}$Tl, as a typical example, we analyze the band structure and configuration in $^{187}$Tl in detail. To this end, we list the total wavefunctions in terms of the single-particle orbitals of the bands in $^{187}$Tl in Table 4.

From Table 4, we can recognize that the band 1 originates near purely from the 22nd single particle orbital coupling with the prolate even-even $^{186}$Hg core. Seen from Table 3, the 22nd orbital contains mixing of 54.9% $|5f_{7/2}\frac{1}{2}\rangle$, 23.0% $|5p_{3/2}\frac{1}{2}\rangle$ and 10.7% $|5h_{9/2}\frac{1}{2}\rangle$ configurations. Since the largest component is $|5f_{7/2}\frac{1}{2}\rangle$, the band 1 can be assigned as the one arising mainly from the configuration $[530]\frac{1}{2}^- (\pi f_{7/2})$. Meanwhile, from Table 4, we can see that the band 2 consists of mixing of about 93% 20th and 7% 19th orbitals. Seen from Table 3, the 20th orbital contains 84.3% of $|5h_{9/2}\frac{3}{2}\rangle$ configuration. Thus, we can infer that the band 2 originates from the $[532]\frac{3}{2}^-$ configuration. Similarly, combining Table 4 with Table 3, we can recognize that the band 5, 6 originates mainly from the 23rd, 21st single particle orbital, respectively, the 21st orbital contains 87.4% of $|6i_{13/2}\frac{1}{2}\rangle$
Table 1: The deformation parameters and the main components of the single-particle levels $|\nu\rangle$ near the Fermi surface in terms of the Nilsson levels of the bands in $^{183}\text{Tl}$ (the initial values of the deformation parameters are taken as those of $^{185}\text{Tl}$ in Ref. [3].)

| band     | $\beta$ | $\gamma$ | $\nu\rangle$ wave function in terms of $|Nl/\Omega\rangle$ |
|----------|---------|----------|--------------------------------------------------|
|          | initial value | fitted value | initial value | fitted value | |
| band 3   |                      |           |                                   | [19] 0.856$|5h_{11/2}\frac{1}{2}\rangle$ + 0.425$|5f_{5/2}\frac{1}{2}\rangle$ − 0.182$|5f_{7/2}\frac{1}{2}\rangle$ |
| $([505\frac{3}{2}^-])$ | −0.162 | −0.168 | 0 | 15° | |
|          |                      |           |                                   | [20] 0.986$|5h_{9/2}\frac{5}{2}\rangle$ + 0.103$|5h_{9/2}\frac{5}{2}\rangle$ |
|          |                      |           |                                   | [21] 0.764$|5h_{9/2}\frac{5}{2}\rangle$ + 0.601$|5f_{7/2}\frac{1}{2}\rangle$ − 0.169$|5h_{9/2}\frac{5}{2}\rangle$ |
|          |                      |           |                                   | [22] 0.819$|5h_{9/2}\frac{5}{2}\rangle$ + 0.385$|5h_{9/2}\frac{1}{2}\rangle$ − 0.210$|5f_{5/2}\frac{3}{2}\rangle$ |
|          |                      |           |                                   | [23] 0.733$|5h_{9/2}\frac{5}{2}\rangle$ + 0.392$|5h_{9/2}\frac{1}{2}\rangle$ + 0.378$|5h_{9/2}\frac{3}{2}\rangle$ |
| band 6   |                      |           |                                   | [19] 0.995$|4g_{9/2}\frac{3}{2}\rangle$ |
| $([660\frac{1}{2}^+])$ | 0.267 | 0.270 | 0 | 0 | |
|          |                      |           |                                   | [20] 0.967$|4d_{3/2}\frac{5}{2}\rangle$ + 0.217$|4g_{7/2}\frac{3}{2}\rangle$ + 0.130$|4g_{9/2}\frac{5}{2}\rangle$ |
|          |                      |           |                                   | [21] 0.951$|6i_{13/2}\frac{3}{2}\rangle$ + 0.545$|6g_{9/2}\frac{1}{2}\rangle$ |
|          |                      |           |                                   | [22] 0.945$|6i_{13/2}\frac{3}{2}\rangle$ + 0.511$|6g_{9/2}\frac{1}{2}\rangle$ |
|          |                      |           |                                   | [23] 0.902$|4d_{3/2}\frac{5}{2}\rangle$ + 0.251$|4s_{1/2}\frac{1}{2}\rangle$ + 0.216$|5d_{5/2}\frac{3}{2}\rangle$ |

