The suggested presence of tetrahedral symmetry in the ground-state configuration of the $^{96}_{40}\text{Zr}_{56}$ nucleus

J Dudek$^{1,2}$, D Curien$^{1,2}$, D Rouvel$^{1,2}$, K Mazurek$^{3}$, Y R Shimizu$^{4}$ and S Tagami$^{4}$

$^1$ Institut Pluridisciplinaire Hubert Curien, IN2P3-CNRS, France
$^2$ Université de Strasbourg, 23, rue du Loess, BP 28, F-67037 Strasbourg Cedex 2, France
$^3$ The Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences ul. Radzikowskiego 152, PL-31432 Kraków, Poland
$^4$ Department of Physics, Faculty of Sciences, Kyushu University, Fukuoka 812-8581, Japan

E-mail: Jerzy.Dudek@unistra.fr, Dominique.Curien@iphe.cnrs.fr, David.Rouvel@iphe.cnrs.fr, Katarzyna.Mazurek@ifj.edu.pl, Shimizu@phys.kyushu-u.ac.jp and Tagami@phys.kyushu-u.ac.jp

Received 28 November 2013, revised 13 December 2013
Accepted for publication 14 December 2013
Published 29 April 2014

Abstract
We discuss predictions made by large scale calculations using the realistic realization of phenomenological nuclear mean-field theory. The calculations indicate that certain zirconium nuclei are tetrahedrally symmetric in their ground states. After a short overview of past research into nuclear tetrahedral symmetry we analyse the predictive capacities of the method and focus on the $^{96}_{40}\text{Zr}_{56}$ nucleus, which is expected to be tetrahedral in its ground state.

Keywords: point-group symmetries, nuclear tetrahedral symmetry, mean-field methods, zirconium ground-state properties

(Some figures may appear in colour only in the online journal)

1. Nuclear point-group symmetries: the search for tetrahedral symmetry—a short overview

The analysis of point-group symmetries of molecules has become one of the standard tools of molecular quantum mechanics. These symmetries often result from the relative positions of the constituent atoms (e.g. positions of hydrogen atoms in the CH$_4$ molecule) and in this sense their presence may be considered rather intuitive. In contrast, there seem to be no intuitively direct analogies with atomic nuclei, which can be considered compact objects whose volume is nearly equal to the sum of the volumes of the constituent nucleons. Moreover, the underlying strong interactions, both non-central and non-local, are much more complex than the Coulomb interactions governing molecular structure.

Despite that, the molecular-geometry guided intuition has been followed by certain authors, who have constructed group-theoretical models of nuclei based on the idea of modelling in terms of alpha clusters. As an example, analogous to the tetrahedral symmetry of methane molecules, the nuclear tetrahedral symmetry induced by four $\alpha$-clusters in $^{16}\text{O}$ has been discussed in e.g. [1].

Nuclear mean-field theory is one of the most successful tools used in the study of nuclear structure. Today, the most frequent realizations of this theory are: a. The phenomenological one (the so-called macroscopic–microscopic method); b. the relativistic mean field theory based on the Dirac formalism, and; c. the Hartree–Fock theory. The first of these is technically the best adapted to study nuclear geometrical symmetries. This is true in particular for the phenomenological Woods–Saxon realization of the approach,
according to which the central potential is constructed as
\[ V_{WS}(\vec{r}; V_0, R_0, a_0) \equiv \frac{V_0}{1 + \exp \left[ \text{dist}_4(\vec{r}; R_0)/a_0 \right]} \]  

(1)

where \( \Sigma \) denotes the nuclear surface and \( \text{dist}_4(\vec{r}; R_0) \) the distance of the point \( \vec{r} \) from the surface. Above, \( V_0, R_0 \) and \( a_0 \) are adjustable parameters characterising the potential depth, radius and diffusivity, respectively. In our approach, they are fixed once for all, i.e. for all the nuclei in the periodic table and independent of deformation—hence the name: ‘universal parameterisation’.

According to the above definition, the potential contains a constant diffusivity parameter and therefore has an overall linear dependence of the argument of the exponential on the distance of a given point \( \vec{r} \) from the nuclear surface. [This is in contrast to some alternative forms used in the literature, in which the diffusivity is treated as a position-dependent quantity.] It follows that the resulting Hamiltonian has exactly the same symmetry as the underlying nuclear surface. Of course similar can be said about the spin-orbit potential of the Woods–Saxon type. Consequently, the analysis of the point-group symmetries of the Woods–Saxon mean-field Hamiltonian can be reduced to the analysis of the point-group symmetries of the underlying nuclear surfaces.

