RESTORATION OF THE BROKEN D2-SYMMETRY IN THE MEAN FIELD DESCRIPTION OF ROTATING NUCLEI

F. Dönau, Jing-ye Zhang,* and L.L. Riedinger*

Institut für Kern- und Hadronenphysik, FZ Rossendorf, 01314 Dresden
* Department of Physics and Astronomy, University of Tennessee, TN 37996

Abstract

Signature effects observed in rotational bands are a consequence of an inherent D2-symmetry. This symmetry is naturally broken by the mean field cranking approximation when a tilted (non-principal) axis orientation of the nuclear spin becomes stable. The possible tunneling forth and back between the two symmetry-related minima in the double-humped potential-energy surface appears as a typical bifurcation of the rotational band. We describe this many-body process in which all nucleons participate by diagonalizing the nuclear Hamiltonian within a selected set of tilted and non-tilted cranking quasiparticle states. This microscopic approach is able to restore the broken D2 symmetry and reproduce the quantum fluctuations between symmetry-related HFB states which emerge as splitting of the band energies and in parallel staggering in intraband M1 transitions.

1. Introduction

The Tilted Cranking (TAC) Model [1] has been a rather fruitful mean field approach to treat the angle degree of freedom connected with non-principal axis orientations of the rotational axis in deformed nuclei. This mean-field theory resulted in the microscopic description of $\Delta I=1$ rotational band structures, in particular, those which manifest themselves by strong magnetic dipole transitions observed in several mass regions. However, the tilted-axis rotation implies unavoidably the spontaneous breaking of the signature symmetry, i.e. the familiar D2 symmetry in deformed nuclei with respect to a 180 degree rotation is lost. Here we consider the consequences of this symmetry breaking and a possible way of its restoration for a typical example, the $K = 7/2$ ground-state band in $^{175}$Hf. The situation is illustrated in fig. 1 which shows the dependence of the potential energy surface (PES) on the tilt angle $\vartheta$ for three frequencies as obtained from a TAC calculation. Due to the D2 symmetry of the deformed density, these PES are mirror symmetric. The potential minima determine the stable rotational axes of uniformly rotating selfconsistent quasiparticle (qp) states, which turn out to be tilted for the lowest and non-tilted for the excited configuration.

At low frequency there appears two symmetry-related minimum points $\vartheta_o$ and $-\vartheta_o$ separated by a substantial barrier. Correspondingly, there exist two different quasiparticle states with stably tilted, symmetry-broken spin orientations. In the TAC model one of these tilted states is selected to represent the intrinsic state of the considered $\Delta I=1$ band. This is a good

1This axis is defined by the direction of the expectation value $\langle I \rangle$ of the nuclear spin vector $I$ for a given state.
approximation as long as the possible quantal motion between the different minima can be neglected. As seen in fig. 1 the two equivalent minima approach each other with increasing rotational frequency and finally merge into a single minimum at $\vartheta = 0$, then corresponding to the stable rotation about the short, so-called collective deformation axis. The latter is a principal axis rotation (PAC) having naturally good signature symmetry. The onset of the quantal motion is observed experimentally as the beginning of the well-known $\Delta I = 1$ staggering effect (signature splitting) in the band energies and a corresponding staggering of the $B(M1)$ strength [2] of subsequent $\Delta I = 1$ transitions.

