# Theoretical analysis of <sup>111,113</sup>I by a Microscopic framework of calculation

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**Abstract:** The Projected shell model is used to study the fine details of the high spin states of <sup>111,113</sup>I nuclei. In the present work the negative parity yrast bands of these iodine nuclei are studied. Some of the nuclear structure properties like yrast spectra, Yrast band diagrams and Moment of inertia are calculated for these nuclei and a good agreement of these nuclear structure properties with their observed values is obtained.

**Keywords:** Theoretical analysis; yrast bands; <sup>111,113</sup>I.

## 1. Introduction

The neutron-deficient odd-mass nuclei in the Z > 50 transition region show collective features which have generated considerable theoretical and experimental interest. The traditional theoretical approaches used for the interpretation of the collective properties of these nuclei are based on models of deformed rotors [1] or anharmonic vibrators [2]. Some microscopic theories like perturbation expansion [3] and the interacting boson-fermion model [4] had been applied for a more detailed understanding of the collectivity of transitional nuclei with 49<Z<61. The  $h_{11/2}$  band in the intermediate <sup>111</sup>I isotope is unknown, but an isomeric  $I^{\pi}=11/2^{-}$  state has been proposed, together with the decay  $\sqrt{rays}$ , following a NORDBALL experiment in conjunction with charged particle and neutron ancillary detectors [5]. Paul et al [6], presents a new level scheme for <sup>111</sup>I, deduced from two <sup>58</sup>Ni+<sup>58</sup>Ni experiments, while the previously assigned  $\sqrt{10}$  rays [5] could not be confirmed. The experiments [6] were undertaken to investigate the high-spin structure of <sup>111</sup>I, in particular the  $\pi h_{11/2}$ band, in order to complete the systematics of the light odd-A iodine isotopes. Nuclei near the Z=50closed proton shell exhibit a novel collective structure that coexists with the expected single particle structure. Starosta et al. [7] reports on the wealth of structure information extracted from a high-spin study of the <sup>113</sup>I nucleus, which has three protons and ten neutrons outside the doubly closed <sup>100</sup>Sn core.Extensive experimental and theoretical investigations have been dedicated to the study of <sup>113</sup>I over the last decade [7-9]. These investigations have been mainly focused on the high-spin intruder bands and phenomena related to them, but have also led to the construction and interpretation of the low-spin part of the level scheme. A portion of the level scheme of <sup>113</sup>I is shown by P. Petkov et al [10]. As in other neutron-deficient odd iodine isotopes, the dominant feature is the negative-parity yrast band based on a low-K prolate  $\pi h_{11/2}$  orbital. In a recent work [6], a comprehensive systematic study of the level energies of these bands from <sup>109</sup>I to <sup>127</sup>I can be found. In recent years, the projected shell model (PSM) [11] has become quite successful in explaining a broad range of properties of deformed nuclei in various regions of nuclear periodic table. The purpose of the present work is to interpret the negative parity bands observed in <sup>111,113</sup>I in the framework of PSM.

#### 2. Theory of PSM

In this section, we give a brief outline of PSM. The Hamiltonian used in the present work is quadrupole plus pairing type and is of the form

$$\hat{H} = \hat{H}_{o} - \frac{\chi}{2} \sum_{\mu} \hat{Q}_{\mu}^{\dagger} \hat{Q}_{\mu} - G_{M} \hat{P}^{\dagger} \hat{P} - G_{Q} \sum_{\mu} \hat{P}_{\mu}^{\dagger} \hat{P}_{\mu}$$
(1)

Where  $\hat{H}_o$  is the spherical single-particle Hamiltonian which contains a proper spin-orbit force. The second term in Eq. (1) is the quadrupole-quadrupole (*QQ*) interaction and  $\chi$  represents its strength whose value is adjusted in a self-consistent manner such that it would give the empirical deformation,  $\varepsilon_{2,}$  as predicted in mean-field calculations, and the last two terms in Eq. (1) are the monopole and quadrupole pairing interactions, respectively. The hexadecapole deformation,  $\varepsilon_4$ , has also been included in the mean-field Nilsson potential to reproduce experimental energies correctly. The strength  $\chi$  of the quadrupole-quadrupole term can be obtained via self-consistent conditions with a given deformation parameter,  $\beta_2$ . The present calculations are performed by considering three major shells (N=3, 4 and 5) for both protons and neutrons.

