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COLLECTIVE ROTATION OF NUCLEI WITH TETRAHEDRAL SYMMETRY*

N. Schunck

Department of Physics, University of Surrey, Guildford, GU2 7XH, UK

J. Dudek

IReS IN_2P_3-CNRS/Université Louis Pasteur
F-67037 Strasbourg Cedex 2, France

and S. Frauendorf

Nuclear Structure Laboratory
University of Notre Dame, IN 46556, USA

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Collective rotation of tetrahedral nuclei is analyzed within a three-dimensional cranking model. The favored orientation of the rotational frequency vector with respect to the turning nucleus as function of angular momentum is obtained from the total energy calculations. A new quantum number, resulting from the particular symmetry of the cranking Hamiltonian of the nuclei with tetrahedral nuclei is discussed. Some consequences for the structure of the rotational bands are presented.

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1. Introduction: motivations and calculation technique

Low-lying energy minima associated with high-rank symmetries of the nuclear surface, such as the tetrahedral and octahedral ones, have been predicted to exist in several neutron- and proton-rich nuclei by both phenomenological and self-consistent mean-field calculations [1, 2]. In this paper, we present for the first time the main features of rotating nuclei of

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tetrahedral symmetry following the microscopic three-dimensional cranking calculations. Our study focuses on ^{110}Zr which is predicted to be one of the best candidates for the tetrahedral symmetry in the medium-mass range.

In our analysis, the shape of the nucleus is described by the standard expansion of the nuclear surface onto the basis of spherical harmonics, with the deformation parameters $\alpha_{\lambda,\mu}$. In a 3-dimensional cranking approach, the rotation is described by a set of three Lagrange parameters often referred to as a rotational frequency vector $\vec{\omega}$, whose orientation is specified by the two spherical (also called 'tilt') angles θ and φ. The single-particle Hamiltonian in the rotating frame reads:

$$\hat{h}^{\vec{\omega}} = \hat{h}_0 - \vec{\omega} \cdot \hat{j}\,, \tag{1}$$

where $\hat{h}_0$ is the Hamiltonian at $\vec{\omega} = \vec{0}$, and $\hat{j}$ represents the three components $\{\hat{j}_x, \hat{j}_y, \hat{j}_z\}$ of the nucleonic angular-momentum operator. We use the Woods–Saxon mean-field Hamiltonian with the parameterization of [3]. In a no-pairing approach, the total energy in the rotating-frame (total Routhian) is the sum of the liquid drop- and the shell-energies:

$$R(\vec{\omega};\ \theta,\varphi) = R_{\text{macro}}(\vec{\omega};\ \theta,\varphi) + R_{\text{shell}}(\vec{\omega};\ \theta,\varphi)\,. \tag{2}$$

We use the LSD parametrization of [4] for the macroscopic energy. The expectation values of the components of the angular momentum $\hat{j}$ are:

$$j_\mu(\,\vec{\omega}) = \sum_\nu \langle \varphi_\nu^{\vec{\omega}} | \hat{j}_\mu | \varphi_\nu^{\vec{\omega}} \rangle\,, \tag{3}$$

where $\varphi_\nu^{\vec{\omega}}$ are the single-particle wave-functions in the rotating frame. The total angular momentum is obtained from the expectation values of

$$j^{\,2}(\vec{\omega}) = j_x^2(\vec{\omega}) + j_y^2(\vec{\omega}) + j_z^2(\vec{\omega}) \quad \leftrightarrow \quad I(I+1)\,. \tag{4}$$

The total energy in the laboratory frame can then be obtained from the canonical transformation:

$$E(\vec{\omega};\ \theta,\varphi) = R(\vec{\omega};\ \theta,\varphi) + \vec{\omega} \cdot \hat{j}(\vec{\omega})\,. \tag{5}$$

The total energy as function of spin, $E(I;\,\theta,\varphi)$, is calculated by interpolation of the $E(\omega;\theta,\varphi)$. We used a mesh of $N = 11$ frequencies with a step $\Delta\omega = 0.05$ MeV.