The microscopic description of the signature bifurcation goes beyond the concept of the mean field. When the spin orientation is artificially fixed along a principal deformation axis as done in the 1-dimensional (PAC) cranking model, the signature effect appears as an intrinsic excitation (in fig. 1: $3 \rightarrow 4$) within the same mean field. However, this cranking axis happens to be unstable for the lowest configuration as seen in fig. 1. The two-dimensional cranking (TAC) brings the spin orientation into a stable but tilted direction which is manifested nicely in the geometrical spin dependence of the $\gamma$ radiation amplitudes [4]. Hence, in order to build a bridge between the PAC and the TAC picture, one must give up the simple determinantal form of the qp solutions in favor of an appropriate superposition of those states implying both tilted and non-tilted ones. It will be demonstrated that a direct diagonalization of the nuclear Hamiltonian within a small set of relevant quasiparticle states provides the desired framework for obtaining the mixing amplitudes of this superposition. This approach, denoted later on as diagonalized superposition of quasiparticles (DISQ), has some features of the Generator coordinate method when identifying the orientation angle $\vartheta$ as the collective variable in the spirit of reference [5]. However, we purposely include also an excited configuration...
not obtainable by a continuous change of the angle variable. The inclusion of the excited signature partner qp state is necessary in order to complete the configuration space. At higher frequency in the lowest PES only the symmetrical combination of the tilted qp states survives while merging into the favored signature PAC state, whereas the antisymmetric component simultaneously disappears. One may relate the signature effect to the picture of quantum tunneling [3], but the tunneling under the barrier seems to play only a partial role. The explicit presence of an excited signature-partner state above the barrier is important as well. The practical performance of the DISQ approach is technically ambitious because the PAC and TAC quasiparticle states are complicated many-body states forming in addition a non-orthogonal basis set. The setting up of the Hamiltonian matrix in such a basis and the subsequent calculation of the transition matrix elements were enabled by applying here the tools recently developed [4] in order to derive the overlaps and Hamiltonian kernel for non-orthogonal Hartree-Fock-Bogoliubov (HFB) states.

2. Hamiltonian
The study of the symmetry restoration relies on a rotational invariant many-body Hamiltonian which consists of three parts: a spherical average field part with the chemical potential term, a residual monopole pairing plus quadrupole interaction, and the usual cranking term:

\[ H' = h_{\text{sph}} - \lambda N + \sum_{\tau=p,n} G_{\tau} P_{\tau}^+ P_{\tau} - \frac{\kappa}{2} \sum_{\mu} Q_{\mu}^* Q_{\mu} - \omega I_x. \] (1)

The spherical mean field part \( h_{\text{sph}} \) is taken to be the modified oscillator Hamiltonian at zero deformation. The parameters \( G_{\tau} \) and \( \kappa \) determine the coupling strength of the factorized pairing and quadrupole force, respectively, where for the latter we assumed the same strength for protons and neutrons. The last term implying the cranking frequency \( \omega \) aligns the angular momentum direction (i.e. the spin orientation) along the x-axis. The self-consistent (s.c.) mean-field solutions corresponding to the above Hamiltonian \( H' \) (because of the cranking term, a Routhian) are constructed by means of the following tilted mean-field cranking Hamiltonian denoted also as the qp Routhian:

\[ h' = h_{\text{sph}} - \lambda N + \sum_{\tau=p,n} \Delta_{\tau} (P_{\tau}^+ + P_{\tau}) - \hbar \omega_0 \beta (\cos \gamma Q_0 + \sin \gamma / \sqrt{2} (Q_2 + Q_{-2})) - \omega (\cos \partial I_x + \sin \partial I_z). \] (2)

Here a two-dimensional cranking term, \( -\omega (\cos \partial I_x + \sin \partial I_z) \), is needed to obtain intrinsic qp states with a tilted spin orientation that is rotated subsequently to the space-fixed x axis of the lab system. The pairing gaps \( \Delta_{\tau} \) and quadrupole deformation parameters \( (\beta, \gamma) \) are determined by the usual selfconsistent conditions

\[ \Delta_{\tau} = G_{\tau} < P_{\tau} > \]
\[ h\omega_0 \beta \cos \gamma = \kappa < Q_0 >, \quad h\omega_0 \beta \sin \gamma / \sqrt{2} = \kappa < Q_2 >, \]
\[ < Q_1 >= < Q_{-1} >= 0. \]

where the \(< Q_{\mu=0,\pm1,\pm2} >\) and \(< P_{\tau=\pm1/2} >\) are the expectation values with respect to the considered qp state. The eigenstates of the Routhian \( h' \) are the Hartree-Fock-Bogoliubov determinantal states determined by the actual occupation of the many quasiparticle orbitals involved.

The Hamiltonian \( h' \) coincides with the TAC model \([1]\) and we construct our qp states with the oscillator basis including the proton shells \( N = 3, 4, 5 \) and neutron shells \( N = 4, 5, 6 \). The selfconsistency of the pairing plus quadupole Hamiltonian is easily obtained by choosing appropriate values of the deformation parameters and pairing gaps and subsequently matching the strength constants from eqs. 1 - 3. Hence, the tilted quasiparticle states are formed by standard methods. From a solution of the HFB equation (cf. \([5]\)), i.e. \([h', a_i^+] = e'_i a_i^+\), the quasiparticle operators \( a_i^+ \) and the Routhian energies \( e'_i \) are calculated for given set of parameters \( \beta, \gamma, \Delta, \omega, \vartheta \).

