High-Spin Consequences of Octupole Shape in Nuclei around ^{222}Th

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The effect of an octupole component in the intrinsic mean field at high spin is demonstrated by a Woods-Saxon-Bogolyubov cranking calculation. The nature of nuclear rotation becomes nearly collective instead of collective plus single-particle, because octupole couplings with Δl up to 3 "dilute" the high-j shells. Theory is consistent with experimental data on ^{222}Th and could be tested further by studying the properties of rotating quasiparticles in neighboring odd-mass nuclei.

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An interesting development in nuclear structure physics during the last few years has been the discovery that intrinsic reflection symmetry is spontaneously broken in the ground state of certain nuclei, contrary to previous beliefs. Better theoretical insight has been achieved into the microscopic origin of intrinsic "octupole shape" and its consequences for nuclear spectroscopy,[1-7] in conjunction with a range of new experiments.[8-15]

For rotational bands, molecular spectroscopy suggests that reflection asymmetry is characterized by spin states I of alternating parity $p=(-1)^I$, connected by collective $E1$ transitions. This situation was in fact recently observed[14,15] in nuclear spectroscopy at high spins ($I\sim 4$–17) for the nucleus ^{222}Th, which had previously been identified theoretically as a good candidate for reflection asymmetry.[3] It was also observed[11,13] in the nearby transitional nucleus ^{218}Ra. In analogy with low spins,[7] one might hope to learn more about the structure and symmetries at high spins through a study of low-lying quasiparticle states. The quasiparticles in rotating nuclei manifest themselves by the presence of various bands with distinctive properties.[16] We shall find that there is indeed an intimate interplay between rotation and the octupole mode, which helps to explain the ^{222}Th data and should be interesting to explore in the future. Any alternative interpretations of data, for example with α clusters,[13,15,17] should be distinguishable if there is a substantial difference in physical content.

Theoretical calculations of the single-particle states in an octupole-deformed rotating potential have been carried out previously,[18,19] but those calculations did not include the pair field and addressed different physical questions. The Hamiltonian in the present work is

$$\hat{H}=\hat{H}_{\rm WS}(\beta_2,\beta_3,\ldots)+\hat{H}_{\rm pair},$$

where $\hat{H}_{\rm WS}$ is a Woods-Saxon single-particle Hamiltonian[20] and $\hat{H}_{\rm pair}$ is a monopole pairing interaction, with parameters taken from Dudek and co-workers. The Woods-Saxon potential can have axially symmetric deformation with quadrupole (β_2), octupole (β_3), and higher multipole terms. Cranking constraints, $-\lambda\hat{N}$ and $-\omega\hat{I}_x$, are added to $\hat{H}$ before the eigensolutions are determined. The Fermi level, λ, is set to give the desired number of particles, $\langle\hat{N}\rangle$, in the vacuum on the average. Similarly, a prescribed finite rotational frequency, $\omega>0$, gives rise to angular momentum in the vacuum, $\langle I_x\rangle>0$. The constrained problem leads to equations whose solutions are quasiparticle configurations in a field characterized by a self-consistently determined "gap" parameter Δ (for details and original references see Cwiok *et al.*[23]). The eigenvalues which emerge from these equations are called "Routhians" rather than "energies," following the terminology of classical mechanics, since the value of the Hamiltonian in a rotating frame of reference is not identical with the energy.

Symmetries of the rotating potential are exploited to simplify the cranking equations. In recent years most authors have used symmetry under $\hat{R}_x$ and the associated quantum number, r, called "signature." With intrinsic parity broken it is, however, necessary to return to the original suggestion of Goodman[24] and use symmetry under $\hat{S} = \hat{\pi}\hat{R}_x^{-1}$, where $\hat{\pi}$ denotes the intrinsic parity operator. To distinguish from the signature, we shall refer to the associated quantum number as the simplex, s. The simplex of the rotating vacuum is $+1$, and the simplex of excited states is obtained by multiplying with the simplex of each quasiparticle. The spins and parities which occur in rotational bands[25] are, for $s = 1$,