Table 2: The deformation parameters and the main components of the single-particle levels $|\nu\rangle$ near the Fermi surface in terms of the Nilsson levels of the bands in $^{185}\text{Tl}$ (the initial values of the deformation parameters are taken from Ref. [3].)

| band     | $\beta$ | $\gamma$ | $\nu\rangle$ wave function in terms of $|Nl/\Omega\rangle$ |
|----------|---------|----------|--------------------------------------------------|
|          | initial value | fitted value | initial value | fitted value | |
| band 2   |                      |           |                                   | [18] 0.993$|5h_{11/2}\frac{3}{2}\rangle$ |
| $([532\frac{3}{2}^-])$ | 0.245 | 0.247 | 0 | 0 | |
|          |                      |           |                                   | [19] 0.872$|5h_{9/2}\frac{5}{2}\rangle$ − 0.420$|5f_{5/2}\frac{1}{2}\rangle$ + 0.183$|5f_{7/2}\frac{1}{2}\rangle$ |
|          |                      |           |                                   | [20] 0.910$|5h_{9/2}\frac{3}{2}\rangle$ + 0.335$|5f_{5/2}\frac{1}{2}\rangle$ + 0.195$|5f_{7/2}\frac{1}{2}\rangle$ |
|          |                      |           |                                   | [21] 0.997$|5h_{11/2}\frac{11}{2}\rangle$ |
|          |                      |           |                                   | [22] 0.764$|5f_{7/2}\frac{1}{2}\rangle$ + 0.475$|5p_{3/2}\frac{1}{2}\rangle$ + 0.321$|5h_{9/2}\frac{5}{2}\rangle$ |
| band 3   |                      |           |                                   | [19] 0.681$|5h_{11/2}\frac{3}{2}\rangle$ + 0.449$|5f_{5/2}\frac{1}{2}\rangle$ − 0.352$|5f_{7/2}\frac{1}{2}\rangle$ |
| $([505\frac{3}{2}^-])$ | −0.162 | −0.164 | 0 | 15° | |
|          |                      |           |                                   | [20] 0.976$|5h_{9/2}\frac{5}{2}\rangle$ + 0.121$|5h_{9/2}\frac{5}{2}\rangle$ |
|          |                      |           |                                   | [21] 0.770$|5h_{9/2}\frac{3}{2}\rangle$ + 0.332$|5f_{7/2}\frac{1}{2}\rangle$ − 0.182$|5h_{9/2}\frac{3}{2}\rangle$ |
|          |                      |           |                                   | [22] 0.815$|5h_{9/2}\frac{3}{2}\rangle$ + 0.394$|5h_{9/2}\frac{1}{2}\rangle$ − 0.221$|5f_{5/2}\frac{3}{2}\rangle$ |
|          |                      |           |                                   | [23] 0.752$|5h_{9/2}\frac{3}{2}\rangle$ − 0.392$|5h_{9/2}\frac{1}{2}\rangle$ − 0.372$|5h_{9/2}\frac{3}{2}\rangle$ |
| band 6   |                      |           |                                   | [19] 0.999$|4g_{9/2}\frac{3}{2}\rangle$ |
| $([660\frac{1}{2}^+])$ | 0.267 | 0.268 | 0 | 0 | |
|          |                      |           |                                   | [20] 0.935$|4d_{3/2}\frac{5}{2}\rangle$ + 0.235$|4g_{7/2}\frac{3}{2}\rangle$ + 0.151$|4g_{9/2}\frac{5}{2}\rangle$ |
|          |                      |           |                                   | [21] 0.941$|6i_{13/2}\frac{3}{2}\rangle$ + 0.337$|6g_{9/2}\frac{1}{2}\rangle$ |
|          |                      |           |                                   | [22] 0.952$|6i_{13/2}\frac{3}{2}\rangle$ + 0.298$|6g_{9/2}\frac{1}{2}\rangle$ |
|          |                      |           |                                   | [23] 0.921$|4d_{3/2}\frac{5}{2}\rangle$ + 0.238$|4s_{1/2}\frac{1}{2}\rangle$ + 0.208$|5d_{5/2}\frac{3}{2}\rangle$ |
Table 3: The deformation parameters and the main components of the single-particle levels $|\nu\rangle$ near the Fermi surface in terms of the Nilsson levels of the bands in $^{187}$Tl (the initial values of the deformation parameters are taken from Ref. [6].)

