ATOMIC NUCLEI WITH TETRAHEDRAL AND OCTAHEDRAL SYMMETRIES*

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We present possible manifestations of octahedral and tetrahedral symmetries in nuclei. These symmetries are associated with the O_h^D and T_d^D double point groups. Both of them have very characteristic finger-prints in terms of the nucleonic level properties — unique in the Fermionic universe. The tetrahedral symmetry leads to the four-fold degeneracies in the nucleonic spectra; it *does not preserve* the parity. The octahedral symmetry leads to the four-fold degeneracies in the nucleonic spectra as well but it *does preserve* the parity. Microscopic predictions have been obtained using mean-field theory based on the relativistic equations and confirmed by using 'traditional' Schrödinger equation formalism. Calculations are performed in multidimensional deformation spaces using newly designed algorithms. We discuss some experimental fingerprints of the hypothetical new symmetries and possibilities of their verification through experiments.

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1. Introduction

The phenomenon of the shape coexistence in nuclei is related to one of those 'intuitive' mechanisms that can be relatively easily imagined in terms of classical physics and geometry. This is perhaps one of the reasons why a conceptual progress in this important sub-field of nuclear structure physics has been relatively slow — although important successes such as finding an evidence for 'prolate-spherical-oblate' shape coexistence or for a coexistence between the super-deformed and normal-deformed nuclear configurations have been achieved. The examples of the shape coexistence just mentioned

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are related directly to fundamental symmetries of the nuclear mean-field: (pseudo) SU_3 and the so-called pseudo-spin symmetries (*cf. e.g.* Ref. [1], [2]). Studying the symmetries that will be discussed in this paper may shed some light on yet another microscopic mechanism possibly present in nuclei: the spontaneous symmetry breaking leading to *unusually high single-nucleon degeneracies* that may appear in *deformed* nuclei.

The most common, one may think, triaxial-ellipsoid nuclear shapes have for a long time *not* received as thorough an attention from the experimental point of view as they should have — even though in many models, such as cranking model or mean-field theory based models, the tri-axiality and the so-called γ -deformation play an important role. Only recently an attempt to observe the quantum wobbling mechanism in nuclei has forced considering a simultaneous combination of several experimental manifestations of the non-axial shapes in nuclei. To our knowledge, there has been so far no experimental effort undertaken, in terms of searches for an evidence of nonaxially symmetric nuclear shapes, with the exception of the ellipsoidal ones.

In terms of the conceptual progress, the so-called C_4 -symmetry hypothesis is particularly worthwhile mentioning, Ref. [3]. Although no consistent evidence of its presence in experimental results on super-deformed nuclei exists so far (and rather numerous arguments against), no systematic search, neither theoretical nor experimental in terms of normally deformed nuclei has ever been undertaken, and it remains to be seen which nuclei can possibly built-up C_4 -symmetric configurations with the elongation that are not very different from their ground-state elongation.

Recently, an idea originally proposed in Ref. [4] has been re-analyzed in terms of the possible presence of the pyramid-like (tetrahedral) shapes in nuclei, Ref. [5], with a conclusion that extremely strong nuclear shell effects leading to a tetrahedral symmetry may exist in nature on a sub-atomic level. In this presentation we would like to address a slightly more general problem of possible existence in nuclei of both *octahedral* and *tetrahedral* symmetries; these symmetries are mathematically related but cause very different physical implications.

Octahedral and tetrahedral symmetries are characterized by a relatively large number of symmetry elements. Compared to classical D₂-symmetry group that is composed of 4 elements (three rotations through an angle of π about three mutually perpendicular axes plus the identity transformation) and characterizes a family of tri-axially deformed nuclei, a group of symmetry of a classical tetrahedron, T_d, contains 24 symmetry elements and that of a classical octahedron, O_h , 48 symmetry elements¹. As a result of such a high degree of symmetry, the T_d^D or O_h^D invariance implies an unusually high degeneracy of the single particle states — eigen-solutions to the Schrödinger equation. More precisely, the double tetrahedral, T_d^D -symmetry group generates two two-dimensional and one four-dimensional irreducible representations. This fact manifests itself through double and quadruple degeneracies of the single-nucleonic levels — an unusual situation given the fact that so far, for the deformed nuclei, only the double (*i.e.* Kramers) degeneracies of the single-nucleonic levels have been considered.