$$I = 0^+, 1^-, 2^+, 3^-, \ldots;$$

for $s = -1$,

$$I = 0^-, 1^+ \cdot 2^-, 3^+, \ldots;$$

for $s = -i$,

$$I = \tfrac{1}{2}^-, \tfrac{3}{2}^+, \tfrac{5}{2}^-, \tfrac{7}{2}^+, \ldots;$$

and for $s = i$,

$$I = \tfrac{1}{2}^+, \tfrac{3}{2}^-, \tfrac{5}{2}^+, \tfrac{7}{2}^-, \ldots.$$

In the reflection-symmetric case, both r and π are good quantum numbers and $s = -\pi r$. Then the unnatural-parity states in a band have a vanishing norm.

There is no mechanism within the model which can given an energy shift between positive- and negative-parity states in a band. However, the calculated parity content of a quasiparticle state, $\langle \hat{\pi} \rangle$, might be a useful quantity for the analysis of such parity splitting where it occurs experimentally. In the spirit of the core-quasiparticle approach of Ref. 7, the in-band parity splitting would be obtained to lowest order by multiplying the phenomenological parity splitting of the core, i.e., the reference band,[16] by the $\langle \hat{\pi} \rangle$ for each quasiparticle.

The nucleus ^{222}Th was chosen for a first application of the Woods-Saxon-Bogolyubov cranking method with reflection asymmetry since suggestive data are available for this nucleus.[14,15] The deformation of the single-particle potential was held fixed at the ground-state equilibrium shape defined by the minimum of the Strutinsky energy surface in Fig. 1: $\beta_2 = 0.114$, $\beta_3 = 0.096$, $\beta_4 = 0.0678$, $\beta_5 = 0.0067$, and $\beta_6 = 0.0028$. An additional cranking calculation was carried out for comparison at the reflection-*symmetric* saddle-point shape, $\beta_3 = 0$. The potential energy of deformation in Fig. 1 also has a secondary minimum for spherical shape; cranking solutions at this point would be equivalent to multi-quasiparticle excitations in a spherical Woods-Saxon well.

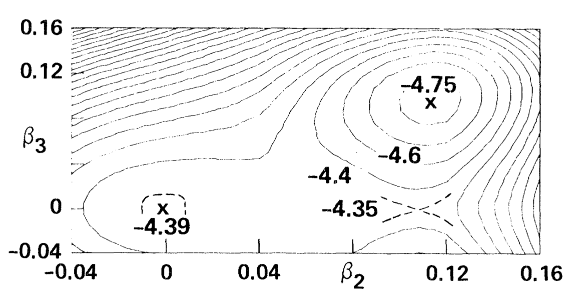

FIG. 1. Potential energy of β_2 and β_3 deformation for the nucleus ^{222}Th at angular momentum $I = 0$, calculated from the present Woods-Saxon model by Strutinsky renormalization to the macroscopic energy formula of Ref. 2. Appropriate β_4, β_5, and β_6 values were determined at each point. Indicated values are in megaelectronvolts.