| band                  | $\beta$ initial value | $\beta$ fitted value | $\gamma$ initial value | $\gamma$ fitted value | $\nu$ wave function in terms of $|Nlj\Omega\rangle$ |
|-----------------------|-----------------------|-----------------------|------------------------|------------------------|---------------------------------------------------|
| band 1 \((530\frac{1}{2}^+\rangle\) | 0.250                 | 0.253                 | 0                      | 0                      | $\langle 18 \rangle \cdot 0.997|5h_{11/2}\frac{3}{2}\rangle$ \(+\langle 19 \rangle \cdot 0.849|5h_{9/2}\frac{1}{2}\rangle + 0.429|5f_{5/2}\frac{1}{2}\rangle - 0.169|5f_{7/2}\frac{1}{2}\rangle \) \(+\langle 20 \rangle \cdot 0.909|5h_{9/2}\frac{3}{2}\rangle + 0.325|5f_{5/2}\frac{3}{2}\rangle + 0.191|5f_{7/2}\frac{3}{2}\rangle \) \(+\langle 21 \rangle \cdot 1.000|5h_{11/2}\frac{3}{2}\rangle \) \(+\langle 22 \rangle \cdot 0.741|5f_{7/2}\frac{1}{2}\rangle + 0.480|5p_{3/2}\frac{1}{2}\rangle + 0.327|5h_{9/2}\frac{1}{2}\rangle \) |
| band 2 \((532\frac{3}{2}^+\rangle\) | 0.234                 | 0.237                 | 0                      | 0                      | $\langle 18 \rangle \cdot 0.997|5h_{11/2}\frac{3}{2}\rangle$ \(+\langle 19 \rangle \cdot 0.868|5h_{9/2}\frac{1}{2}\rangle + 0.410|5f_{5/2}\frac{1}{2}\rangle - 0.162|5f_{7/2}\frac{1}{2}\rangle \) \(+\langle 20 \rangle \cdot 0.916|5h_{9/2}\frac{3}{2}\rangle + 0.312|5f_{5/2}\frac{3}{2}\rangle + 0.189|5f_{7/2}\frac{3}{2}\rangle \) \(+\langle 21 \rangle \cdot 1.000|5h_{11/2}\frac{3}{2}\rangle \) \(+\langle 22 \rangle \cdot 0.766|5f_{7/2}\frac{1}{2}\rangle + 0.469|5p_{3/2}\frac{1}{2}\rangle + 0.300|5h_{9/2}\frac{1}{2}\rangle \) |
