Nuclear Tetrahedral Symmetry: Possibly Present Throughout the Periodic Table

J. Dudek\(^1\), A. Goźdz\(^{1,2}\), N. Schunck\(^1\) and M. Miśkiewicz\(^2\)

\(^1\)Institut de Recherches Subatomiques IN2P3-CNRS/Université Louis Pasteur
F-67037 Strasbourg Cedex 2, France

\(^2\)Katedra Fizyki Teoretycznej Uniwersytet Marii Curie-Skłodowskiej,
PL-20031 Lublin, Poland

More than half a century after the fundamental, spherical shell structure in nuclei has been established, theoretical predictions indicate that the shell-gaps comparable or even stronger than those at spherical shapes may exist. Group-theoretical analysis supported by realistic mean-field calculations indicate that the corresponding nuclei are characterized by the \(T^D_d\) ('double-tetrahedral') group of symmetry, exact or approximate. The corresponding strong shell-gap structure is markedly enhanced by the existence of the 4-dimensional irreducible representations of the group in question and consequently it can be seen as a geometrical effect that does not depend on a particular realization of the mean-field. Possibilities of discovering the corresponding symmetry in experiment are discussed.

PACS numbers: PACS numbers: 21.10.-k, 21.60.-n, 21.60.Fw

A possibility that atomic nuclei exhibit tetrahedral symmetry - in quantum physics so far discussed mainly as a property of certain molecules, metal clusters or fullerenes - has a definite interest for all the related domains of physics. While in the above mentioned objects the underlying interactions are electromagnetic, the nuclear tetrahedra (pyramid-like nuclei with 'rounded edges and corners') are expected to be stabilized primarily by the strong interactions. Within the nuclear mean-field theories, a convenient framework for discussing this phenomenon is provided by the spontaneous symmetry breaking mechanism. It is analogous to the one associated with the existence of numerous deformed nuclei, e.g. ellipsoidal ones. According to such a mechanism all nuclei are governed by rotationally-invariant elementary nucleon-nucleon interactions, yet, for some specific low energy configurations their total energy becomes lower when the corresponding mean-fields take non-spherical shapes. Mathematically different but physically analogous mechanism of spontaneous symmetry breaking is related to a discrete symmetry: the inversion. The underlying elementary interactions, although inversion-invariant, do not guarantee that all the resulting low energy nuclear configurations lead to stable inversion-invariant shapes, and there is a growing experimental evidence of the existence in nature of the octupole deformations, usually pear-shape type, cf. e.g. Ref. \(^{2}\). It turns out that the tetrahedral nuclei do break spontaneously both the spherical symmetry and the symmetry by inversion (see below).

In the past there has been a number of studies published that address the question of the non-axially symmetric octupole deformations. Using the Strutinsky method and considering a space composed of 2 (quadrupole) + 4 (octupole) + 5 (hexadecapole) + 6 (multipolarity 5) = 17 deformations, the authors of Ref. \(^{2}\) have suggested that an ensemble of isomeric states of tetrahedral symmetry may exist in the region of light Radium nuclei pointing to the importance of the so far neglected \(\alpha_{32}\) deformation. Using the Hartree-Fock approach in their symmetry-unconstrained variant, Takami et al., Ref. \(^{3}\), obtain in some light \(Z = N\) nuclei an \(\alpha_{32}\) instability. In Ref. \(^{4}\) this and other exotic octupole deformations were studied in the \(^{32}\)S nucleus, while in \(^{5}\), a similar hypothesis has been advanced theoretically for a group of nuclei around \(A \sim 70\).