The octahedral double point group, O_h^D , contains an inversion among its symmetry elements with the consequence that the parity of single-nucleonic levels is preserved by the solutions to the octahedrally-symmetric Hamiltonians. In this case we find six irreducible representations, three of them characterized by the positive parity of the underlying single-particle states and three other by the negative parity. Within each of the two parities we find two two-dimensional and one four-dimensional irreducible representations and it follows that the corresponding levels can be occupied by up to two and up to four nucleons, respectively.

2. Symmetries of the nuclear mean-field

In this section we are going to summarize the mathematical concepts underlying the present study. This summary will be followed by a few illustrations of the discussed principles in the case of the nuclear T_d^D and O_h^D symmetries.

2.1. General aspects of discrete symmetries in multi-fermion systems

We consider a deformed mean-field nuclear Hamiltonian; the corresponding operator can always be written down in the form

$$\hat{\mathcal{H}} = \hat{\mathcal{H}}(\vec{r}, \vec{p}, \vec{s}; \hat{\alpha}), \qquad (1)$$

where \vec{r} , \vec{p} and \vec{s} are the position, linear momentum and spin operators, respectively, and where $\hat{\alpha} \leftrightarrow \{\alpha_{\lambda,\mu}\}$ represents an ensemble of all parameters that define nuclear shapes; here we are using the multipole deformation parameters that are particularly well suited for analyzing the point-group symmetry properties.

¹ On the level of symmetries of the Schrödinger equation for the nucleons (fermions) the classical symmetry groups need to be replaced by the so-called double (or spinor) groups that contain a double set of symmetry elements. In the mentioned groups this means 8, 48 and 96 symmetry elements for the double D_2^D , T_d^D and O_h^D groups, respectively.

Consider a group \mathcal{G} with the symmetry operators (group elements)

$$\{\hat{\mathcal{O}}_1, \hat{\mathcal{O}}_2, \dots \hat{\mathcal{O}}_f\} \Leftrightarrow \mathcal{G}.$$
 (2)

Assuming that \mathcal{G} is the group of symmetry of Hamiltonian $\hat{\mathcal{H}}$ implies that all elements of the group commute with $\hat{\mathcal{H}}$:

$$[\tilde{\mathcal{H}}, \tilde{\mathcal{O}}_k] = 0 \quad \text{with} \quad k = 1, 2, \ \dots f \,. \tag{3}$$

Of course, operators $\hat{\mathcal{O}}_k$ may, but do not need to commute among themselves. Suppose that the group in question has irreducible representations (irreps)

$$\{\mathcal{R}_1, \mathcal{R}_2, \ldots \mathcal{R}_r\}.$$
(4)

(The reader unfamiliar with the terminology used in group theory does not need to know at this point more than the fact that the irreps can be characterized by their dimensions.) Suppose that the irreps in question have dimensions

$$\{d_1, d_2, \ldots d_r\},\tag{5}$$

respectively. Then the eigenvalues ε_{ν} of the problem

$$\mathcal{H} \Psi_{\nu} = \varepsilon_{\nu} \Psi_{\nu} \tag{6}$$

appear in multiplets: d_1 -fold degenerate, d_2 -fold degenerate, ... etc.

The point groups of interest for us in nuclear physics applications differ from those usually discussed in crystallography. Since the eigenstates of the problem in Eq. (6) are spinors it follows that all 360° space-rotations must not give the identity, \mathcal{I} , but rather $-\mathcal{I}$ (change in phase). The classical crystallographic point groups 'adapted' to provide this feature are called double or spinor point groups and their names are written with the superscript D, as seen already above. Among 32 standard point groups usually considered in quantum mechanics applications (cf. Ref. [6] for a detailed presentation) there are only two that are of interest for the present study: the tetrahedral and the octahedral double point groups, T_d^D and O_h^D , respectively. The important physical reason for that interest is that among the corresponding irreps there are some with dimensions d = 4; all other double point-groups of possible interest in subatomic physics generate exclusively the double degeneracies at most.

