Triaxial rotation-axis flip triggered by an isoscalar *np* pair

P. C. Srivastava,¹ S. Åberg,² and I. Ragnarsson²

¹Department of Physics, Indian Institute of Technology, Roorkee 247 667, India ²Mathematical Physics, Lund University, Post Office Box 118, S-221 00, Lund, Sweden (Received 4 October 2016; published 24 January 2017)

We show that the rotation axis of a triaxial nucleus may flip from the intermediate axis ($\gamma = -30^{\circ}$) to the smallest axis ($\gamma = +30^{\circ}$) due to the polarization by an aligned T = 0 np pair. The example we discuss is the triaxial N = Z nucleus ⁶⁴Ge where the isoscalar $\pi(g_{9/2}) \otimes \nu(g_{9/2})$ pair aligns to $i^{\pi} = 9^+$ in ⁶⁶As and flips the rotation from $\gamma \approx -30^{\circ}$ to $\gamma \approx 30^{\circ}$. Calculations are performed in the spherical shell model as well as in the cranked Nilsson-Strutinsky model, supporting the suggested scenario. The role of the np interaction in forming the np pair is discussed in both models.

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The possibility for atomic nuclei to exist with stable triaxial shapes has been discussed since the 1950s [1,2]. The nucleus may show a triaxial ground-state deformation, or the triaxiality could appear in some excited states. Shell effects associated with certain particle numbers and deformations are considered to be responsible for the appearance of triaxiality [3]. Particularly interesting features of triaxiality may appear in N = Z nuclei where shell effects from protons and neutrons are in phase and where the np interaction plays an important role.

The rotational pattern of excited states of the triaxial nucleus is expected to exhibit unique features, such as quantized wobbling motion [4] (experimentally observed in some nuclei around ¹⁶³Lu [5]) or chiral band structures [6]. In an even-even nucleus with a stable triaxial ground-state deformation, the ground-state rotational band is expected to look similar to a band of a deformed axially symmetric nucleus, i.e., no direct sign of triaxiality. However, as discussed below, electromagnetic properties are sensitive to triaxiality and may be used to determine the triaxiality as well as the rotational axis.

In this Rapid Communication we discuss the rotational features of N = Z nuclei that possess large triaxiality, i.e., $\gamma \approx 30^{\circ}$ because of shell effects. At low-spin values due to pairing, the rotation is then generally expected to be favored around the intermediate axis ($\gamma = -30^{\circ}$) that corresponds to the axis with the largest moment of inertia. However, if angular momentum-aligned particles in high-j shells are added to the triaxial core, a competition of the rotation axes takes place since the aligned particles favor positive- γ rotation [7,8]. For N = Z nuclei neutron-proton interactions become important. Recently evidence for a spin-aligned neutron-proton paired phase has been reported from the level structure of ⁹²Pd in Ref. [9]. Also, favorable configurations are observed built from maximal aligned isoscalar-coupled nucleon pairs in high-*i* shells, see, e.g., Ref. [10]. The particular favoring of forming such an np pair implies a building block with a large spin vector that could flip the rotation axis of a triaxial rotor.

A favorable case for this phenomenon is the even-even nucleus ⁶⁴Ge. Its ground state is suggested to be triaxial in several calculations (see, e.g, Refs. [11–13]) as well as from data [11]. Adding a strongly *np*-coupled isoscalar pair in the $g_{9/2}$ shell $\pi(g_{9/2}) \otimes \nu(g_{9/2})$ adds an angular momentum vector of i = 9 to the triaxial core. A T = 0 rotational band in ⁶⁶As is

thus formed by coupling the ground-state band (gsb) of ⁶⁴Ge to the i = 9 np pair. The triaxial rotor may then flip the rotation axis from the *intermediate* axis (negative- γ rotation) in ⁶⁴Ge, and the 9⁺ band in ⁶⁶As corresponds to a rotation around the *smallest* axis (positive- γ rotation). A candidate for this 9⁺ band has been observed [14].

To investigate this idea in detail we perform calculations based on the (laboratory frame) shell model (SM) as well as the (intrinsic frame) cranked Nilsson-Strutinsky (CNS) model. It is shown that an experimental verification implies measuring reduced transitional strengths B(E2) as well as spectroscopic quadrupole moments.