The relevant s.c. tilt angle \( \vartheta_o \) is derived from the requirement \([1]\) that the (here two-dimensional) spin orientation determined by the expectation values \(< I_x >, < I_z >\) of the spin operator \( I \) becomes parallel to the cranking direction, i.e. in our two-dimensional case
\[
\frac{\omega_x}{\omega_z} = \tan(\vartheta_o) = \frac{< I_x >}{< I_z >}.
\]

This parallel condition is equivalent to finding the local minimum in the PES (cf. fig. 1) of the selected qp configuration.

3. Selection of quasiparticle states in \(^{175}\text{Hf}\)

As mentioned above, a similar description of signature-splitting effects within a more conventional GCM approach was tried previously in ref. \([3]\). These authors considered a set of up to 30 quasiparticle states forming a path of tilt angles through the PES including the two minimal points, but all these qp states develop continuously in the lowest sheet of the PES, i.e. the qp states follow adiabatically the minimum configuration. However, the outcome of this attempt was not really satisfactory. The inclusion of an excited configuration seems to be crucial for treating the signature effects. The previous results indicate the situation that more experience is needed in order to learn more about both the physics of the large amplitude collective motion and the generator coordinate method. Our calculations below should be also considered as exploratory studies in this direction.

To simplify the task, we consider all mean field parameters in \( h' \), except the tilt angle \( \vartheta \), to be fixed. The adopted deformation parameters for the \( K = 7/2 \) band under study are \( \varepsilon_2 = 0.258 \), \( \varepsilon_4 = 0 \), and \( \gamma = 0 \). The pairing gaps are \( \Delta_p = 0.75 \text{ MeV} \) and \( \Delta_n = 0.69 \text{ MeV} \), respectively. Aiming in this paper to extend the TAC mean-field approach in the simplest manner, we include only the four tilted s.c. qp states marked in PES of fig. 1 in the diagonalization.
of $H'$. Two of the selected points correspond to the symmetrical TAC minima of the two stably tilted qp states, denoted below as $| \pm \vartheta_0 \rangle$. The third point belongs to the metastable maximum point of the favored signature PAC configuration at $\vartheta = 0$, and the fourth point is placed also at $\vartheta = 0$ into the minimum of the unfavored signature PAC configuration (fig. 1). These four states are suggested to play the key role for describing the signature-splitting effects. Needless to say, the normal PAC model is able to describe the signature splitting of non-tilted rotational bands quite successfully [6]. Thus, it is suggestive to include the above four states which merge naturally into the usual PAC signature partners at higher frequency. A systematic study for a larger set of points will be done elsewhere.

By construction, the qp states of the Routhian $h'$ are intrinsic states which belong to different spin orientations $\pm \vartheta_0$. Therefore, before the final $4 \times 4$ diagonalization of $H'$ is done, one has to transform all intrinsic qp states to a common lab system via an appropriate rotation. In this respect, we remind the reader that the spin orientation of a rotational invariant Hamiltonian is a space-fixed vector.

As a result of the cranking term $\omega I_x$, the common spin orientation of all included qp states is made parallel to the x axis. The rotation of a tilted intrinsic state $| \vartheta \rangle$ reads explicitly as

$$| \vartheta_{\text{lab}} \rangle := e^{-i\vartheta I_y} | \vartheta_0 \rangle$$

where $I_y$ is the y-component of the angular-momentum operator. The corresponding density distribution considered in the lab frame of reference is sketched in fig. 2. Note that the tilted qp state changes its density in space for the signature operation i.e. while rotating 180 degrees about the common x-axis. This common spin orientation along the x axis is taken later on also as the quantization axis for the electromagnetic transition operators.
For these explorative studies we did not try to precisely match the interaction strengths, nor run the qp states to selfconsistent deformations. Since a quite flexible computer code is available, several improvements can be made e.g. the inclusion of particle number projection and angular momentum projection in x direction by rotating the qp states in gauge space and about the space-fixed x axis. It is intended to build into the code also a hexadecupole interaction, in order to account for a possible $\epsilon_4$ deformation of the qp states.