The experimental verification of the discussed phenomenon does not exist so far. We believe that the mechanism related to \(\alpha_{32}\) deformations is just a visible part of an iceberg: a phenomenon whose physical consequences are much richer than what has been discussed so far. First of all, the corresponding \(T^D_d\) symmetry is nearly unique: only \(T^D_d\) and the octahedral \(O^h\) point-group symmetries produce in deformed nuclei the nucleonic level degeneracies higher that 2. More precisely: some states must carry 2-fold and some 4-fold degeneracies. The corresponding nuclear hamiltonians are invariant with respect to the very large number of 48 different symmetry elements (in the case of the \(O^h\) this number would be 96). The depth of the nuclear mean-field potential and the number of its bound states depend only very weakly on deformation: the 4-fold degeneracy mechanism at non-zero \(\alpha_{32}\) implies larger interspacing and helps in producing very large shell-gaps that are comparable to or larger than at least some of the gaps at spherical shapes. Moreover, since the argument is geometrical in nature the predicted strong shell-gaps propagate all over the periodic table in a repetitive fashion independently of a particular realization of the mean-field approach. This mechanism is far from being an exoticity of a few nuclei here and there. Its presence is predicted in dozens if not hundreds of nuclei. Among unique quantum features it should be noted the prediction that some nucleonic orbitals should have the...
expectation value of parity close to zero - nearly complete disappearance of the quantum characteristic that is otherwise dominating in the micro-world of nuclear interactions. Another unique element foreseen concerns the collective (especially low spin) rotation of the quantum tetrahedra: the corresponding predicted structures of rotational bands will be very different for even ($T_d$-group) and odd ($T_{d}^1$-group) nuclei since both the number of the irreps associated with these groups and the dimensions of the corresponding irreps are very different as well, see e.g. Refs. [6, 7].

The mathematical background of our considerations is well known and can be summarized in a few lines. Consider a nuclear deformed mean-field Hamiltonian $\hat{H} = \hat{H}(\vec{r}, \vec{p}, \vec{s}; \hat{a})$ where $\hat{a}$ represents the ensemble of all the deformations $\{\alpha_{\lambda\mu}\}$ and a group of symmetry $G$ with the symmetry operators $\{\hat{O}_1, \hat{O}_2, \ldots, \hat{O}_f\}$ $\subseteq G$, so that: $[\hat{H}, \hat{O}_k] = 0$, for $k = 1, 2, \ldots, f$. Suppose that the group in question has irreducible representations $\{R_1, R_2, \ldots, R_r\}$ with the dimensions, respectively: $\{d_1, d_2, \ldots, d_r\}$. Then the eigenvalues $\varepsilon_\nu$ of the problem $\hat{H} \Psi_\nu = \varepsilon_\nu \Psi_\nu$, $\forall \nu$, appear in multiplets: $d_1$-fold degenerate, $d_2$-fold degenerate, $\ldots$, $d_r$-fold degenerate. Since the nuclear mean-field Hamiltonians do not depend explicitly on time, it follows that each eigen-energy must be at least twice degenerate (Kramers theorem). In terms of irreducible representations of $G$ this property manifests itself for the deformed nuclei through the presence of two-dimensional irreducible representations or pairs of conjugated one-dimensional ones.

The point-group symmetries of the nuclear mean-field Hamiltonian can be very often directly connected to the corresponding deformation parameters: if $R(\vartheta, \varphi)$ denotes the nuclear surface, expanding it into a series of spherical harmonics $Y_{\lambda\mu}(\vartheta, \varphi)$ with the numerical coefficients $\alpha_{\lambda\mu}$ (deformation parameters) provides a natural classification scheme. Indeed, setting all $\alpha_{\lambda\mu}$ to zero one obtains a sphere, posing $\alpha_{2,2,0} = \pm 2.0 \neq 0$ gives the most important example of the (ellipsoidal) $D_{2h}$-symmetry, by setting $\alpha_{1,1,0} = 0 \neq 0$ we obtain an example of the octupole-axial ($C_{2s}^0$) symmetry; many other combinations of the non-zero deformation parameters may lead to more 'realistic' realizations of the symmetry groups in nuclei. It can be shown using elementary properties of the spherical harmonics that in the case of the pure octupole deformations the following relations between the nuclear shape and the double point-group symmetries of the fermion Hamiltonians hold:

- Deformation $\alpha_{30}$: implies the $C_{6v}$-symmetry group with infinitely many 1-dimensional irreps., characterized by the so-called K-quantum numbers;
- Deformation $\alpha_{31}$: implies the $C_{2v}$-symmetry that generates only 1 two-dimensional irrep;
- Deformation $\alpha_{32}$: implies the $T^D_d$-symmetry of 2 two-dimensional and 1 four-dimensional irreps;
- Deformation $\alpha_{33}$: implies the $D_{2h}^+$-symmetry, and generates 3 two-dimensional irreps.