CNS calculations have been performed for two N = Znuclei, namely, the even-even ⁶⁴Ge and the odd-odd ⁶⁶As on the (ε_2, γ) plane with implicit minimization of the ε_4 deformation. Pairing is neglected, implying less accuracy for calculated low-spin states, whereas calculated deformations, related to B(E2) values and spectroscopic moments, are less sensitive to pairing. For details of the CNS calculation, see Ref. [15] and references therein. The set of new parameters introduced in Ref. [16] is used.

Total-energy surfaces on the (ε_2, γ) plane from the CNS calculation are shown for ⁶⁴Ge (Fig. 1) and ⁶⁶As (Fig. 2). Axial symmetry corresponds to $\gamma = 0^{\circ}, -120^{\circ}$ (prolate shapes) and $60^{\circ}, -60^{\circ}$ (oblate shapes) with noncollective rotation (particle-hole excitations) for $\gamma = 60^{\circ}$ and -120° . The rotation takes place around the smallest axis for $\gamma > 0^{\circ}$, the intermediate axis for $-60^{\circ} < \gamma < 0^{\circ}$, and around the longest axis in the sector $-120^{\circ} < \gamma < -60^{\circ}$. There are 4 + 4 valence particles and 5 + 5 valence particles outside the ⁵⁶Ni core in ⁶⁴Ge and ⁶⁶As, respectively. At low spins they are placed essentially in the *pf* orbitals (referring to the pseudospin partners $p_{3/2}, f_{5/2}$), whereas particles have to be lifted to the $g_{9/2}$ orbitals to obtain higher-spin values.

The ground-state deformation for ⁶⁴Ge is found to be triaxial with $\gamma \approx 30^{\circ}$ and $\varepsilon_2 \approx 0.22$. This agrees with other mean-field calculations, see, e.g., Refs. [11–13]. At I = 0 (no rotation) the same minimum is seen [Fig. 1(a)] in all three sectors, but as I increases the minimum is lowest for rotation around the middle axis, i.e., for $\gamma \approx -30^{\circ}$. At I = 4 the rotation around the middle axis is favored by more than 1 MeV as compared to rotation around the other axes. If pairing

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FIG. 1. CNS calculated total-energy surfaces on the (ε_2, γ) plane for the ground-state band of ⁶⁴Ge. Surfaces are shown for angular momenta $I^{\pi} = 0^+, 2^+, 4^+, 8^+$. Contour line separation is 0.4 MeV.

is included in the CNS calculation we expect that the rotation around the middle axis is even more favored since pairing generally makes the moment of inertia around the middle axis largest (cf. the irrotational flow moment of inertia). This band should thus be identified with the ground-state band with observed states $I^{\pi} = 0^+ - 8^+$ [11].

For ⁶⁶As we consider the configuration with the two odd particles placed in the $g_{9/2}$ shell. This configuration may be identified with the observed T = 0 band with 9^+ , 11^+ , and 13^+ [14,17] where the 9^+ state is found to be isomeric [18]. In Fig. 2 it is seen how the minimum at positive γ values is clearly lowest in energy for this configuration, found at $\varepsilon \approx 0.29$ and $\gamma \approx 37^{\circ}$. The two particles in $g_{9/2}$ have thus changed the equilibrium γ deformation from $\gamma \approx -30^{\circ}$ in 64 Ge to $\approx +30^{\circ}$ in 66 As. The Coriolis force acts to align the collective spin vector with the spin vector of the aligned np pair. This mechanism is strengthened by the increase in the γ deformation towards noncollective rotation as the spin increases and implies that the total rotational vector is mainly in the x direction, i.e., along the shortest axis. At $I^{\pi} = 17^+$ we notice two minima: one at $\gamma \approx 60^{\circ}$ and one at $\gamma \approx 20^{\circ}$. We identify the nonvrast minimum at $\gamma = 60^{\circ}$ as the terminated state of the 9⁺ rotational band. In Fig. 3 the energies of this band are compared with data showing excellent agreement.