| band 3 \((505\frac{3}{2}^+\rangle\) | -0.162                | -0.162                | 0                      | 0                      | $\langle 19 \rangle \cdot 0.695|5h_{11/2}\frac{3}{2}\rangle + 0.447|5f_{5/2}\frac{1}{2}\rangle - 0.360|5f_{7/2}\frac{1}{2}\rangle \) \(+\langle 20 \rangle \cdot 0.986|5h_{9/2}\frac{9}{2}\rangle - 0.101|5h_{9/2}\frac{3}{2}\rangle \) \(+\langle 21 \rangle \cdot 0.780|5h_{9/2}\frac{9}{2}\rangle + 0.348|5f_{7/2}\frac{1}{2}\rangle - 0.169|5h_{9/2}\frac{1}{2}\rangle \) \(+\langle 22 \rangle \cdot 0.825|5h_{9/2}\frac{3}{2}\rangle + 0.382|5h_{9/2}\frac{3}{2}\rangle - 0.201|5f_{7/2}\frac{1}{2}\rangle \) \(+\langle 23 \rangle \cdot 0.741|5h_{9/2}\frac{3}{2}\rangle - 0.386|5h_{9/2}\frac{1}{2}\rangle - 0.384|5h_{9/2}\frac{3}{2}\rangle \) |
| band 5 \((606\frac{1}{2}^+\rangle\) | -0.189                | -0.192                | 0                      | 0                      | $\langle 23 \rangle \cdot 0.997|6i_{13/2}\frac{1}{2}\rangle \) \(+\langle 24 \rangle \cdot 0.991|6i_{13/2}\frac{1}{2}\rangle \) \(+\langle 25 \rangle \cdot 0.974|6i_{13/2}\frac{1}{2}\rangle \) \(+\langle 26 \rangle \cdot 0.931|6i_{13/2}\frac{1}{2}\rangle + 0.298|6i_{13/2}\frac{3}{2}\rangle \) \(+\langle 27 \rangle \cdot 0.805|6i_{13/2}\frac{1}{2}\rangle + 0.471|6i_{13/2}\frac{3}{2}\rangle + 0.219|5i_{13/2}\frac{3}{2}\rangle \) |
| band 6 \((660\frac{1}{2}^+\rangle\) | 0.267                 | 0.265                 | 0                      | 0                      | $\langle 19 \rangle \cdot 0.995|4g_{7/2}\frac{3}{2}\rangle \) \(+\langle 20 \rangle \cdot 0.967|4d_{5/2}\frac{5}{2}\rangle + 0.217|4g_{7/2}\frac{3}{2}\rangle + 0.131|4g_{9/2}\frac{5}{2}\rangle \) \(+\langle 21 \rangle \cdot 0.935|6i_{13/2}\frac{1}{2}\rangle + 0.334|6g_{9/2}\frac{1}{2}\rangle \) \(+\langle 22 \rangle \cdot 0.946|6i_{13/2}\frac{3}{2}\rangle + 0.303|6g_{9/2}\frac{3}{2}\rangle \) \(+\langle 23 \rangle \cdot 0.906|4d_{3/2}\frac{3}{2}\rangle + 0.245|4s_{1/2}\frac{3}{2}\rangle + 0.214|5d_{5/2}\frac{3}{2}\rangle \) |
Table 4: The theoretically predicted main components of the wavefunctions of the bands 1, 2, 3, 5 and 6 in $^{187}$Tl in terms of the single-particle levels