However, the link between the above scheme and the realistic calculations is not always direct - especially when the point-groups rich in structure are concerned. Any isomeric minimum is, within the mean-field theory, associated with the presence of energy-gaps in the corresponding single particle spectra - usually the larger the gap, the more stable the implied equilibrium deformation. Within a given symmetry (given irrep) the non-crossing rule implies that the single-particle energies tend

![FIG. 1: Results of the realistic calculation of the proton single-particle energies in function of the $\alpha_{32}$ deformation corresponding to the $T^D_d$ symmetry (top) compared to the analogous dependence in function of $\alpha_{31}$ (bottom, $C_{2s}^0$-group). The numbers in front of the Nilsson labels give the expectation values of parity at the extremes of the deformation axes. None of the Nilsson quantum numbers is a good quantum number at tetrahedral deformations: each label gives the full set of quantum numbers of the strongest basis state. (Results obtained using a standard deformed Woods-Saxon potential.)](image-url)
towards an equidistant distribution when deformation increases. If a given group admits only one irreducible representation each level can carry at most two nucleons. When the corresponding irreducible representations have higher dimensionality, e.g. four (the corresponding curves are marked with the double Nilsson labels \([Nn\lambda]Ω\) in Fig. 1) more particles may reside on one single energy level, leading, in some other place of the energy scale to effectively diminishing the number of levels and possibly increasing the shell gaps. The features discussed above are followed very closely by the realistic calculation results of Fig. 1 where, in addition, the extremes on the horizontal axes have been chosen in such a way that by comparing the labels on the left- and on the right-hand side of the Figure one can read how quickly the parity mixing sets in when the deformation increases (the curves are symmetric with respect to 0). The parity mixing at \(|α_{32}| ≃ 0.15\) is so strong, that the typical calculated parity expectation values are \((\sim ±0.5)\).

Several observations deserve emphasizing. First of all, there is a qualitative difference in the deformation dependence in the two studied cases as predicted by the considerations based on the point-group symmetries presented above: at \(|α_{31}| > 0.15\) the level distribution can already be considered ‘nearly uniform’ except for a relatively small gap at \(Z = 56\) that decreases slowly with increasing deformation. In contrast, the spectrum in function of \(α_{32}\) reveals strongly increasing gaps at \(Z = 32, ΔE > 2\) MeV, at \(Z = 40\) with \(ΔE ≃ 3\) MeV and a huge gap at \(Z = 56, 58\); the latter can be seen as a \(\sim 4\) MeV separation in the spectrum ‘cut across’ by a single, usual (i.e. twice degenerate) orbital. These deformed gap-sizes are comparable to- or larger than- the strongest spherical gaps at \(Z = 20, 28, 40\) or even \(Z = 50\), that are known in the medium heavy nuclei; neutron results are similar.

Not all the gaps have an equal impact on the existence (or not) of the well defined minima on the total energy surfaces. More extended calculations whose results will not be presented here in detail can be summarized as follows: The strongest tetrahedral-symmetry effects appear at proton numbers \(Z_t = 16, 20, 32, 40, 56 – 58^*, 70^*, 90 – 94^*\), where the asterisks denote the gaps that are particularly strong (up to \(\sim 3\) MeV or so). A clear proton-neutron symmetry exists in the calculations leading to the related tetrahedral neutron gaps at \(N_t = 16, 20, 32, 40, 56 – 58^*, 70^*, 90 – 94^*, 112\) and 136/142.

Typically, tetrahedral minima on the total energy surfaces are accompanied by an oblate- and/or a prolate-symmetry minima. The energy cuts corresponding to the paths from the tetrahedral minima down to the ground state have been calculated in function of increasing \(β_2\) by performing a minimization with respect to the \(γ\) deformation as well as, simultaneously, \(\{α_{3μ}; μ = 0, 1, 2, 3\}\) and \(\{α_{4μ}; μ = 0, 1, 2, 3, 4\}\), 10-dimensional minimization, using the standard Strutinsky method. These results are presented in Fig. 1 for \(^{90}\)Zr\(_{40}\), \(^{108}\)Zr\(_{68}\), \(^{160}\)Yb\(_{90}\) and \(^{242}\)Fm\(_{142}\) nuclei, whose tetrahedral equilibrium deformations are calculated at \(α_{32} = 0.13, 0.13, 0.15\) and \(0.11\), respectively. The right-hand side minima (Fig. 2)