In the CNS picture, the driving force of a particle in the $g_{9/2}$ shell towards positive γ is related to how the alignment of

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FIG. 2. The same as in Fig. 1 but for the 9⁺ band in ⁶⁶As. Surfaces are shown for angular momenta $I^{\pi} = 9^+, 11^+, 15^+, 17^+$. Note the secondary minimum at $\gamma = 60^\circ$ (noncollective rotation) for $I = 17^+$.

angular momentum varies with γ . For $\gamma \gtrsim 30^{\circ}$ the alignment of the lowest $g_{9/2}$ orbit is close to maximal i = 9/2 already at zero rotation. Putting two particles in the $g_{9/2}$ shell the driving effect is strengthened. Maximal effect is obtained for one proton and one neutron in the same orbit, i.e., an isoscalar pair with maximal aligned angular momentum i = 9 at a low-energy cost.

We thus find that adding a np pair to the triaxial groundstate band of ⁶⁴Ge flips the rotation axis from intermediate to smallest axis in ⁶⁶As. This scenario is physically intuitive and clear from the CNS intrinsic-frame mean-field description. We now study the same bands in the laboratory frame shellmodel method. In the SM calculation, ⁵⁶Ni is taken as the inert core with the spherical orbits $1p_{3/2}$, $0f_{5/2}$, $1p_{1/2}$, and $0g_{9/2}$ forming the basis space. The jj44b interaction developed by Brown and Lisetskiy [19] is used here. The shell-model calculation is performed using the code ANTOINE [20].

We identify the measured $9^+ T = 0$ band in ⁶⁶As with the lowest calculated band with (about) one proton and one neutron occupying the $g_{9/2}$ shell. The isoscalar coupling of the *np* pair to maximal spin i = 9 is indeed very favorable, cf. the discussion in Ref. [9]. In both SM and CNS calculations the 9^+ state comes out as very favored in energy. Energies calculated in the SM for the ground-state band of ⁶⁴Ge and the 9^+ band of ⁶⁶As are compared to data in Fig. 3. Both calculated bands show very good agreement with data. CNS



FIG. 3. Measured energies of the ground-state (T = 1) band of ⁶⁴Ge and the 9⁺ (T = 0) band of ⁶⁶As (band 4 in Ref. [17]) are compared to SM and CNS calculations. Energies are renormalized to band-head energies; in the SM and unpaired CNS calculations the excitation energy of the 9⁺ state in ⁶⁶As is calculated to 1.96 and 0.99 MeV, respectively. In the CNS two 17⁺ states are shown where the dashed line marks the yrast state, and the solid line corresponds to a continuation of the 9⁺ band structure, see Fig. 2.

calcutated energies of the 9⁺ band in ⁶⁶As also are found to well reproduce measured energies. In the neighboring odd-odd N = Z nucleus ⁶²Ga a 9⁺ band with the same structure has been observed up to termination $I = 9^+ \cdots 17^+$ [21]. In the CNS calculation the gsb of ⁶⁴Ge is found to be too compressed as compared to the data. This is in line with the expectation that the calculated moment of inertia is too large due to the neglect of pairing.

It is interesting to compare the mechanism of the strongly coupled isoscalar *np* pair in the SM and in the CNS. In the SM the coupling of a $(g_{9/2})^2$ isoscalar pair to maximal angular momentum i = 9 is exceptionally favored with a diagonal matrix element of -2.1 MeV. This can be compared to the corresponding matrix element of coupling an isovector pair in $g_{9/2}$ to maximal spin i = 8 being 0.2 MeV, that is a difference of about 2.3 MeV. In the CNS no explicit np interaction is included. However, an implicit np interaction is included by the requirement of the same deformation of neutrons and protons. One proton and one neutron (that is an isoscalar pair) in the same $g_{9/2}$ orbit then becomes very favorable, in particular, at large positive γ deformation where an alignment of i = 9 is obtained at low-energy cost. If instead an isovector pair is added in $g_{9/2}$, e.g., two protons or two neutrons, the two particles occupy the two most favorable $g_{9/2}$ states, one with alignment i = 9/2 and the other with i = 7/2 (Pauli principle), i.e. in total with alignment i = 8. The two lowest $g_{9/2}$ states have an energy split of about 2 MeV at the 9⁺ deformation of ⁶⁶As. This means that in the CNS the isovector i = 8 state comes about 2 MeV higher in energy than the isoscalar i = 9state, i.e., a very similar energy difference as obtained from the SM diagonal matrix elements.