With the help of such an approach it was shown for the first time in [2], that the non-trivial nuclear point-group symmetries, such as the tetrahedral one, can be easily realised with the help of realistic nuclear Woods–Saxon Hamiltonians with the single deformation parameter \( \alpha_{32} \). The calculated single-particle nucleonic spectra were shown to satisfy the two-fold and four-fold degeneracies related to the \( E_r \) and \( E^* \) (two-dimensional) and \( G \) (four-dimensional) irreducible representations of the tetrahedral group, cf figures 3 and 4 in the above reference. Moreover, it was shown that the local minima on the total potential energy surfaces corresponding to tetrahedral symmetry are obtained thus paving the way towards the idea of new, richer forms of shape coexistence in atomic nuclei. Such a coexistence may involve non-axial symmetries, i.e. different from the prolate/oblate quadrupole or pear-shape octupole symmetries discussed abundantly so far in the literature.

At the same time it has been suggested [2] that the new point-group symmetries generate new chains of magic numbers analogous to the well known ones: \( (Z/N)_{\text{spherical}} = 8, 20, 28, 50, 82 \) and 126 was generated by spherical symmetry. The prediction of the tetrahedral magic numbers \( (Z/N)_{\text{tetrahedral}} = 56, 64, 70, 90, 112 \) and 136 was formulated in the same article, where only moderately heavy and heavy nuclei were studied.

Extending realistic calculations which involve tetrahedral symmetry of nuclear shapes represented by the \( T_4 \) group and \( \alpha_{32} \) deformation parameter, from now on referred to as tetrahedral, it was shown that a combination of quadrupole and tetrahedral components may lead to a new class of shapes, symmetric with respect to the \( D_{3d} \) group. The latter describes, in the nuclear context, some exotic superdeformed shapes, with the spherical harmonic expansion in terms of the leading axial-quadrupole, \( \alpha_{20} \), and tetrahedral, \( \alpha_{32} \), components combined, as suggested in [3] (cf also [4], the latter focussed on the Hg-Pb region, and [5].)

Unfortunately, the names used sometimes in the literature to describe the related nuclear geometry such as ‘non-axial octupole shapes’, hide the presence of possibly very distinct symmetry effects. Indeed, the nuclear octupole deformations \( \alpha_{31}, \alpha_{32}, \alpha_{33} \) imply very different point-group symmetries. It may then become useful to design distinct spectroscopic criteria associated with each of these symmetries, e.g. in terms of the energy-versus-spin staggering (see below), approximate level degeneracies or specific branching ratios among the electromagnetic transitions; all these depending on the dominating\(^5\) symmetry.

The mean-field theory studies were continued in [6], where the tetrahedral-symmetry induced ‘magic’ gaps in the single-particle nuclear spectra have been found to include \( (Z/N)_{\text{tetrahedral}} = 16, 20, 32, \) and 40 for the relatively light nuclei, and 142 for the heaviest ones. In this context the role of the four-fold degeneracies, alternatively, the four-dimensional irreducible representations of the tetrahedral group, as the background of the large tetrahedral shell gaps has been emphasised. Moreover, the predictions related to the new forms of (tetrahedral) shape-isomerism have been formulated for \( ^{80}\text{Zr}, ^{106}\text{Zr}, ^{166}\text{Yb} \) and \( ^{212}\text{Fm} \).

These calculations have been extended in [7], employing the Skyrme Hartree–Fock technique with the SLy4 parameterisation. These results suggested that the very exotic \( ^{106–112}\text{Zr} \) nuclei are tetrahedral in their ground states [cf also [8]]. In [7], yet another research direction has been proposed and illustrated, viz. the application of group representation theory to calculate the symmetry-induced characteristic intensity branching ratios of the electromagnetic transitions emitted by the tetrahedrally symmetric nuclear quantum rotor [cf figure 4 in [7]].

A more general ‘theory of nuclear stability’ based on the point-group symmetries has been formulated in [9], where, moreover, the illustrations related to the tetrahedral symmetry minima in \( ^{88}\text{Zr}, ^{90}\text{Zr} \) and \( ^{110}\text{Zr} \) nuclei can be found, together with the indication that the axial-symmetry octupole-shape minima are in a direct competition with the tetrahedral ones, all at the zero quadrupole deformation. These calculations indicate that the nuclei in question should manifest strong octupole transitions and thus strong \( B(E3) \) values which according to theory, certainly do not correspond to the quadrupole-(super)deformed minima predicted in \( ^{88}\text{Zr} \) and \( ^{110}\text{Zr} \).

Independently, the Hartree–Fock mean-field calculations focused on the \( Z = N \) nuclei in [10], confirmed both the...
presence of the superdeformation and the instability of the spherical con-
figuration with respect to the $\alpha_{32}$ deformation in the tetrahedral doubly-magic nucleus $^{80}\text{Zr}_{40}$ showing the strongest effect in $^{96}\text{Zr}$. The data are from [13].