2.2. Four-fold degeneracies of nucleonic levels and energy gaps

The degeneracies of single-nucleonic levels are related to the symmetries of the underlying potential. They may imply a presence of strong gaps in the single particle spectra and thus play an important role in stabilizing certain nuclear configurations. Indeed, if a large energy gap appears at the Fermi level of a given nucleus, in order to excite (*i.e.* destabilize) the corresponding configuration for instance through bombarding with external particles, there will be a large energy necessary as compared to the situations where the gaps are small. This mechanism is very well known in spherical nuclei in which the 'magnetic' [(2j + 1)-fold] degeneracy of the nucleonic levels gives rise to the large ('magic') gaps and implies indeed a strong increase in stability of the corresponding nuclei, like *e.g.* in ²⁰⁸Pb.

What has been until recently unknown is that the single-particle spectra in deformed nuclei may generate gaps as large as those in the spherical ones (!) and that apparently the T_d^D and/or O_h^D symmetries play an important role there. The quantitative predictions related to the strong shell-gaps presented below, can be qualitatively understood as follows.

The property of saturation of the nuclear forces leads, among others, to a relatively weak dependence on the proton and neutron numbers of the depth of the mean nuclear potential. In fact in several nuclear physics considerations this weak dependence has been neglected altogether assuming that the potential depth remains constant (this will of course *not* be the case in the present study when performing the realistic calculations and the argument is brought here for the sake of a qualitative consideration only). At a constant depth of the potential, an enhanced appearance of single-particle gaps in the spectra is more likely if the increased degeneracy of levels is allowed. The above statement is based on 'empirical' knowledge and has no rigorous mathematical foundation².

3. Octahedral and tetrahedral symmetries: shapes

One of the important mathematical aspects of working with the octahedral and tetrahedral symmetries is related to modeling of these symmetries with the help of spherical harmonics when parameterizing the nuclear surface Σ :

$$\Sigma: \quad \mathcal{R}(\vartheta,\varphi;\hat{\alpha}) = R_0 \ c(\hat{\alpha}) \left[1 + \sum_{\lambda=2}^{\lambda_{\max}} \sum_{\mu=-\lambda}^{\lambda} \alpha_{\lambda,\mu} \ Y_{\lambda,\mu}(\vartheta,\varphi) \right].$$
(7)

² In fact the single-particle spectra that differ in terms of the level degeneracies, if obtained with the mean-field potentials of (nearly) constant depths will differ in terms of the average level spacing: the higher the degeneracies — the larger the average level spacing. For the realistic nuclear Hamiltonians there is no general theorem that allows to predict the presence (or absence), of the large gaps in the single particle spectra although some aspects like *e.g.* the influence of the spin-orbit interaction potential on such gaps are, to some extent, predictable.

Above, $\hat{\alpha} \equiv \{\alpha_{\lambda,\mu}; \lambda = 2, 3, ..., \lambda_{\max}; \mu = -\lambda, -\lambda + 1, ..., +\lambda\}$, R_0 is the nuclear radius parameter, and $c(\hat{\alpha})$, a function whose role is to insure that the nuclear volume remains constant, independent of the deformation.

3.1. Octahedral deformations

We can demonstrate that there exist special combinations of spherical harmonics that can be used as a basis for surfaces with octahedral symmetry. The lowest order of the octahedral deformation, called by convention the first, is characterized by the fourth rank spherical harmonics. By introducing a single parameter o_1 we must have in this case

$$\alpha_{40} \equiv +o_1; \quad \alpha_{4,\pm 4} \equiv +\sqrt{\frac{5}{14}} o_1,$$
(8)

i.e. three hexadecapole deformation parameters must contribute simultaneously and with proportions $\sqrt{5/14}$ fixed by the octahedral symmetry requirement. No deformation with $\lambda = 5$ is allowed and the next possible



Fig. 1. Comparison of two octahedrally deformed nuclei. Left: octahedral deformation of the first order, $o_1 = 0.10$; right: octahedral deformation of the second order, $o_2 = 0.04$.