| band   | $I^\pi$ wavefunction $|\nu K\rangle$ |
|--------|--------------------------------------|
|        |                                      |
| band 1 | $^{15}_2^-$ 0.981$|22\frac{1}{2}\rangle + 0.189|19\frac{1}{2}\rangle$ |
|        | $^{15}_2^-$ 0.981$|22\frac{1}{2}\rangle + 0.190|19\frac{1}{2}\rangle$ |
|        | $^{23}_2^-$ 0.980$|22\frac{1}{2}\rangle + 0.192|19\frac{1}{2}\rangle$ |
|        | $^{39}_2^-$ 0.979$|22\frac{1}{2}\rangle - 0.196|19\frac{1}{2}\rangle$ |
|        | $^{35}_2^-$ 0.979$|22\frac{1}{2}\rangle - 0.197|19\frac{1}{2}\rangle$ |
|        |                                      |
| band 2 | $^{17}_2^-$ 0.964$|20\frac{3}{2}\rangle + 0.263|19\frac{1}{2}\rangle$ |
|        | $^{21}_2^-$ 0.955$|20\frac{3}{2}\rangle - 0.294|19\frac{1}{2}\rangle$ |
|        | $^{25}_2^-$ 0.947$|20\frac{3}{2}\rangle - 0.321|19\frac{1}{2}\rangle$ |
|        | $^{29}_2^-$ 0.939$|20\frac{3}{2}\rangle + 0.343|19\frac{1}{2}\rangle$ |
|        | $^{33}_2^-$ 0.932$|20\frac{3}{2}\rangle + 0.362|19\frac{1}{2}\rangle$ |
|        | $^{37}_2^-$ 0.925$|20\frac{3}{2}\rangle + 0.378|19\frac{1}{2}\rangle$ |
|        |                                      |
| band 3 | $^{9}_2^-$ 0.815$|20\frac{3}{2}\rangle + 0.444|21\frac{3}{2}\rangle + 0.231|23\frac{3}{2}\rangle$ |
|        | $^{11}_2^-$ 0.728$|20\frac{3}{2}\rangle + 0.518|21\frac{3}{2}\rangle - 0.299|23\frac{3}{2}\rangle$ |
|        | $^{13}_2^-$ 0.500$|20\frac{3}{2}\rangle + 0.479|21\frac{3}{2}\rangle + 0.399|23\frac{3}{2}\rangle$ |
|        | $^{15}_2^-$ 0.584$|20\frac{3}{2}\rangle + 0.544|21\frac{3}{2}\rangle - 0.388|23\frac{3}{2}\rangle$ |
|        |                                      |
| band 5 | $^{13}_2^{13}_2^+ 0.720|23\frac{11}{2}\rangle + 0.520|24\frac{11}{2}\rangle + 0.350|25\frac{11}{2}\rangle$ |
|        | $^{15}_2^{15}_2^+ 0.580|23\frac{11}{2}\rangle - 0.560|24\frac{11}{2}\rangle + 0.450|25\frac{11}{2}\rangle$ |
|        | $^{17}_2^{17}_2^+ - 0.620|23\frac{11}{2}\rangle - 0.390|27\frac{5}{2}\rangle + 0.390|26\frac{5}{2}\rangle$ |
|        |                                      |
| band 6 | $^{17}_2^{17}_2^+ - 0.952|21\frac{1}{2}\rangle - 0.298|22\frac{3}{2}\rangle$ |
|        | $^{21}_2^{21}_2^+ - 0.943|21\frac{1}{2}\rangle - 0.326|22\frac{3}{2}\rangle$ |
|        | $^{25}_2^{25}_2^+ 0.936|21\frac{1}{2}\rangle + 0.347|22\frac{3}{2}\rangle$ |
|        | $^{29}_2^{29}_2^+ 0.930|21\frac{1}{2}\rangle + 0.363|22\frac{3}{2}\rangle$ |
|        | $^{33}_2^{33}_2^+ - 0.924|21\frac{1}{2}\rangle - 0.377|22\frac{3}{2}\rangle$ |
|        | $^{37}_2^{37}_2^+ 0.919|21\frac{1}{2}\rangle + 0.388|22\frac{3}{2}\rangle$ |
|        | $^{41}_2^{41}_2^+ 0.915|21\frac{1}{2}\rangle + 0.398|22\frac{3}{2}\rangle$ |
configuration, and the 23rd consists of almost purely the $|6i_{13/2}^{13/2}\rangle$ configuration. Therefore, the bands 5, 6 are based on the configuration $\pi[606]^{13/2}$, $\pi[660]^{13/2}$, respectively. The above calculated results of the bands 1, 2, 5 and 6 are consistent with the prediction of Ref. [6]. And the configuration assignment of the bands 1 and 2 is a corroboration of that in Ref. [6]. Furthermore, the $[530]^{1/2}_{1/2} \ (f_{7/2})$ band involves about 10% $h_{9/2}$ configuration and the $[532]^{3/2}_{3/2} \ (h_{9/2})$ band involves only about 4% $f_{7/2}$ configuration. On the other hand, similar results are obtained for the corresponding bands in $^{183,185,187}$Tl.