Electromagnetic (E2) quadrupole transition-matrix elements as well as spectroscopic quadrupole moments can be calculated in both the CNS (approximately) and the SM models (using effective charges). In the CNS the moments

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can be relateapproximately to the triaxiality through the relations [4,22],

$$B(E2; I+2, K \to I, K) = \frac{5}{6\pi} \langle I+2K20|IK\rangle^2 Q_{22}(x)^2,$$
(1)

and

$$Q_{\text{spec}}(I,K) = -2\langle II20|II\rangle\langle IK20|IK\rangle Q_{20}(x), \quad (2)$$

where x is the rotation axis. These relations work very well for arbitrary values of I (and K) for axially symmetric shapes. For axially asymmetric (triaxial) shapes, the expressions are approximately correct for large spin values. The full spin vector then is assumed along the x axis, i.e., $I \approx I_x \gg I_z$, and K is set to zero in Eqs. (1) and (2). To use the expressions for arbitrary triaxial shapes at small values of I, the relations are of course approximations but still expected to give results accurate enough for the present discussion.

The two (charge) quadrupole moments in Eqs. (1) and (2) are defined along the rotation axis x as

$$Q_{20}(x) = 2\langle x^2 \rangle - \langle y^2 \rangle - \langle z^2 \rangle, \qquad (3)$$

and

$$Q_{22}(x) = \sqrt{\frac{3}{2}}(\langle z^2 \rangle - \langle y^2 \rangle), \tag{4}$$

where the averages are taken over the proton distribution at the considered nuclear shape. Assuming the same density shapes as the potential parametrization, (ε_2, γ) , $Q_{22}(x)$, and $Q_{20}(x)$ are calculated easily from analytical expressions. The two moments for ⁶⁴Ge and ⁶⁶As are shown in Fig. 4 versus the triaxiality parameter γ covering the region $-60^{\circ} < \gamma < +60^{\circ}$. This corresponds to rotation around the middle axis ($\gamma < 0^{\circ}$) and around the smallest axis ($\gamma > 0^{\circ}$). In the limit of small quadrupole deformation, the expressions



FIG. 4. Variation with triaxiality of intrinsic quadrupole moments $Q_{20}(x)$ and $Q_{22}(x)$ for ⁶⁴Ge (dashed lines) and ⁶⁶As (solid lines). Quadrupole deformations are taken from CNS calculations $\varepsilon_2 = 0.22$ and $\varepsilon_2 = 0.29$ for I = 0 in ⁶⁴Ge and I = 9 in ⁶⁶As, respectively.

simplify to $Q_{20}(x) = -\frac{4}{5}r_o^2 A^{2/3}eZ\varepsilon_2 \sin(\gamma + 30^\circ)$ and $Q_{22}(x) = \frac{2\sqrt{2}}{5}r_o^2 A^{2/3}eZ\varepsilon_2 \cos(\gamma + 30^\circ)$, i.e., B(E2) is proportional to the geometrical distance [on the (ε_2, γ) plane] to the $\gamma = -120^\circ/60^\circ$ axis, and Q_{spec} is proportional to the distance to the $\gamma = -30^\circ$ axis.

The limit $\gamma = 60^\circ$, corresponding to noncollective rotation with the rotational axis coinciding with the (oblate) symmetry axis, gives $Q_{22}(x) = 0$ that implies B(E2) = 0. It is interesting that there is also a γ value where the spectroscopic moment vanishes $Q_{\text{spec}} = 0$. This occurs when nuclear size along the rotation axis (measured as $\langle x^2 \rangle$) coincides with the mean value of the sizes along the perpendicular axes, see Eq. (3). For small quadrupole deformations this occurs at $\gamma = -30^\circ$. For the calculated deformations for ⁶⁴Ge and ⁶⁶As we find that $Q_{\text{spec}} = 0$ for $\gamma \approx -40^\circ$, see Fig. 4.

If a nucleus with a strong triaxiality ($\gamma = 30^{\circ}$) rotates around the smallest axis or the intermediate axis (i.e., $\gamma =$ $+30^{\circ}$ or $\gamma = -30^{\circ}$), the Q_{22} values [related to the B(E2)values] differ by a factor of ~ 1.5 , whereas the spectroscopic moments deviate by an order of magnitude. A calculation of the spectroscopic moment together with the B(E2) value in the SM is thus a way to determine a rotation axis in the intrinsic frame picture and to cross-check the scenario suggested by the CNS calculations.