are deformations with spherical harmonics of $\lambda = 6$. Similarly, we introduce one single parameter, o_2 , with the help of which the next allowed octahedral deformation, called *of the second order*, and depending on the 6th rank spherical harmonics can be defined. We must have:

$$\alpha_{60} \equiv +o_2; \quad \alpha_{6,\pm 4} \equiv -\sqrt{\frac{7}{2}} o_2.$$
(9)

The *third order* octahedral deformation is characterized by the 8^{th} rank spherical harmonics and we can demonstrate that it can be defined with the help of a single parameter, o_3 , where:

$$\alpha_{80} \equiv +o_3; \quad \alpha_{8,\pm 4} \equiv \sqrt{\frac{28}{198}} o_3; \quad \alpha_{8,\pm 8} \equiv \sqrt{\frac{65}{198}} o_3.$$
(10)

Of course, the basis of the octahedrally deformed surfaces is infinite, but the increasing order of the octahedral deformations implies immediately a twice as fast increase in the rank of the underlying multipole deformations; the possibility of having such a situation in real nuclei is unlikely and the expansion series can be cut off quickly.

3.2. Tetrahedral deformations

In a similar fashion, the tetrahedral deformation basis can be introduced in terms of the standard spherical harmonics. The first order tetrahedral deformation, t_1 , is characterized by a single octupole deformation with $\lambda = 3$ and $\mu = 2$ and we have

$$\alpha_{3,\pm 2} \equiv t_1 \,. \tag{11}$$

The second order tetrahedral deformation, t_2 , is characterized by multipolarity $\lambda = 7$ (observe that the multipoles with $\lambda = 4, 5$ and 6 are not allowed at all by the symmetry studied) and we have

$$\alpha_{7,\pm 2} \equiv t_2; \qquad \alpha_{7,\pm 6} \equiv -\sqrt{\frac{11}{13}} t_2.$$
(12)



Fig. 2. Comparison of two tetrahedrally deformed nuclei. Left: tetrahedral deformation of the first order, $t_1 = 0.15$; right: tetrahedral deformation of the second order, $t_2 = 0.05$.

The third order tetrahedral deformation, t_3 , is characterized by $\lambda = 9$ and by definition we must have:

$$\alpha_{9,\pm 2} \equiv t_3; \quad \alpha_{9,\pm 6} \equiv +\sqrt{\frac{13}{3}} t_3.$$
(13)

Strictly speaking, the bases of these exotic deformations are of the infinite order. However, for the nuclear physics applications, it is important to observe that also the rank of the spherical harmonics increases very rapidly so that the importance of the components with the high multipolarity becomes quickly negligible.

4. Octahedral and tetrahedral symmetries: shell structure

In the following we are going to illustrate some characteristic features of the single particle level spectra and of the shell structures associated with the octahedral and tetrahedral symmetries.

4.1. Octahedral symmetry: O_h^D -symmetric single particle spectra

An example of the single particle spectra corresponding to the octahedral symmetry is shown in Fig. 3.

Let us remark first that the single particle energy curves are *not* symmetric with respect to the change in sign of the octahedral deformation, similarly as in the case of the very well known hexadecapole deformation.

Secondly, and more importantly, let us observe that the octahedrallysymmetric Hamiltonian preserves the parity. This follows from the fact that the corresponding shapes are modeled with the help of the spherical harmonics of the *even rank* only, *cf.* Eqs (8)–(10). It is well known (*cf. e.g.* Ref. [7]) that the O_h^D group has six irreducible representations, two of them four-dimensional and the remaining four two-dimensional. This implies that the solutions to the Schrödinger equation split naturally into six families, *cf.* Eqs (4)–(6). From the physics point of view it is important to notice that within each parity we have a symmetric repartition of the irreps: one four-dimensional and two two-dimensional ones within each parity, as it can be seen in Fig. 3.