In order to investigate the deformation nature of band 3 in $^{183,185,187}$Tl, we illustrate at first the calculation error $\chi^2 = \frac{1}{N} \sum_j (E_j^{cal} - E_j^{exp})^2$ of the energy spectrum of band 3 in $^{187}$Tl (where $N$ is the number of levels in the band) with respect to the value of $\gamma$ at several $\beta$’s in the upper panel of Fig. 2. We also display the variation of the calculated energy spectrum against the value of $\gamma$ at the best fitted $\beta (-0.162)$ and the comparison

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**Figure 1:** Comparison of calculated energy levels of the rotational bands in $^{183,185,187}$Tl with the experimental data (taken from Refs. [6, 8]).
Figure 2: Upper panel: calculation error $\chi^2$ against the deformation parameter $\gamma$ at several axial deformation parameter $\beta$’s of the band 3 in $^{187}$Tl. Lower panel: variation of the calculated energy spectrum of the band 3 in $^{187}$Tl with fixed $\beta = -0.162$ against the value of $\gamma$ and comparison with experimental data. The experimental data are taken from Ref.[6].

with experimental data of the band in the lower panel of Fig. 2. The upper panel of Fig. 2 shows that the variation of the axial deformation parameter $\beta$ (except for that with angular deformation parameter $\gamma$ in special region) does not affect the calculation error $\chi^2$ so drastically as that of the $\gamma$ does. Combining the upper panel and the lower panel of Fig. 2, one can notice clearly that, for zero $\gamma$, the calculation error $\chi^2$ is quite large (about 60) and the calculated level sequence is not consistent with experiments. As the $\gamma$ increases to 3-5 degrees, the calculated level sequence becomes consistent with the experimental one and the $\chi^2$ decreases to about $10^{-1}$. For the value of $\gamma$ in the region 3 to 14 degrees, the calculation error $\chi^2$ maintains around $10^{-1}$. When $\gamma = 15^\circ$, the $\chi^2$ with $\beta = -0.162$ becomes suddenly the minimum ($\sim 10^{-4}$) of the $\chi^2(\beta, \gamma)$ and
the calculated energy spectrum agrees with experimental data very well. As $\gamma$ increases from 15 degrees further, the $\chi^2$ increases to around $10^{-3}$, even to $10^{-1}$. Moreover, in the case of $\beta = -0.162$, even though the calculated energies of the states with lower angular momentum do not deviate from experimental data obviously, the ones with higher angular momentum do drastically. It is then evident that, when the deformation parameters $(\beta, \gamma) = (-0.162, 15^\circ)$, the calculated energy spectrum agrees best with experimental data. It indicates that the band 3 of $^{187}$Tl is in triaxial oblate deformation. In addition, from Table 4, we notice that the band 3 in $^{187}$Tl originates mainly from the 20th single particle orbital. As can be seen from inspecting Table 3, the 20th orbital contains 97.2% of $|5h_9/2\pi\rangle$ configuration. Therefore, the band 3 can be identified as the one arising from the proton configuration $[505]_{2^+}^\pi \times (\pi h_{9/2})$ coupled to a triaxial oblate deformed core. It provides then
Figure 4: Upper panel: calculation error $\chi^2$ against the deformation parameter $\gamma$ at several axial deformation parameter $\beta$’s of the band 3 in $^{185}$Tl. Lower panel: variation of the calculated energy spectrum of the band 3 in $^{185}$Tl with fixed $\beta = -0.164$ against the value of $\gamma$ and comparison with experimental data. The experimental data are taken from Ref. [6].
Figure 5: Upper panel: calculation error $\chi^2$ against the deformation parameter $\gamma$ at several axial deformation parameter $\beta$’s of the band 5 in $^{187}$Tl. Lower panel: variation of the calculated energy spectrum of the band 5 in $^{187}$Tl with fixed $\beta = -0.192$ against the value of $\gamma$ and comparison with experimental data. The experimental data are taken from Ref. [6].
a corroboration of the conjecture in Ref. [6]. Similar results for the bands 3 in $^{183,185}$Tl are obtained, too (the calculation errors $\chi^2$ of the energy separations against the value of $\gamma$ at several $\beta$’s and the comparison of the calculated energy spectrum with $\gamma \in (0^\circ, 29^\circ)$ and $\beta = -0.168 (-0.164)$ with experimental data are illustrated in Fig. 3 (4) for $^{183}$Tl ($^{185}$Tl)). The deformation parameters can then be fixed as $(-0.168, 15^\circ)$, $(-0.164, 15^\circ)$ for the band 3 of $^{183}$Tl, $^{185}$Tl, respectively. These results confirm the assumption that the band originated from orbital $[505]{9\over 2}^- (\pi h_{9/2})$ may be in triaxial oblate deformation[6]. Besides, from the calculation error $\chi^2$ and the comparison between the obtained energy spectrum with $\beta = -0.192$ and the experimental data of the band $[606]{13\over 2}^+$ shown in Fig. 5, one can recognize that the band 5 ($[606]{13\over 2}^+$ band) is also a triaxial oblate deformation band (with $(\beta, \gamma) = (-0.192, 11.3^\circ)$).