FIG. 2: Results of the multidimensional minimization of the total nuclear energies projected on the quadrupole deformation axis. The gamma deformation as well as all other deformations vary along the \(β_2\)-axis following the minimization, for each curve separately. The left-hand side insert shows an exaggerated (for better visibility) view of the tetrahedral shape at \(α_{32} = 0.3\), roughly twice the calculated equilibrium deformation. The right-hand side insert shows for comparison an oblate shape surface at \(β_2 = 0.20, γ = 60^º\) i.e. roughly at the calculated equilibria.

for \(^{80}\)Zr and \(^{160}\)Yb nuclei are at oblate deformations; the corresponding energies visible in the Figure are, respectively, at \(1.4\) MeV and \(0.1\) MeV above the prolate g.s. minima, the latter not shown in order not to perturb the legibility of the figure. For the other two nuclei the right-hand side minima correspond directly to the prolate ground-states; in the Fm case the tetrahedral minimum lies particularly high (\(7.1\) MeV above the g.s.). One can see from the Figure that the calculated barriers are of the order of \(1\) MeV, similarly to those encountered in the case of the experimentally known prolate/oblate shape coexistence. Unfortunately, lack of information about the collective inertia parameters makes it impossible to speculate about the isomeric half-lives at present.

An experimental identification of proposed \(T^D\) symmetry may rely on one or combination of several criteria.

First of all, within the class of the single-particle excitations, the presence of the four-fold degeneracies will manifest itself by the presence of a multitude of particle-hole transitions of close-lying energies. For instance if both the particle and the hole states are associated to the exact-symmetry four-fold degenerate levels, one should expect a sixteen-fold exactly degenerate multiplet of transitions. (In realistic situations the nuclear polarization effects are expected to be in general different for various 1p-1h excitations and the predicted 16-fold degeneracy in the associated decay lines will only be approximate) If
of the low-lying collective rotational excitations not much is known at present as far as nuclear tetrahedral quantum rotor behavior is concerned. In a formal treatment of the rotational spectra of the tetrahedral symmetry molecules, the corresponding rotor Hamiltonians are expanded in terms of tensor operators that are constructed out of \( \hat{I}_x, \hat{I}_y, \hat{I}_z \) angular momentum operators. The nuclear rotor Hamiltonians can be constructed analogously: we have performed the corresponding calculations and the preliminary results indicate characteristic degeneracies of the rotor levels clearly different than those of the ‘traditional’ ellipsoidal rotors.

Fortunately, qualitative criteria of the ‘yes/no’ type can be formulated that are related to the rotational decay of the tetrahedral nuclei and this in a nearly model-independent way. The starting point in the considerations is the so-called simplex-invariance, i.e. the invariance of the Hamiltonian with respect to the product of parity, \( \hat{\pi} \) and \( \hat{R}_y \), a 180° rotation about, say, \( O_y \)-axis: \( \hat{S} = \hat{\pi} \cdot \hat{R}_y \). This invariance implies, as discussed in more detail in Ref. \[8\], that the rotational energies form two parity-doublet sequences (four parity-doublet \( E2 \)-bands) as illustrated schematically in Fig. \[8\]. Both the ‘usual’ axial-octupole shape nuclei and the tetrahedral nuclei obey to the simplex symmetry and thus must produce the parity-doublet bands. However, the tetrahedral nuclei, in contrast to the ‘usual’ octupole-type ones are not expected to produce the \( E1 \) inter-band transitions since the nuclear pyramids, due to their high symmetry, will not have any significant dipole moments.

A particularly appealing, ‘academic case’ possibility corresponds to a pure tetrahedral symmetry with no other multipole deformations present. In such an ideal case the dipole and quadrupole moments are expected to be zero and the first non-vanishing moments will have \( \lambda = 3 \). In such a case the parity-doublet energies at the right-hand side in Fig. \[8\] would be connected by pure \( E3 \)-transitions rather than \( E2 \)-transitions.

In summary: We suggest that the tetrahedral symmetry in nuclei should be present among many isomeric states throughout the periodic table. We predict the proton and neutron numbers for which this effect should be the strongest. The four-fold \( T1D \) degeneracy of related deformed nucleonic orbitals is a unique feature - only the inversion-conserving octahedral \( O6h \) symmetry may provide in deformed nuclei the degeneracies higher than two (more precisely: four-fold).

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