Among the three doubly-magic tetrahedral nuclei, i.e. $^{96}\text{Zr}_{40}$, $^{90}\text{Zr}_{46}$, and $^{110}\text{Zr}_{50}$, only the second one is stable. Consequently, the experimental results concerning the reduced probabilities for the $B(E3)$ transitions can be found in the literature only for this one, and for a few neighbouring nuclei. The existing results are presented in table 1, showing that the measured value for $^{96}\text{Zr}$, i.e. $B(E3) = 57 \pm 4$ W.u., clearly dominates. To our knowledge this is the largest $B(E3)$ value ever measured. Given the fact that the theory predictions favour the dominance of the $\alpha_{32}$ over $\alpha_{30}$, cf also the results in figures 3–4 below, one is tempted to suggest that these very

Table 1. Experimental values of the $B(E3)$ reduced transition probabilities in Weisskopf units for to the first $3^-$ excitation, in the vicinity of the tetrahedral doubly-magic nucleus $^{80}\text{Zr}_{40}$ showing the strongest effect in $^{96}\text{Zr}$. The data are from [13].

| Z versus N | 54 | 56 | 58 | 60 |
|------------|----|----|----|----|
| $\omega_{\text{Pd}}$ | —  | —  | 29 ± 10 |
| $\omega_{\text{Ru}}$ | 14 ± 3 | —  | —  | —  |
| $\omega_{\text{Mo}}$ | 31 ± 4 | 35 ± 3 | —  | —  |
| $\omega_{\text{Zr}}$ | 57 ± 4 | —  | —  | —  |
| $\omega_{\text{Sr}}$ | 18.3 ± 11 | —  | —  | —  |
big values should be attributed to the presence of the tetrahedral rather than octupole-axial symmetry. (For the domination of the $\alpha_3$ over $\alpha_2$ deformation, the reader is referred to figure 4 in [9] and to [14].) Finally, an overview of the tetrahedral symmetry oriented nuclear shell-effect calculations focussing on the rare earth nuclei can be found in [15].

More recent microscopic calculations addressing the issue of nuclear tetrahedral symmetry have been performed using advanced projection techniques [16] including the generator coordinate approach and various forms of nuclear interactions, varying between the phenomenological and the self-consistent Gogny Hartree–Fock approach. These calculations fully confirm the importance of tetrahedral symmetry on the nuclear level, the symmetry which strongly enhances nuclear stability properties. The calculations demonstrate in particular the existence of the privileged spin-parity combinations of the nuclear states forming the tetrahedral sequences (‘bands’), structures whose properties will be helpful in analysing the results of dedicated experiments, cf [17] and more particularly [18].

2. Testing the method’s prediction capacity in terms of nuclear non-axial configurations

Whereas nuclear quadrupole deformations are characterised by a single non-axiality parameter, $\alpha_2$, octupole non-axial degrees of freedom are characterised by three: $\alpha_2$, $\alpha_3$ (tetrahedral) and $\alpha_4$. According to the shape parameterisation in terms of the spherical harmonics, the non-axiality is determined by the $\phi$-dependence of the spherical harmonics $Y_{\mu}^{\ell} (\theta, \phi) \propto P_{\mu}^{\ell} (\cos \theta) \exp (i \mu \phi)$ and it follows that this dependence is identical for the non-axial quadrupole and tetrahedral symmetry shapes.
model calculations can be qualified as realistic; we believe that so too are the predictions for the nucleus of $^{96}\text{Zr}$, which will be discussed next.

3. Two competing octupole modes: the $^{96}\text{Zr}$ case

The calculations by the present authors, and by the authors cited above, leave no doubt that: a. the two octupole modes, i.e. $\alpha_{32}$ representing tetrahedral ($T_d$) symmetry, and $\alpha_{30}$ representing axial ($C_{∞}$) symmetry compete on the total energy maps in the zirconium region, and b. tetrahedral symmetry most often wins the competition. The strong presence of the collective octupole mode in the region as manifested by the experiment, cf. table 1 and surrounding text, clearly confirms this prediction. It then follows that the tetrahedral symmetry should be the dominating factor, and it will be instructive to illustrate the microscopic origin of this mechanism.

Figures 3 and 4 illustrate the characteristic dependence of the proton single-particle Woods–Saxon energies (the neutron levels present very similar features and are not shown here) on the two competing deformations. Observe that whereas for tetrahedrally symmetric shapes the gap at $Z = 40$ extends to very large deformations of about $\alpha_{32} \approx 0.3$, the same gap decreases continuously as a function of $\alpha_{30}$. Similar observations can be made about the gap at $Z = 56$ (in the case of protons this gap is close to the zero-binding limit, what is not the case for the neutrons). The origin of this systematic difference can be traced back to the four-fold degeneracies of the majority of the single-particle levels in the case of tetrahedral symmetry. The corresponding levels can be identified in figure 4 as marked with the double Nilsson labels. Due to the fact that the dominating majority of levels belong to this category the average inter-level spacing is systematically larger in the tetrahedral symmetry case leading to overall larger spacings.