The very existence of the six independent classes of single-particle wavefunctions is a special feature that has not been observed so far on the subatomic level. Any experimental evidence alluding to such a structure will be of a great interest, and this, on the very basic level: numerous point-group symmetries have been exploited to a large extent and for a long time in solid-state and molecular physics and the theoretical understanding of the



Fig. 3. An example of single particle spectra for protons (top) and neutrons (bottom) valid around ¹⁷⁰Yb nucleus in function of the octahedral deformation of the first order (o_1) . The four-fold degenerate levels are marked with the full lines; the two-fold degenerate levels with the dashed lines. The curves are labeled with the Nilsson labels; the numbers in the curly brackets give the percentage of validity of each label. For further comments see the text.

underlying phenomena has profited in an important way. The mean-field theories based on the strong interactions have not advanced towards the 'exotic' point-group symmetries so far.

Results in Fig. 3 show extremely large (over 3 MeV each) gaps at Z = 70 and N = 114. This in itself is an important observation: the gaps of this order of magnitude belong to the strongest known in nuclear structure

physics. Their sizes exceed *e.g.* the sizes of the shell-gaps responsible for the stabilization of the superdeformed nuclear configurations. Below we will demonstrate that these gaps may lead to static octahedral deformations in nuclei, but our experience with the 'more traditional' gaps of this size suggests that they may have an important influence, among others, on the collective oscillation properties.

4.2. Tetrahedral symmetry: T_d^D -symmetric single particle spectra

The tetrahedral shell structure has been studied in some detail especially in order to establish the particularly strong tetrahedral magic gaps, *cf.* Ref. [5]. The corresponding tetrahedral shell closures are predicted at:

 $Z_t = 16, 20, 32, 40, 56, 70, 90, 100, 112, 126,$

for the protons, and

$$N_t = 16, 20, 32, 40, 56, 70, 90, 100, 112, 136,$$

for the neutrons, showing strong similarities between the proton and neutron spectra.

Instead of over-viewing the whole series of various mass ranges we will limit ourselves to presenting one region only. An example of the single particle spectra corresponding to the tetrahedral symmetry is shown in Fig. 4 for the nuclei in the vicinity of the 226 Th. In this case the energy curves are symmetric with respect to the change in sign of the deformation, unlike the octahedral deformation case discussed above. Within the first order tetrahedral deformation the corresponding tetrahedral gaps visible in the figure, valid for the actinide mass range, are of the order of 2 MeV.

In principle one could think that optimal conditions to observe the particularly stable tetrahedral nuclei would correspond to the combining of the 'doubly magic' proton and neutron configurations. Such a suggestion would have been natural in the case of the strongest *i.e.* spherical shell gaps, but in the context of the 'secondary' shell structures it is insufficient (or incorrect). The reason is that the tetrahedral minima arise as a result of a competition with comparably strong (or stronger) shell closures, notably at the spherical or at the prolate deformed shapes. In such a case, a moderately strong tetrahedral shell effect may be sufficient to produce a reasonably stable tetrahedral minimum when *the competing* shell effects are weak, non-existent, or giving rise to the positive shell energies at *e.g.* spherical shapes: such a situation often takes place at certain particle numbers that are *between* the traditional magic numbers corresponding to the spherical shell closures. In the next section we are going to illustrate this mechanism in some detail.



Fig. 4. Examples of the single particle proton (top) and neutron (bottom) spectra in function of the tetrahedral deformation of the first order, t_1 . For further comments see text and also Fig. 3. Large gaps at Z = 70 and 90/94 as well as at N = 112 and 136/142 deserve noticing.

5. Octahedral and tetrahedral symmetries: stability

The problem of stability of nuclei with the tetrahedral and/or octahedral symmetries is directly related to the properties of the total potential energy surfaces. Calculations employing the Strutinsky Woods–Saxon method can be considered realistic in the context and offer *a priori* quick and reliable estimates. However, one needs to take into account several competing defor-

mation degrees of freedom³ in order to avoid overestimating the heights of the potential barriers that separate tetrahedral/octahedral minima from the other structures on the total energy landscapes. To solve this type of a problem an algorithm has been designed that minimizes the potential energies in an arbitrary subspace of the multipole expansion space $\{\alpha_{\lambda\mu}\}$. Preliminary results of this kind of calculations have been published in Ref. [5]. More extensive calculations are in progress and here we are going to limit ourselves to a global illustration of the shell effects on the potential energies. They will include the macroscopic energy contributions calculated by using the most recent version of the liquid drop model of Ref. [8].

