A self-consistent quantal description of high-$K$ states
in the tilted-axis cranking model

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Abstract

A self-consistent and quantal description of high-$K$ bands is given in the framework of the tilted-axis cranking model. (With a $\theta = 90^\circ$ tilt angle with respect to $x$-axis, this cranking model is equivalent to the $z$-axis cranking.) The numerical results of the HFB calculations in this framework are compared with experimental data for two quasi-particle excited bands with $K^\pi = 6^+$ in $^{178}$W.

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The nuclear shell structure shows us that most of nuclei are deformed except some doubly and singly closed shell nuclei and a few of their neighbours. According to microscopic calculations [1], most of the deformed ground states have prolate shape. In addition, the presence of high-$K$ isomers in the well deformed region ($A \simeq 160 \sim 180$) indicate axial symmetry is well conserved in many nuclear excited states [4]. Then, $K = \sum_i \Omega_i$ is a good quantum number in a wide range of nuclear states. ($\Omega_i$ denotes the projection of single-particle spins on the quantization axis, or $z$-axis.) In such a situation, nuclear collective rotation is restricted along the $x$-axis, and yrast states (lowest states for given spin) are pictured in terms of one-dimensional static rotations.

The conventional self-consistent (one-dimensional) cranking calculations (SCC) about the $x$-axis are able to express the yrast states in such a way that the solutions at lower spins correspond to the ground-state rotational band (g-band) and those at higher spins to the rotation-aligned states (s-band). Although there are arguments about the validity of the cranking model in the band crossing region [3,4], SCC works well outside this region and is known as a useful tool in many microscopic high-spin calculations, in particular, in the cases where low-$K$ states are concerned.

In recent studies of high-spin physics, new types of nuclear rotations have been discovered in experiments, and explained by theoretical models. These rotations are not restricted any longer to rotations about the $x$-axis: for example, rotations of the magnetic dipole moment in near-magic nuclei (magnetic rotations [5]), tilted-axis rotations of triaxial deformed nuclei (chiral rotations [6]), and dynamical two-dimensional rotations in the multi-bands crossing region (wobbling motions [7]). In these phenomena, high-$K$ states play significantly important roles, especially in the context of tilted rotations. Microscopic treatments of these phenomena are presented principally by means of the tilted-axis cranking (TAC) model [5,8,9].

However, as for self-consistent descriptions of these multi-quasi particle excited high-$K$ states, there have been fewer attempts except a well known prescription to exchange the corresponding Hartree-Fock-Bogoliubov (HFB) solutions for the second solutions with
negative energy [10].

TAC calculations developed by Frauendorf [5] have been playing important roles to understand several high-K phenomena, but the method is not fully self-consistent because it fixes the deformation parameters and gap parameters through the iteration procedure.

Considering the increasing importance of such high-K states it is necessary to search for a tilted-axis version of SCC for the purpose of physically natural descriptions of high-K states.

At the same time, quantum mechanical treatments are required for the description of rotational bands of multi-quasi particle excited states because the single-particle (quasi-particle) degree of freedom has an essential role in these states in addition to the collective degree of freedom that can be treated in a semi-classical way. Angular momentum projection onto mean-field solutions is one of the methods which fulfill the requirement.

In a previous paper [11], we have compared numerical results from the self-consistent tilted-axis cranking calculations with experimental data in $^{182}$Hf, and suggested that these tilted-rotation minima can correspond to the high-K bands as a good approximation.

In this letter, the above suggestion is examined within the regime of the tilted-axis cranking model by means of (1)a mean-field approach based on the HFB method and (2)a quantal approach based on angular momentum projection. Then, attempts are made to describe rotational bands of high-K two quasi-particle excited states with the tilted-axis cranking model in a microscopic, fully self-consistent and quantal manner.

First of all, let us present our semi-classical picture of high-K bands. It is accepted that a band head of these bands is produced by a two or more quasi-particles excitation that contributes to building total angular momentum ($I$) along the quantization axis, or $z$-axis. On the other hand, it is assumed that rotational members in the high-K bands build their total angular momentum by collective rotation about the $x$-axis, as well as single-particle (quasi-particle) angular momentum along the $z$-axis. Therefore, the vector addition of these two angular momenta gives rise to a total angular momentum vector which is tilted away from $x$- and $z$-axes. The tilt angle ($\theta_{cl}$ which is defined as an angle of the total angular
momentum from the \( x \)-axis) can be thus evaluated as

\[
\theta_{\text{el}}^{I=K+\alpha} = \arcsin \left( \frac{K}{I} \right) = \arcsin \left( \frac{1}{1 + \alpha/K} \right),
\]

(1)
in which \( K \) represents the spin value for the band head and \( I = K + \alpha \) for the \( \alpha \)-th member in the band.