From the calculations one may recognize that the deformation parameter $\gamma$ influences the results more drastically than the axial deformation parameter $\beta$. Analyzing the obtained single particle configuration we know that the states in the bands $[505]{9\over 2}^-$ and $[606]{13\over 2}^+$ involve much more complicated single particle Nilsson configurations than the other bands. Such a result is consistent with that once given for nucleus $^{127}$I in Ref. [20].

We infer then that the reason for the $\gamma$-degree of freedom to play more important role than $\beta$ may be that it induces more obvious mixing among the single particle Nilsson configurations.

## 4 Conclusion and Remarks

In summary, we have systemically calculated the energy spectra, the deformations and wavefunctions of the rotational bands in nuclei $^{183,185,187}$Tl in the particle triaxial-rotor model with variable moment of inertia. The calculated energy spectra of the bands agree quite well with the experimental data. The configuration of the bands in $^{187}$Tl is analyzed in detail as an example. Meanwhile we have also calculated the variation of the configuration of single-particle levels against the deformation parameters $\beta$ and $\gamma$. Considering both the parameters fitted and the agreement between calculated results and experimental data, we conclude that the rotation-aligned band structures observed in $^{183,185,187}$Tl are due to one of the $[530]{1\over 2}^-$, $[532]{3\over 2}^-$, $[660]{1\over 2}^+$ proton configurations coupled to a prolate deformed core. Meanwhile, the negative parity bands built upon the $\frac{9}{2}^-$ isomeric states in $^{183,185,187}$Tl are formed by a proton with the $[505]{9\over 2}^-$ configuration coupled to a core with triaxial oblate deformation $(\beta, \gamma) = (-0.168, 15^\circ)$, $(-0.164, 15^\circ)$, $(-0.162, 15^\circ)$, re-
respectively, and the positive parity band on the \( \frac{13}{2}^+ \) isomeric state in \(^{187}\text{Tl}\) is generated by a proton with configuration \([606]\frac{13}{2}^+\) coupled to a triaxial oblate core with deformation parameters \((\beta, \gamma) = (-0.192, 11.3^\circ)\). In short, the nuclei \(^{183,185,187}\text{Tl}\) involve quite rich shape coexistence. Meanwhile our present calculation provides a clue that the triaxial deformation may arise from the mixing of single particle Nilsson configurations. To understand it much better, more investigations are required.

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