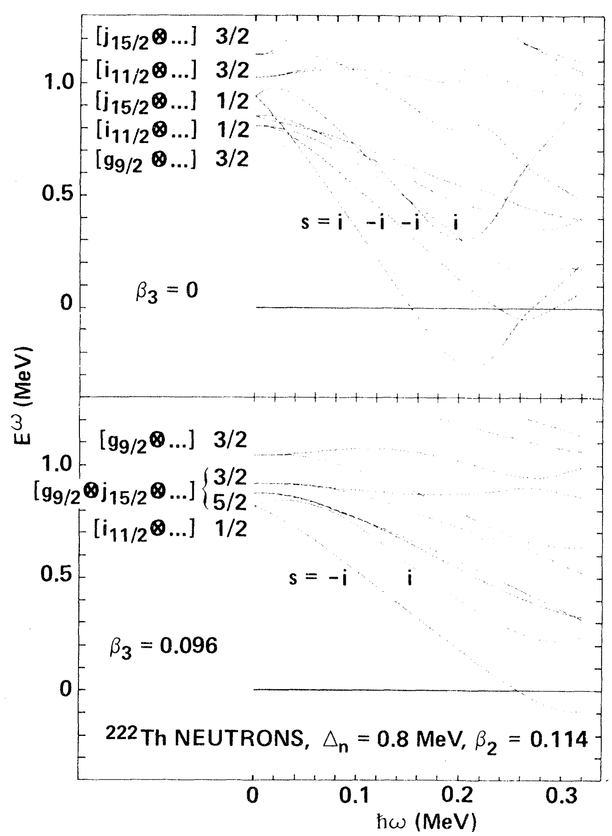

FIG. 2. Neutron quasiparticle Routhians, E^ω, vs rotational frequency, ω, from a Woods-Saxon-Bogolyubov cranking calculation for ^{222}Th at a fixed deformation with (bottom) and without (top) intrinsic reflection asymmetry. In order to suppress a profusion of irregularities at the crossings, we have arbitrarily fixed the pair gap Δ_n (but not the Fermi level) in this diagram. All other results in this Letter were obtained with self-consistent pairing.

Neutron quasiparticle Routhians, E^{ω}, obtained by solving the cranking equations are plotted in Fig. 2 versus rotational frequency, ω, at both the $\beta_3 = 0.096$ equilibrium shape (bottom) and the $\beta_3 = 0$ constrained equilibrium (top). The negative slope of a quasiparticle Routhian, $-dE^{\omega}/d\omega$, is equal to its rotation-aligned angular momentum $\langle \hat{j}_x \rangle$. An essential difference between the reflection-asymmetric and -symmetric cases can be seen in Fig. 2. At $\beta_3 = 0$, large alignment is acquired by the $j_{15/2}$ intruder states; they slope down rapidly with increasing ω and exchange character under a weak interaction with "holelike" solutions (not shown in Fig. 2). The physically observable consequence would be a band crossing and a "backbend" at relatively low rotational frequency along the yrast line.[26] Backbending was predicted for nuclei around ^{222}Th by earlier calculations[27] which did not include octupole deformation. For $\beta_3 \neq 0$, however, no orbital slopes down much more than the others and many orbitals have about equally large alignment. Similar results are obtained for protons. The basic reason is inherent to nuclear shell structure: Whereas quadrupole deformation only perturbs the high-j intruder subshells by couplings to the *next* major energy shell, octupole deformation mixes the intruders with states in the *same* major shell. Thus the high-j orbitals are fragmented by the octupole interaction onto several orbitals, in which the normal-parity valence-shell components contribute a smaller and sometimes inverted alignment. A detailed analysis of such mixing was given in a previous study[6,7] of decoupling factors, i.e., for the special case of $K = \frac{1}{2}$ and $\omega = 0$. Figure 2 shows that the fragmentation persists up to high spins, on the premise that octupole deformation persists up to high spins.

Results with self-consistent Δ_p and Δ_n are shown in the form of backbending plots in Fig. 3, along with the experimental data for ^{222}Th. The solid line represents the vacuum (yrast line) calculated with reflection asymmetry included. The three dashed curves for the symmetric case represent the ground band and two bands obtained by occupation of the lowest quasiparticle orbitals. These two-quasiparticle bands cross the ground band as indicated by the thin dashed lines in Fig. 3, so that a neutron-aligned band would be yrast above $\hbar\omega \sim 170$ keV ($E_\gamma \sim 340$ keV). Clearly the experimental data points fall closer to the solid curve, calculated for $\beta_3 = 0.096$. The deviations from the solid curve might be explained at low spins by spherical configuration mixing into the positive- but not the negative-parity states, as suggested by experimental