## 3. Results and Discussion:

## 3.1 Yrast Spectra in <sup>111,113</sup>I

In Figures 1(a) and 1(b)), the results on yrast spectra for <sup>111,113</sup>I isotopes have been presented. The theoretical spectra have been obtained for that value of quadrupole deformation for which the Potential Energy Surface (PES) of the band-head shows a minima. In case of <sup>111</sup>I, in Figure1(a), the theoretical yrast spectra matches with the experimental values for spin values up to  $19/2^{-}\hbar$ . The comparison of both shows very a reasonable agreement with each other. Also in case of <sup>113</sup>I, in Figure1(b), the agreement of theoretical and experimental values of yrast spectra is very good up to the spin  $19/2^{-}\hbar$  and after that the calculated values show a reasonable agreement with experimental values.



**Figure 1:** Comparison of calculated (PSM) yrast spectra with experimental (EXP) data for negative parity of <sup>111,113</sup>I isotopes.

#### 3.2 Quasi-particle structure of iodine isotopes

To have physical insight in the nucleus and to interpret our numerical results, we have plotted the bands obtained from our calculations before their diagonalization in form of diagram between the energy of different bands and their corresponding spin (I) known as band diagrams. In these diagrams we have also plotted the yrast spectra so that one can find that which particular band is contributing towards the formation of the yrast spectra. Here, we have plotted only the lowest lying energy bands to extract the important physics from them. From the band diagram, one can get the information that, which particular bands contribute towards the formation of the yrast band after their diagonalization. Fig. 2(a) shows the band diagram for  $^{111}$ I isotope, where one can see that upto the spin of  $23/2^{-}$ , the yrast band is formed by the combination of two 1-qp bands having configurations:  $1\pi h_{11/2}[1/2]$ , K =1/2 and  $1\pi h_{11/2}$ [-3/2], K = -3/2. At spin 23/2<sup>+</sup>, there occurs a band crossing of the above mentioned overlapped 1-qp bands by a 3-qp band with configuration:  $1\pi h_{11/2}[1/2] + 2vh_{11/2}[1/2, -3/2], K = -1/2,$ which then alternatively contributes to yrast band up to the spin  $39/2^{\circ}$ . At the spin  $39/2^{\circ}$ , the above mentioned 3-qp band gets mixed with two more overlapped 3-qp bands with configuration:  $1\pi h_{1/2}$ [-3/2] + 2vh<sub>11/2</sub> [1/2,-3/2], K = -5/2, and 1 $\pi h_{11/2}$ [1/2] + 2vh<sub>11/2</sub> [1/2,5/2], K = 7/2, account for the yrast levels up to spin 59/2<sup>-</sup>. Similarly, for <sup>113</sup>I isotope (see Fig. 2(b)), the band diagram shows that the yrast band up to spin 23/2 consists of two overlapped 1-qp bands with configurations:  $1\pi h_{11/2}[1/2]$ , K = 1/2and  $1\pi h_{11/2}[-3/2]$ , K = -3/2, these overlapped 1-qp bands gets crossed by one 3-qp bands with configurations:  $1\pi h_{11/2}[1/2] + 2vh_{11/2}[1/2, -3/2]$ , K = -1/2, which then contributes to the yrast states up to spin 39/2<sup>-</sup>. At this spin, mixture of two more 3-qp band with configuration:  $1\pi h_{11/2}$ [-3/2] +  $2vh_{11/2}$  [1/2,-3/2], K = -5/2, and  $1\pi h_{11/2}$  [1/2] +  $2vh_{11/2}$  [1/2,5/2], K = 7/2, joins the above mentioned 3qp band and this combination then contributes to yrast levels for rest of the calculated spins.