2. Results: new conserved quantum number

In the following we select the $\mathcal{O}_z$ axis of the reference frame to coincide with one of the C_2 and one of the S_4 rotation-inversion symmetry axes of the tetrahedron. Figure 1 shows the variation of the total energy as a function of the two tilt angles θ and φ at low angular momenta. There appear to exist two favoured axes of rotation, characterized by the set of angles $(\theta, \varphi) \equiv (0, \varphi)$ and $(\theta, \varphi) \equiv (\pi/2, \pi/4)$. These two orientations correspond to the C_2^z symmetry axis and another S_4 rotation-inversion symmetry-axis of the tetrahedral point group T_d, respectively.

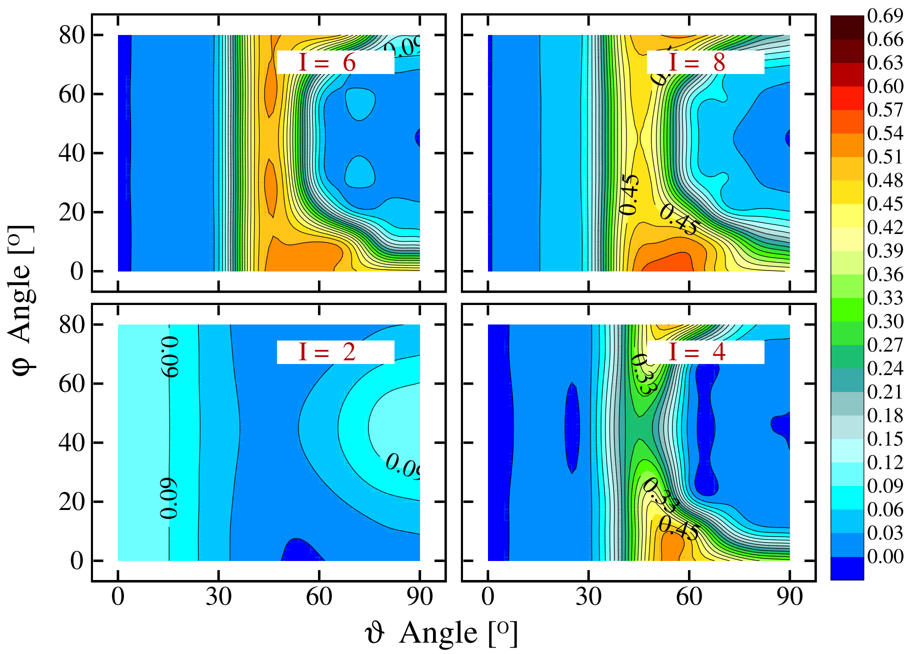

Fig. 1. Total energy in [MeV] as a function of the two tilt angles θ and φ for spins $2\hbar$ to $8\hbar$ in ^{110}Zr. The deformation of the nucleus is fixed and set to $\alpha_{32} = 0.15$, which corresponds to the value in the tetrahedral minimum [2].

As long as the stable axis of rotation coincides with the $\mathcal{O}_z$-axis of the coordinate system, the yrast energies can be calculated from (1) assuming $\omega_x = 0$ and $\omega_y = 0$ and (2) the nucleus is invariant under C_2^z which implies the conservation of the signature. The related eigenvalues are $r = e^{-i\pi\alpha}$ with $\alpha = 0, 1$. Moreover, there are three equivalent S_4 rotation-inversion axes, one of them coinciding with the z-axis of the Cartesian body-fixed reference frame. The operator performing the 90° rotation-inversion about the z-axis is:

$$S_4^z: \quad \hat{\mathscr{D}}_z = \hat{\mathscr{P}} e^{-i\frac{\pi}{2}\hat{j}_z}\,, \tag{6}$$