According to our calculations, the ground-state minimum of $^{96}\text{Zr}$ corresponds to the tetrahedral deformation with $\alpha_{32} \approx 0.15$ and a small octahedral deformation, with the energy about 1300 keV below the spherical minimum. At the strict symmetry limit the excitation (and feeding) of the ground-state through collective transitions coming from either rotational or vibrational excited states is possible only via the octupole $E3$ transitions since the tetrahedral deformed quantum objects have vanishing collective quadrupole and dipole moments. However, such a state may receive transitions of the single-particle strengths from the non-collective particle–hole excitations. The lowest-lying non-collective excitations are expected to come either from the tetrahedral ground-state or from the excited spherical energy minimum giving rise to the $E\left( I = \{j^2\} \right)$ sequences as indicated schematically in figure 5. Since the highest-$j$ neutron orbital above the Fermi level is $g_{7/2}$ one may expect such sequences to terminate at $I^\pi = 6^+$ states. The dedicated analysis of the experimental data in this nucleus including the reduced transition probabilities, negative and positive parity rotational-like sequences and their possible interplay, partly following the lines discussed in [18], is in progress and will be published elsewhere.

4. The possible impact of tetrahedral symmetry

Because of the unusual four-fold degeneracies of single-nucleon levels, tetrahedral symmetry of the mean-field is expected to generate strong shell effects and thus relatively strongly bound ground- or shape-isomeric states. This is expected to justify the presence of the new waiting-point nuclei which would help to explain missing elements of the nucleosynthesis models and modify the known nuclear abundance scheme, in addition to paving the way to new spectroscopic features, new ideas about the structure (and the very definition) of the rotational bands (cf [18] in these proceedings) with new selection rules for the collective rotational transitions.

Acknowledgements

This work is supported by the LEA COPIGAL project 04-113 and by the COPIN-IN2P3 agreement No.06-126.
References

[1] Robson D 1982 Phys. Rev. C 25 1108
[2] Li X and Dudek J 1994 Phys. Rev. C 49 R1250
[3] Li X, Dudek J and Romain P 1991 Phys. Lett. B 271 281
[4] Skalski J 1992 Phys. Lett. B 274 1
[5] Skalski J 1991 Phys. Rev. C 43 140
[6] Dudek J, Góźdź A, Schunck N and Miskiewicz M 2002 Phys. Rev. Lett. 88 252502
[7] Schunck N, Dudek J, Góźdź A and Regan P H 2004 Phys. Rev. C 69 061305(R)
[8] Schunck N and Dudek J 2004 Int. J. Mod. Phys. E 13 213
[9] Dudek J, Mazurek K, Curien D, Dobrowolski A, Góźdź A, Hartley D, Maj A, Riedinger L and Schunck N 2009 Acta Phys. Pol. B 40 713
[10] Yamagami M, Matsuyanagi K and Matsuo M 2001 Nucl. Phys. A 693 579
[11] Olbratowski P, Dobaczewski J, Pwalowski P, Sadiak M and Zberek K 2006 Int. J. Mod. Phys. E 15 333
[12] Zberek K, Majerski P, Heenen P H and Schunck N 2006 Phys. Rev. C 74 5
[13] National Nuclear Data Center http://www.nndc.bnl.gov
[14] Zberek K, Heenen P H and Majerski P 2009 Phys. Rev. C 79 014319
[15] Dudek J, Curien D, Dubray N, Dobaczewski J, Pangon V, Olbratowski P and Schunck N 2006 Phys. Rev. Lett. 97 072501
[16] Tagami S and Shimizu Y R 2012 Prog. Theor. Phys. 127 79
[17] Tagami S, Shimizu Y R and Dudek J 2013 Phys. Rev. C 87 054306
[18] Tagami S, Shimada M, Fujioka Y, Shimizu Y R and Dudek J 2014 Phys. Scr. 89 054013
[19] Zamfir N Y and Casten R F 1991 Phys. Lett. B 260 265
[20] Toh Y et al 2013 Phys. Rev. C 87 041304
[21] Davydov A S and Filippov S 1958 Nucl. Phys. 8 237
[22] Wilets L and Jean M 1956 Phys. Rev. 102 788
[23] Singh B and Farhan A R 2006 Nucl. Data Sheets 107 1923
[24] Döring J et al 1998 Phys. Rev. C 57 2912
[25] Valiente-Dobón J J et al 2005 Phys. Rev. C 71 054309
[26] Schunck N PhD Thesis Strasbourg University http://tel.archives-ouvertes.fr/?language=en