4. Results

The experimental and calculated Routhian energies $E'(\omega)$ are shown in fig. 3 for the frequency interval $\omega = 0.1$ to 0.3 MeV. The experimental frequency and Routhian are obtained from the data with the prescriptions according to TAC [1, 7]. The theoretical curves correspond to TAC, PAC and DISQ approaches, using the same parameters as given previously. To make the comparison with the experimental Routhian better visible, we apply an arbitrary common shift of the theoretical Routhians in fig. 3. The mixing of the four cranking states described above can nicely reproduce the experimental splitting of the Routhian into the two signature branches. The analogous signature splitting of the PAC Routhian (i.e. the energy difference between the two quasiparticle states $|\vartheta = 0, \pm \rangle$ in fig. 2) becomes too small by about a factor three. The TAC Routhian belongs to the energetically favored quasiparticle states (fig. 1) compared to the PAC states but without a signature effect. Finally, the mixing of the PAC and TAC states leads to an increasing signature splitting that reaches at $\hbar \omega = 0.3$ MeV a few hundred keV and a size comparable to the observed splitting.

---

Footnote:

2Including a positive hexadecapole deformation $\epsilon_4$ in the PAC calculation (not considered here) may increase the amount of signature splitting, but it is beyond the scope of this paper to adjust the parameters for the best fit.
In fig. 4 calculated B(M1) and B(E2) values are displayed as a function of the frequency $\omega$, as found with TAC and PAC quasiparticle states and the eigenstates of the DISQ approach. The B(E2) values are calculated straightforwardly with the electric quadrupole operator. Concerning the M1 strength, it is known [2, 8, 7], that the calculation of the $\Delta I = 1$ magnetic dipole transition requires a correction for the nuclear recoil effect similar to the center of mass correction in the electric dipole transition. Therefore, the effective transversal ($\Delta I = 1$) magnetic dipole operator reads as [2]

$$ (\mu_{\Delta I = \pm 1})_{\text{eff}} = \mu_{\pm 1} - g_r I_{\pm 1} $$

where $g_r$ is the so-called gyromagnetic factor of the recoiling core and $\mu_{\pm 1}$ denote the usual magnetic dipole operator in spherical representation, i.e. for the (lab) x-quantization axis one has $\mu_{\pm 1} = \mp 1/\sqrt{2}(\mu_y \pm i\mu_z)$ and accordingly for the transversal spin components $I_{\pm 1}$.

In order to apply a $g_r$-value which is consistent with our cranking quasiparticle states, we take as in [9, 10]:

$$ g_r = \frac{\langle \mu_x \rangle}{\langle I_x \rangle}. $$

The $M1$-transition amplitude for pure TAC states $|\vartheta\rangle$ reduces to a simple expectation value $\langle \vartheta | \mu_{\pm 1} | \vartheta \rangle$. Then, the recoil contribution vanishes automatically since the stability condition (eq. 4) for the tilt angle $\vartheta$ implies a zero perpendicular spin component $\langle I_{\pm} \rangle$ [1]. This is not any more valid for the PAC and mixed states where we calculate the transition amplitude between signature partners as $\langle \alpha = -1/2 | \mu_{+1} | \alpha = +1/2 \rangle$. The above recoil term is important for obtaining the right average size of the B(M1) values. However, it only weakly influences the signature effects and it is not the origin of the resulting bifurcations in fig. 4.

For both the B(M1) and B(E2) values, one realizes in fig. 4 the deficiencies of the pure mean-field cranking states irrespective of whether one relies on TAC or PAC. The TAC approach gives the correct geometrical dependence of the M1 and E2 transition rates. Qualitatively, the tilt angle $\vartheta$ is large for the lowest frequency and, correspondingly, the rotational axis (spin orientation) is relatively close to the symmetry axis. Therefore, for low $\omega$ both the B(M1) and the B(E2) values are expected to be small since the effective deformation and the perpendicular magnetic moment seen along this rotational axis are small. For larger frequencies $\omega$, the tilt angle $\vartheta$ approaches zero and the rotational axis becomes more and more perpendicular to the symmetry axis, which leads to increasing effective deformation and perpendicular magnetic moment, i.e. to ascending B(M1) and B(E2) strength. Hence, this general frequency dependence is reflected by the TAC approach. This is not the case for the PAC states where in particular the B(E2) becomes constant. However, the PAC treatment can describe correctly the development of the signature effect in the B(M1) strength, which is outside the range of TAC.