We will illustrate the results of our preliminary calculations addressing the problem of stability of the deformed nuclei for two discussed symmetries separately.

5.1. Octahedral symmetry: nuclear potential energies

Our preliminary calculations related to the octahedral symmetry suggest particularly strong shell effects at Z = 70 and N = 114 with indications to possibly weaker effect at neighboring particle numbers, *cf.* Sect. 4.1.

Since the existence or nonexistence of the octahedral minima is strongly related to a competition between at least the quadrupole (including sphericity) and the octahedral deformations we are going to illustrate the related effects by comparing the simplified energy cross sections that involve these two deformations. In Fig. 5 we present such energy cross-sections for Z = 70(Ytterbium) nuclei for several isotopes ranging from N = 100 to N = 118. First of all it is worth emphasizing that the octahedral deformation susceptibility is *not* a feature of the 'two magic gaps only': there are many isotopes that manifest the minima of interest here. This follows from the fact that the shape stability is a result of a competition among several deformation degrees of freedom and that a minimum in a given deformation area arises either because of the corresponding shell energies are strongly negative there or because the shell energies are positive and particularly strong elsewhere.

The top part in Fig. 5 illustrates possible tendencies to produce the octahedral-deformation minima, while the bottom part of the figure (in conjunction with the previous one) allows to estimate the relative excitation energy of the exotic minimum with respect to the ground state. It can be seen from this comparison that the excitation energies may vary, in func-

³ As it happens the tetrahedral deformation of the first order (that coincides with the octupole deformation α_{32}) has a tendency to couple with the axially symmetric octupole deformation α_{30} , but other couplings cannot *a priori* be excluded. Similarly, the octahedral deformation of the first order is related to the five hexadecapole degrees of freedom and in order to obtain the realistic barrier estimates we need to consider up to a dozen various deformations.



Fig. 5. Cross-sections of the total nuclear energies in function of the octahedral deformation (top) and competing quadrupole deformation (bottom). Observe very strong effects (the energy scale is compact) of the octahedral deformation in *many* nuclei.

tion of the neutron number, from about 3 MeV to about 12 MeV or so, and consequently it is not only the size of the barrier but also the absolute excitation energy that needs to be taken into account. More precisely, while the high barriers may be seen as an encouraging factor that stabilizes the minima under consideration, the high excitation energies can be seen as a direct measure of difficulties with the population of those states, the larger the energy the more difficult the population.

The nuclei with neighboring Z-values provide a priori several further candidates for the octahedral symmetry studies. At this stage we may conclude that the octahedral 'susceptibility' is not limited to a couple of nuclei only as the single-particle diagrams presented earlier may suggest. But to draw the definite conclusions it will be necessary to complete the more involved, multidimensional potential energy calculations.

5.2. Tetrahedral symmetry: nuclear potential energies

A global 'first-test' analysis aiming at a comparison of the susceptibility towards the occurrence of the tetrahedral shapes among many nuclei has been performed in analogy to the one presented above for the case of the octahedral symmetry. Here we select only one nuclear range focusing at the masses roughly between 230 and 250. The corresponding total potential energy cross-sections are shown in Fig. 6 for illustration; the form of this representation follows the one in Fig. 5.



Fig. 6. Cross-sections of the total nuclear energies in function of the octahedral deformation (top) and competing quadrupole deformation (bottom). For further comments see text and the preceding section.

It can be seen from the figure that there are groups of nuclei susceptible to form the tetrahedral-deformed minima, yet the excitation energies related to those highly symmetric structures may be very high. Indeed, a comparison between the results related to the energy minima in the top part of Fig. 6 with the absolute energy minima of the curves in the bottom part of the figure indicates that the energy differences may vary between (2.5–3) MeV and about 10 MeV or so. We conclude that an optimal choice for experimental test will require a compromise between the barrier heights (possibly large) and the excitation energies (possibly low).

6. Nuclei with tetrahedral symmetry: population, decay and observation possibilities

We believe that the hypothetical tetrahedral structures should be more abundant as compared to the octahedral ones and thus we would like to focus the following discussion on the former rather than on the latter.