In the SM the moments are calculated assuming effective charges $e_{\pi} = 1.5e$ and $e_{\nu} = 0.5e$. In the CNS the values of $Q_{22}(x)$ and $Q_{20}(x)$ are obtained at calculated equilibrium deformations, and B(E2) values and Q_{spec} are subsequently obtained from Eqs. (1) and (2), respectively. Quantum fluctuations are neglected in the CNS calculation. In lowest order we expect the vibrations in the ε, γ directions to give a small positive correction to calculated B(E2) values [since B(E2)is quadratic in $Q_{22}(x)$], whereas no change is expected for the Q_{spec} values (since Q_{spec} is linear in $Q_{20}(x)$), cf. the discussion in Ref. [22].



FIG. 5. B(E2) values for I_i to $I_i - 2$ transitions in ⁶⁴Ge and ⁶⁶As calculated in the SM (solid lines) and the CNS (dashed lines). The B(E2) value for the $2^+ \rightarrow 0^+$ transition in ⁶⁴Ge is measured as 410 e^2 fm⁴ [23].

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FIG. 6. Spectroscopic quadrupole moments Q_{spec} in ⁶⁴Ge and ⁶⁶As calculated in the SM (solid lines) and the CNS (dashed lines).

In Fig. 5, B(E2) values are shown for the bands considered in ⁶⁴Ge and in ⁶⁶As, calculated in the SM and the CNS. In general, the two calculations agree quite well. B(E2) values for the ground-state band in ⁶⁴Ge are somewhat larger in the CNS compared to the SM but with a similar spin variation. The measured B(E2) value for the $2^+ \rightarrow 0^+$ transition [23] 410 e^2 fm⁴ falls in between the two calculations. The gradual drift in triaxiality with increasing spin, suggested by the CNS calculation for ⁶⁶As from $\gamma \approx 30^\circ$ for I = 9 to $\gamma = 60^\circ$ for I = 17, implies a gradual drop towards zero (at $\gamma = 60^\circ$) of B(E2) in the CNS calculation that is also found in the SM calculation (band termination). The small and decreasing B(E2) values in the SM calculation support the CNS scenario that approximately the full spin vector is directed along the smallest rotational axis.

Corresponding results for the spectroscopic moments are shown in Fig. 6. The very small moments for the ground-state band of ⁶⁴Ge, suggested by the CNS calculation, are indeed very similar in the SM calculation. This strongly suggests the view of collective rotation around the intermediate axis ($\gamma \approx -30^{\circ}$) as obtained in the CNS. The Q_{spec} values for the band in ⁶⁶As calculated in the SM are somewhat smaller than the CNS values but with a very similar spin dependence.

The quadrupole moment $Q_{20}(z)$ of an axially symmetric rotor determines both the B(E2) value and the Q_{spec} . If an axial-symmetric rotor is assumed, the quadrupole moment may be extracted from the calculated B(E2) value and then used to calculate Q_{spec} . The Q_{spec} values obtained in this way for the considered states in ⁶⁴Ge become about three times *larger*, and for the states in ⁶⁶As they become about three times *smaller* as compared to the SM calculated Q_{spec} values. This little exercise shows the need for invoking triaxiality with different rotational axes in an intrinsic frame picture, such as the CNS in the understanding of moments calculated from the SM.

To summarize, we have shown how nuclei with maximal triaxiality ($\gamma \approx 30^{\circ}$) may flip the rotation axis, influenced by the isoscalar force. The triaxial nucleus ⁶⁴Ge is suggested to rotate around the intermediate axis ($\gamma \approx -30^{\circ}$) in its ground-state band. When an isoscalar *np* pair is added in

a high-*j* shell $g_{9/2}$, constituting an $I^{\pi} = 9^+$ band in ⁶⁶As, the most favored way to rotate is found to be around the smallest axis ($\gamma \approx 30^\circ$). The scenario is supported by two basically different theoretical models: the deformed mean-field model (CNS) and the spherical SM. In the SM the strong isoscalar np matrix element plays a crucial role. In the CNS no explicit np interaction is included, but the T = 0 np pair is favored by the Pauli principle and the assumption of the same shapes for protons and neutrons. The spin alignment of high-*j* orbits at large positive γ deformations causes a flip of the rotation axis. To experimentally confirm the rotation axis flip it would be highly interesting to perform Coulomb excitation measurements and test the predicted very small spectroscopic moments in ⁶⁴Ge and the high spectroscopic moments in ⁶⁶As.

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