In our present analysis, we select a high-\( K \) band with \( K^\pi = 6^+ \) in \( {}^{178}\text{W} \) because it is well studied in experiments \[12\]. In \( {}^{178}\text{W} \), one \( K^\pi = 6^+ \) state is reported and its configuration assigned as \( \nu \{7/2 \,[514] , \, 5/2 \,[512] \} \).

Let us now explain the theoretical frameworks. The mean-field part is basically the same as the one in our previous work \[11\]: the Hamiltonian (\( \hat{H} \)) consists of spherical (spherical Nilsson Hamiltonian) and residual interaction (the pairing-plus-Q·Q force) parts. The tilted-axis cranked HFB solutions (\( \varphi \)) and corresponding energy (\( E(J) \), with \( J = (J_1^2 + J_2^2 + J_3^2)^{1/2} \)) are obtained by solving the HFB equation by means of the gradient method under the constraints for particle numbers and angular momentum vectors. The tilt angle \( \theta \) is introduced in the latter constraints as \( \langle \hat{J}_1 \rangle = J \cos \theta; \langle \hat{J}_2 \rangle = 0; \langle \hat{J}_3 \rangle = J \sin \theta \). We also constrain the off-diagonal components of the quadrupole tensor to be zero, that is, \( \langle \hat{B}_i \rangle = \frac{1}{2} (\langle \hat{Q}_{jk} \rangle + \langle \hat{Q}_{kj} \rangle) = 0 \), where \( (i, j, k) \) is cyclic. Band heads of high-\( K \) bands are described as solutions for \( \langle \hat{J}_z \rangle = J = K \ (\theta = 90^\circ) \). We call them \( z \)-axis cranking solutions, which are denoted as \( \varphi(K) \). The interaction parameters and configuration space are chosen in the same way as in our previous work \[11\]. The deformation and gap energy parameters for \( J = 0 \) are taken from Ref. \[1\].

The second framework is the quantal part based on the angular momentum projection, which is almost the same as those in Ref. \[13\]. The high-\( K \) bands are described as the projection from the \( z \)-axis cranked HFB state (\( \varphi(K) \)),

\[
|\phi_M^{I=K+\alpha} \rangle = \sum_{K'} g_K^{I} \hat{P}_{MK'} |\varphi(K) \rangle,
\]

(2)
where \( \hat{P}_K^{I} = \sum_q |IKq \rangle \langle IK'q| \) denotes the angular momentum projection operator (\( q \) is a collective symbol for other quantum numbers). The weight function \( g_K^{I} \) is determined
in the course of diagonalizing the generalized eigenvalue equation to obtain the projected
energy spectrum \( \{E^I\} \). On the other hand, the yrast band (corresponding to the g-
band at lower spin) is described in the same manner as Ref. [14]. Namely, we perform the
angular momentum projection for given quantized spin \( I \) on the several HFB states with
the constraint \( \langle \hat{J}_x \rangle = J \), and obtain the projected states \( \phi^I(J) \) with corresponding energy
\( E^I(J) \). We then choose the members for the yrast band \( \phi^I_\text{yrast}(J_{\text{min}}) \) satisfying \( \frac{\partial}{\partial J} E^I(J_{\text{min}}) = 0 \).

Let us analyze the numerical results for the band heads of \( K = 6^+ \) in \(^{178}\text{W}\), that is, \( \varphi(K = 6) \). First, self-consistently calculated quadrupole deformations
are given: \( \beta = 0.28 \) and \( \gamma = 0.0^\circ \). That is to say, this z-axis cranking state possesses well-
deformed prolate shape with almost perfect axial symmetry. Next, also in the HFB part,
we calculate the contributions to the band head spin from single-particle angular momenta
along the z-axis. In our calculations for \(^{178}\text{W}\), the major contributions are from the neutron
negative parity sector (\( \nu^- \)) in the model space. About 98\% of the total angular momentum
of the band head \( (J = K = 6\hbar) \) is produced by spins from two single-particle orbits; \( f_{7/2} \)
and \( h_{9/2} \), which are consistent with the assignment from experiments [12].