The mixing of TAC and PAC states within DISQ indeed can reproduce both the geometrical dependence and the signature bifurcation. Thus, this model achieves the goal for which it was
designed. In particular, for the B(M1) strength one realizes the continuous transition from the TAC to the PAC regime when increasing the rotational frequency.

![Figure 4: Calculated $B(M1)$ in $(\mu N)^2$ (left) and $B(E2)$ values in (eb)$^2$ (right). Dashed curves: TAC, thin solid curves: PAC, thick solid curves: DISQ. The $B(M1)$ values show the developing signature bifurcation which is consistent with the energy signature splitting seen in fig 3. There is no signature effect in the $B(E2)$ values since the quadrupole deformation of two signature partners is about the same.]

5. Summary

The proposed DISQ approach, i.e. basically the superposition of appropriate mean-field quasi-particle states by diagonalization, is found to heal the apparent deficiencies of the mean-field cranking model related to the signature symmetry. This microscopic approach accomplishes the description of the gradually growing admixture of the intrinsic signature oscillation to the rotational motion seen experimentally as an expanding bifurcation of the band energies and in parallel in the $B(M1)$ transition strength. This splitting is a signal for the smooth transition from the TAC to the PAC regime, which is definitely out of the reach of the mean-field approximation.

The actual calculations performed for $^{175}$Hf included the total Routhian energy as well as the M1 and E2 transition strength as a function of frequency in the interval $\hbar \omega = 0.1 - 0.3$ MeV. The expected trends for the increasing development of the signature splitting and simultaneous staggering of the $B(M1)$ transitions between the two signatures partners can be nicely described within our approach.

The signature restoration in an odd-A nucleus considered in this paper is a relatively simple case of restoring the signature symmetry. However, the DISQ method is intended to be applied also to more complex situations, e.g. to odd-odd nuclei and triaxial nuclei where the bifurcation patterns are more complicated (c.f. [3]). For triaxial shapes additional stability points exist in the corresponding potential energy surface opening the possibility of novel tunneling modes.
between them. The study of those situations will be a new interesting subject. The DISQ approach is, of course, a general method which might be appropriate for other types of large amplitude motion, e.g. $K$-ismeric decay and band-crossing phenomena.

In a more general context, the symmetry restoration by the DISQ approach can be considered as a successful example for treating the many-body quantum motion in a double humped potential. The splitting process resembles the picture of a phase transition in a finite system where the rotational frequency plays the role of an order parameter. At low $\omega$ values with practically vanishing splitting, the nucleus can stay in a symmetry-broken phase having accidentally one of the stable orientations $\pm \theta_0$. For increasing $\omega$ values the system more and more bifurcates in two phases, realizing the required D2 symmetry. There is obviously a continuous transition region between the signature-broken TAC and the signature-conserving PAC regime.

Acknowledgements. This work is supported by the U. S. Department of Energy through contract no. DE-FG05-96ER40983 and by German Federal Ministry of Education, Science, Research and Technology. We like also to thank S. Frauendorf for important discussions.

References

[1] S. Frauendorf, Nucl. Phys. A557 (1993) 259c

[2] I. Hamamoto, Phys. Lett. 102B (1981) 225; 106B (1981) 281

Scientific, Singapore)

[3] T. Horibata, M. Oi and N. Onishi, Phys. Lett. 355 (1995) 433

[4] F. Dönauf, Phys. Rev. C58 (1998) 872

[5] P. Ring and P. Schuck, The Nuclear Many-Body Problem, Springer Verlag, 1980

[6] W. F. Mueller et al., Phys. Rev. C50 (1994) 1901

[7] S. Frauendorf and J. Meng, Z. Phys. 356 (1996) 263

[8] I. Hamamoto and H. Sagawa, Nucl. Phys. A327 (1979) 99

[9] M. Diebel, A. N. Mantri, and U. Mosel, Phys. Scr. 24 (1981) 164;

Nucl. Phys. A345 (1980) 72

[10] A. Ansari, E. Wüst, and K. Mühlhans, Nucl. Phys. A415 (1984) 215