**Figure 2:** Band diagrams of (a) <sup>111</sup>I and (b) <sup>113</sup>I isotopes for negative parity. Only the important lowest lying bands in each configuration are plotted. The yrast band is also shown (filled squares).

## 3.3 Backbending of moment of inertia in yrast bands

The backbending in moment of inertia, observed in the rotational spectra of deformed nuclei, carries important information on the interplay between the ground band and bands with lignment of a pair of quasiparticles. Thus, an yrast sequence is formed by states of both bands such that the lower spin states are mainly of the ground band, and the major component of the higher spin states belongs to the bands with aligned quasiparticles. In figures 3(a) and 3(b), the theoretical results of moment of inertia  $2J^{(1)}$  versus rotational frequency are compared with the experimentally observed ones for  $\Delta I = 2$  for <sup>111,113</sup>I, respectively.

The kinetic moment of inertia  $2J^{(1)}$  is defined as

$$2J^{(1)} = \frac{2I-1}{\omega},$$
 (2)

where the transition energy  $E_{\gamma} = E(I) - E(I-2)$  is related to the rotational frequency through

$$\hbar\omega = \frac{E_{\gamma}}{\sqrt{(l+1)(l+2) - K^2} - \sqrt{(l-1)l - K^2}}$$
(3)

In following sub-sections 3.3, back-bending phenomenon for negative-parity yrast bands <sup>111,113</sup>I has been discussed. The experimental and theoretical back-bending data for <sup>111,113</sup>I isotopes are plotted for negative- parity in Figs. 3(a) and 3(b). First of all, for <sup>111</sup>I (see Fig. 3(a)), the experimental back-bending occurs at the spin of  $27/2^{-}$ , whereas PSM results predict back-bending at the spin of  $23/2^{-}$ , which correspond to the rotational frequencies ( $\hbar^2 \omega^2$ ) of 0.117MeV<sup>2</sup> and 0.199 MeV<sup>2</sup> respectively. Moreover, it is also observed from the band diagram (Fig. 2(a)) for <sup>111</sup>I that the band crossing occurring at 23/2<sup>-</sup> is in consistent with the phenomenon of back-bending taking place at the same spin, which supports the accuracy of calculated results. Also in case of <sup>113</sup>I isotope, the experimental backbending is observed at the spin of  $27/2^{-}$  and theoretical back-bending calculated by PSM occurs at the spin of  $23/2^{-}$  with rotational frequencies of 0.114 MeV<sup>2</sup> and 0.199 MeV<sup>2</sup> respectively. Also, it is observed from the band diagram that the band crossing for <sup>113</sup>I (See Fig. 2(b)) occurs at  $23/2^{-}$ , which confirms the accuracy of calculated results.



**Figure 3:** Twice the kinetic moment of inertia  $(2\mathfrak{J}^{(1)})$  plotted against angular frequency squared  $(\hbar^2 \omega^2)$  in comparison with the experimental data for (a) <sup>111</sup>I and (b) <sup>113</sup>I for negative-parity yrast bands.

## 4. Conclusions

The projected shell model calculations carried out for odd mass <sup>111,113</sup>I isotopes show satisfactory agreement with observed yrast spectra. The calculated values of yrast energies are all along higher than the observed negative parity yrast energies for <sup>111,113</sup>I. In the present PSM calculations the backbending phenomenon is observed and it occurs at corresponding band crossing in the band plots. This model proposes that this phenomenon occurs by the alignment of a 3-qp state which is formed by a quasineutron state plus a pair of quasiproton states. Thus, it is established that the yrast negative

parity states do not arise from a single band, they arise from one quasiparticle (1-qp) or three quasiparticle (3-qp) bands. Besides this, the results suggest that the low lying yrast spectra in <sup>111,113</sup>I arise from a single band whereas the higher angular momentum states could be thought to be arising from a superposition of bands which indicates the possibility of co-existence of shapes in <sup>111,113</sup>I at higher spins.

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