where $\hat{\mathscr{P}}$ stands for the parity. For the stable $\mathcal{O}_z$-axis rotation the yrast states are obtained by setting $\vec{\omega} = \{0, 0, \omega_z\}$, and the so-constrained operator (1) commutes with (6) thus leading to another conserved quantum number. Since the quantum number associated with $\hat{\mathscr{S}}_z = \hat{\mathscr{P}} e^{-i\pi\hat{j}_z}$ is traditionally called *simplex*, the former will be referred to as *doublex*. We have: $\hat{\mathscr{D}}_z^2 = \hat{\mathscr{R}}_z$. For an even system of fermions: $\hat{\mathscr{D}}_z^4 = 1$ wherefrom it follows that the eigenvalues d of $\hat{\mathscr{D}}$ verify: $d = e^{-i\pi\delta}$ with $\delta = 0, \frac{1}{2}, 1, \frac{3}{2}$. The relation between the signature and the doublex also implies that: $\delta = \frac{\alpha}{2}$ or $\delta = \frac{\alpha}{2} + 1$; with $\alpha = 0, 1$, we have indeed four different doublex eigenvalues. Consequently, using the signature is in fact redundant and we can work with the doublex only.

It is well-known that, for ellipsoidal even-even nuclei, the rotational bands built on top of an intrinsic configuration with a given signature can only contain either states of even spin ($\alpha = 0$) or odd spin ($\alpha = 1$) [5]. The conservation of the doublex specifies the projection of the total angular momentum and puts additional constraints on the parity of the states. Let us denote by $|\Psi\rangle$ the mean-field wave-function of the nucleus. In a tetrahedral system, $|\Psi\rangle$ is not an eigenvector of the operators $\hat{I}^2$, $\hat{I}_z$ and $\hat{\mathscr{P}}$. However, it can be expanded onto a basis of such states with good angular momentum, parity and K quantum number. We have

$$|\Psi\rangle = \sum_{IK,\pi} c_{IK,\pi} |\Phi_{IK,\pi}\rangle \;\; \rightarrow \;\; \hat{\mathscr{D}}_z |\Psi\rangle = \sum_{IK,\pi} c_{IK,\pi}\, \pi e^{-i\frac{\pi}{2}K} |\Phi_{IK,\pi}\rangle\,. \tag{7}$$

However, since the doublex symmetry is conserved, $|\Psi\rangle$ must also be an eigenstate of $\hat{\mathscr{D}}_z$, with the eigenvalue $e^{-i\pi\delta}$. This leads to: $e^{-i\pi\delta} = \pi e^{-i\frac{\pi}{2}K}$ for all $I \geq |K|$ and π. Given the fact that $\alpha = 0$ is associated with $\delta = 0, 1$ while $\alpha = 1$ with $\delta = \frac{1}{2}, \frac{3}{2}$, the above phase relation leads to the following solutions:

$$\delta = 0 \quad \pi = +1: \quad K = \;\ldots -8, -4, 0, +4, +8, \ldots\; I \text{ even}\,, \tag{8}$$

$$\pi = -1: \quad K = \;\ldots -6, -2, \quad +2, +6, \ldots\; I \text{ even}\,, \tag{9}$$

$$\delta = \frac{1}{2} \quad \pi = +1: \quad K = \;\ldots -7, -3, \quad +1, +5, \ldots\; I \text{ odd}\,, \tag{10}$$

$$\pi = -1: \quad K = \;\ldots -5, -1, \quad +3, +7, \ldots\; I \text{ odd}\,, \tag{11}$$

$$\delta = 1 \quad \pi = +1: \quad K = \;\ldots -6, -2, \quad +2, +6, \ldots\; I \text{ even}\,, \tag{12}$$

$$\pi = -1: \quad K = \;\ldots -8, -4, 0, +4, +8, \ldots\; I \text{ even}\,, \tag{13}$$

$$\delta = \frac{3}{2} \quad \pi = +1: \quad K = \;\ldots -5, -1, \quad +3, +7, \ldots\; I \text{ odd}\,, \tag{14}$$

$$\pi = -1: \quad K = \;\ldots -7, -3, \quad +1, +5, \ldots\; I \text{ odd}\,. \tag{15}$$

3. Summary

We show by a microscopic 3-dimensional cranking analysis that at low spins, the favoured axes of rotation for tetrahedral nuclei are the rotation-inversion symmetry axes of the T_d point group of symmetry. This leads to 8 characteristic families of rotational bands, *cf.* Eqs. (8)–(15), that conserve the doublex- simultaneously with signature-symmetry.

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