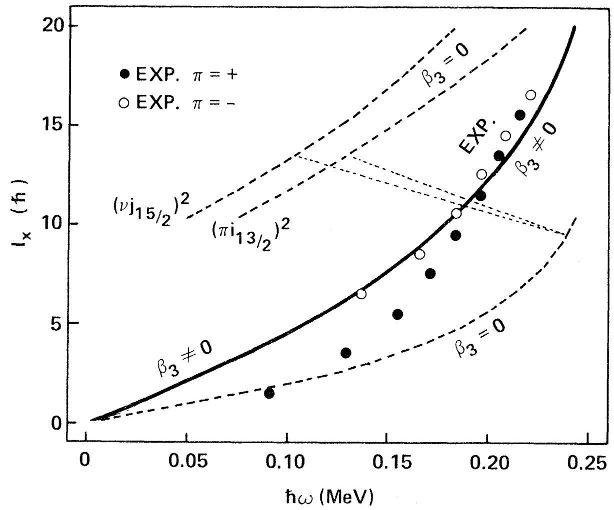

FIG. 3. Angular momentum, I_x, vs rotational frequency, ω, calculated for bands in ^{222}Th with (solid curve) and without (dashed curves) intrinsic reflection asymmetry. The experimental points are marked at $I_x = I + \frac{1}{2}$ and $\hbar\omega = \frac{1}{2}(E_{I+1} - E_{I-1})$.

systematics,[28] while at high spins a small additional contribution to I_x is expected from rotational couplings to axially asymmetric octupole modes.[29] Thus the solid line corresponding to $\beta_3 = 0.096$ in Fig. 3 accounts plausibly for the response to rotation of the deformed configuration, as manifested in the data.

The absence of a sharp backbend clearly distinguishes the $\beta_3 \neq 0$ case (solid curve) from $\beta_3 = 0$ (dashed curves in Fig. 3). For $\beta \neq 0$, neutron alignment does set in at the highest spins shown in Fig. 3 but does not fulfill the condition for backbending,[26] $V < j^2/4J$, where j is the alignment of the two neutrons, J is the ground-band moment of inertia, and V is the interband interaction. This is because j is smaller by a factor of almost 2 for $\beta_3 \neq 0$ relative to $\beta_3 = 0$, and J is larger by a factor of more than 2. V is about 60–120 keV for both cases, which is roughly equal to the critical value for backbending at $\beta_3 \neq 0$ but an order of magnitude smaller than the critical value at $\beta_3 = 0$. Needless to say, experimental data at higher spins would be very interesting, though a discussion of the phenomena that might set in lies beyond the scope of this Letter.

An easier experimental task would be to probe the core structure at intermediate spins by observing one-quasiparticle Routhians in neighboring odd-A nuclei. The lowest Routhian in most reflection-*symmetric* nuclei can be expected to come from a high-j intruder shell and to have the simplex $s = i$.

This is the case in the upper part of Fig. 2, where the neutron high-j intruder shell is $j_{15/2}$. However, for $\beta_3 \neq 0$ in the lower part of Fig. 2, an anomaly occurs in that the lowest neutron Routhian has $s = -i$, characteristic of $i_{11/2}$, and also a positive $\langle \hat{\pi} \rangle$. Specifically, $\langle \hat{\pi} \rangle = +0.70$ and $\langle \hat{j}_x \rangle = 3.5$ at $\hbar\omega = 0.14$ MeV, distinctly different from the $j_{15/2}$ values -1 and 6.7, respectively, at $\beta_3 = 0$. Anomalous yrast Routhians were also calculated for the odd-*proton* neighbors of ^{222}Th at $\beta_3 \neq 0$. Two Routhians with only small simplex splitting came lowest for $\beta_3 \neq 0$, both with $\langle \hat{\pi} \rangle \sim -0.2$ and $\langle \hat{j}_x \rangle \sim 3$ at $\hbar\omega = 0.14$ MeV and thus distinctly different from the single $i_{13/2}$ Routhian with positive parity and $\langle \hat{j}_x \rangle \sim 5.5$ obtained for $\beta_3 = 0$. The primary admixture to $i_{13/2}$ is $h_{9/2}$, which alters both the parity and the favored simplex.

In summary, octupole deformation explains the absence of a backbend in ^{222}Th and is expected to manifest itself in odd-A neighboring nuclei by a relatively small alignment in the yrast band ($\langle j_x \rangle \sim 3$–$4$) and a similar alignment in all the side bands ($\langle j_x \rangle \sim 1$–$2$).

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