Then, let us go to an analysis on the rotational members of high-\( K \) bands. First of
all, consider the energy curves with respect to \( \theta \), which are obtained through the HFB
calculations (see Fig.4). Several local minima are seen in these graphs. The lowest ones
are seen at \( \theta = 0^\circ \) corresponding to the yrast states of g-band character where rotations
are supposed to be about the x-axis. Other minima are at \( \theta = 90^\circ \), relevant to high-\( K \)
states whose spin direction is along the z-axis. If the corresponding spin value is the same
as the band head spin \( (K) \), these minima can be naturally considered as the band heads of
high-\( K \) bands. The others are found as tilted-rotation minima whose tilt angles are listed in
Table 4. Tilt angles for these tilted-rotation minima are consistent with \( \theta_\alpha \) in Eq. (4). When
we look at the z-axis components of single-particle spins for the tilted-rotation minima,
they are almost the same as those for the band head. For instance, in the case of a tilted-
rotation minimum at \( \theta = 38^\circ \) for \( J = 10\hbar \), the z-axis spin components of \( f_{7/2} \) and \( h_{9/2} \) in
the \( \nu^- \) sector occupy about 97\% of \( J_z = J \sin \theta \approx 6\hbar \). Furthermore, the distributions of
the $x$-axis components of single-particle spins for these minima are quite similar to those for the lowest minima at $\theta = 0^\circ$ (see Table II). Thus the tilted-rotation minima have dual aspects of collective and single-particle rotations for $x$- and $z$-axes, respectively. In addition, from calculated deformations for the tilted-rotation minima, it can be said that the corresponding states have well-deformed prolate shape ($\beta \simeq 0.28$) with nearly perfect axial symmetry ($\gamma \lesssim 0.3^\circ$). Therefore, this result implies that the tilted-axis cranking version of SCC can realize rotational members of two quasi-particle excited high-$K$ bands as tilted-rotation minima if the proper interaction is chosen.

However, these tilted-rotation minima are expected to be quite unstable from Fig.1. Then, it may be necessary to go beyond the mean-field approximation. As we mentioned above, $|\varphi^{I=K+\alpha}_M\rangle$ in Eq.(2) should be employed.

It is worth looking at angular momentum projection analysis of the band head states $\varphi(K)$. In general, a wave packet breaking the rotational symmetry is expressed as $\sum_{IK} C^I_K |IK\rangle$. Thus, in our case, a probability $|C^I_{K'}|^2$ tells us how much the rotational symmetry is broken by the $z$-axis cranking term. Fig.2 presents the probability distribution for given $I$, that is, $W^I = \sum_{K'} |C^I_{K'}|^2$. Due to signature symmetry breaking by the $z$-axis cranking term, odd-spin components are equally contained in the HFB state as well as even-spin components. This feature is satisfactory for a description of $\Delta I = 1$ bands including high-$K$ bands. A more important feature is a suppression of lower-spin components ($I < 6\hbar$). This feature reflects that the high-$K$ components from the quasi-particle excitation ($K = 6\hbar$) are exclusively obtained through the $z$-axis cranking term in a self-consistent manner. Although higher-spin components remain as a result of symmetry breaking, this feature cannot be a problem for a description of high-$K$ rotational bands because the nuclear structure is preserved adiabatically within the band. In fact, this feature is rather preferable for our quantal expression (Eq.2) because sufficient of high-spin components are included in these HFB states. The probability distribution for given $I$ ($W^I_K = |C^I_K|^2$) shows the major component in $K$-quantum number. We have checked for $6\hbar \leq I \leq 28\hbar$ that the major component
is $K = 6\hbar$ and that the ratios $W^I_{K=6}/\sum_{K=-I}^{I} W^I_{K}$ are always more than 99.99%. From the results above, we can say that not only that our quantal approach works quite well to build almost pure $K = 6\hbar$ intrinsic states for given $I$, but also that the mean-field approach is already very good in terms of producing states having good (high) $K$-quantum number.

Finally, we compare the energy spectrum for the high-$K$ bands of $K^\pi = 6^+$ in $^{178}$W obtained by the tilted-axis cranking version of SCC and the angular momentum projection. Normalizations for the HFB energies are made with respect to the energy for $J = 0$ (i.e., $E(J) - E(0) \rightarrow E(J)$), while for the projected energies normalization is made with respect to the energy at $I = 0$ projected from the HFB state with $J = 0$ (i.e., $E^I(K) - E^0(0) \rightarrow E^I$).

The energies for the band head ($I = K = 6\hbar$) are given as 1.67 MeV (experiment), 1.21 MeV ($z$-axis cranked HFB), and 1.79 MeV (angular momentum projection), respectively. As for the rotational members, it is convenient to look at Fig.3. In spite of the phenomenological Pairing-plus-Q-Q interaction, the projected energies show very good agreement with experimental data. The energies for the tilted-rotation minima reproduce the experimental data to some extent (errors are roughly 400 keV).

The discrepancy of the projected energy of the yrast band at high spin could be due to the problem in the cranking model, which cannot describe the band crossing phenomenon properly. However, this deficiency does not influence the description of the high-$K$ band because it does not meet any band crossing, at least, about $I = 11\hbar$. Another reason can come from the fact that we have adjusted the residual interaction for the mean-field calculations, but not for the projection procedure. This influence is shown in the systematic errors, that is, projected energies for both the yrast and high-$K$ bands tend to overestimate the experimental values.

In summary, within the tilted-axis cranking model, we have investigated self-consistent and quantal descriptions of high-$K$ two-quasi-particle excited bands. The mean-fielded approach shows results consistent with a semi-classical picture of high-$K$ rotational bands,
and through the projection analysis it is found that the mean-field approach has an effect of angular momentum projection suppressing the irrelevant lower-spin components in the symmetry breaking HFB solutions. On the other hand, the quantal approach presents a satisfactory description in terms of restoration of broken rotational symmetry, and can produce more elaborate states taking into account higher-order correlations which are beyond the mean-field approach. According to our numerical calculations, we can conclude that both of the descriptions are good not only qualitatively but also quantitatively, at least, within some limitations owing to the interaction we chose in this study.

As to the future work, we should examine the present method in other situations, for instance, four quasi-particle excitations, proton quasi-particle excitations, negative parity high-$K$ states, and so on.

After a confirmation that the method can describe more general high-$K$ states like the above, it will be interesting to apply methods to predict features for unknown multi-quasi-particle excited high-$K$ bands such as energies and configurations for the band head, rotational properties of the bands, etc. We expect that these methods are quite helpful in experimental searches for new high-$K$ isomers in, say, the $A \simeq 190$ neutron-rich region that has just being explored recently [15].

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FIG. 1. Energy curves of $J = 6 - 11h$ with respect to $\theta$ for $^{178}$W. Arrows indicate the position of tilted-rotation minima.
FIG. 2. Probability distribution $W^I$ for the $z$-axis cranked HFB state of $^{178}\text{W}$ which correspond to the band head $I = K = 6\hbar$. The sum rule for the probability is satisfied to 99.9% up to $I = 29\hbar$. 
FIG. 3. Energy spectrum for $^{178}\text{W}$. “Exp-G” and “Exp-K” denote experimental data for the yrast and $K^\pi = 6^+$ bands, respectively. For the latter, energies are partially shown up to $I = 11\hbar$. “HFB-X” and “HFB-T” denote the one-dimensional cranked HFB energies and tilted-rotation minima in the tilted-axis cranked HFB calculations, respectively. “AMP-Z” (“AMP-X”) corresponds to the projected energy from the $z$- ($x$-) axis cranked HFB state with $K = J = 6\hbar$ ($K = 0, J = 6\hbar$)
TABLES

TABLE I. Tilt angles for given spin $I = K + \alpha$: $\theta_{cl}$ (Eq.(1)) and $\theta_{HFB}$ for $^{178}$W (Fig.1). The band head spin value is $K = 6\hbar$.

| $\alpha$ | $\theta_{HFB}$ | $\theta_{cl}$ |
|---------|----------------|--------------|
| 0       | $90.0^\circ$   | $90.0^\circ$ |
| 1       | $58.5^\circ$   | $59.0^\circ$ |
| 2       | $48.0^\circ$   | $48.6^\circ$ |
| 3       | $42.0^\circ$   | $41.8^\circ$ |
| 4       | $38.0^\circ$   | $36.9^\circ$ |
| 5       | $33.5^\circ$   | $33.1^\circ$ |

TABLE II. Single-particle spins along the $x$-axis for $^{178}$W at $J = 10\hbar$. Percentages are for the ratio of the total spin component along the $x$-axis ($J_x = J \cos \theta$). The symbols in the first line indicate the isospin and parity. For example, $\pi^+(\nu^-)$, means the proton positive-parity sector (neutron negative-parity sector).

| $\theta$ | $\pi^+$ | $\pi^-$ | $\nu^+$ | $\nu^-$ | $J_x = J \cos \theta$ |
|----------|--------|--------|--------|--------|---------------------|
| 0$^\circ$ | 0.6 (6%) | 0.7 (7%) | 4.7 (47%) | 4.0 (40%) | 10.0 (100%) |
| 38$^\circ$ | 0.4 (5%) | 0.6 (7.5%) | 4.0 (50%) | 3.0 (37.5%) | 8.0 (100%) |