In addressing the problem of an experimental discovery of the discussed nuclear symmetries one may first ask a question as to why none of them has so far been observed? Obviously one may advance several hypotheses ranging from the most pessimistic ones ('since they have not been seen so far, perhaps they do not exist') to the most optimistic ones ('the evidence has been already collected, the affirmative answers are stocked on the tapes with the results of already performed experiments — the only problem: nobody has thought about it').

Let us try to discuss this very basic question first: why do we believe in the existence of the new symmetries on the sub-atomic level? The arguments in favor of the existence of these symmetries are based today exclusively on the theory grounds. The present day nuclear microscopic theories are advanced and performant tools 'tuned' to describe the experimental results in numerous sub-fields of our domain. In particular the self-consistent Hartree-Fock methods have reached a high level of predictive power, especially since artificial constraining conditions imposed in the early stages of the development to simplify the computing — are nowadays removed (cf. e.g. Ref. [9] and references therein). In the present context it has been verified in a few cases (a more systematic study is in progress) that the Hartree–Fock iterative procedures started at initial configurations with all symmetries totally broken may converge to the highly symmetric solutions of the type discussed in this paper and moreover, in accordance with the Z and N numbers for which strong shell effects have been predicted. In particular, the numerical coefficients that define the proportions of various multipoles [Eqs (8)-(10)] for the octahedral symmetry and Eqs (11)–(13) for the tetrahedral symmetry predicted by the group theory are reproduced by the self-consistent HartreeFock solutions down to the computer accuracy. One can hardly consider this type of the result accidental. We believe that the remaining question is not: *Whether* but rather: *On what level of probability* the configurations under discussion can be populated and detected?

Preliminary calculations based on the Dirac–Strutinsky calculations give not only the prediction of the very existence of the tetrahedral (octahedral) *shell-structures* but also several indications about the related *spectroscopic properties*. According to those calculations the minima on the potential energy surfaces that correspond to tetrahedral (octahedral) shapes are surrounded by potential barriers whose heights vary between a few hundreds of keV up to a couple of MeV. The excitation energy associated with these minima may vary typically between ~ 1 MeV and several MeV (*cf.* preceding section). It is therefore possible that the minima of interest will lead to isomeric structures analogous to the ones associated with the prolate–oblate shape coexistence known *e.g.* in the Mercury region.

Unlike yrast-trap isomers, whose configurations are related to the particle-hole excitations with the spins nearly parallel to the symmetry axis, the configurations associated with tetrahedral (octahedral) excited nuclei correspond to deformations with no symmetry axes. Therefore the nuclei in question may always decay through rotational transitions down to the band-head, *cf.* Fig. 7. The yrast trap configurations leading to isomers may in principle appear at any spin ranging from 0 to $\sim 30 \hbar$, possibly higher.



Fig. 7. Schematic illustration: structure and possibilities of the decay out of a tetrahedral minimum. Since the lowest-order tetrahedral deformation has the same geometrical features as the octupole deformation α_{32} , the concerned nuclei may generate parity-doublet rotational bands known from the studies of the octupole shapes. Establishing the structure of the bands (parity doublets?), the nature of the inter- and intra-band transitions (dipole? quadrupole? octupole?), the properties of the side-feeding and the decay branching ratios — all that will greatly help identifying the symmetry through experiments.

The isomers associated with new symmetries could be expected mostly at the lowest spins of the order of $I \sim (0 \text{ to } 2) \hbar$, at or near the band-heads.

The new symmetries are expected to be a relatively low spin, but possibly high excitation-energy phenomenon. In reference to Fig. 8 we may conclude that the main difficulty is likely to be associated with the population rate of states that lie low in spin, say $I \sim (0-14) \hbar$, but whose excitation energies correspond to (1-4) MeV or more. Consequently, reactions with light projectiles may be the first choice there. According to such a scenario the target nuclei selected will lie close to the β -stability line so that the final nuclei 'to start with' will most likely also belong to that area.



Fig. 8. A schematic 'phase diagram' illustrating expected positions of the hypothetical low-spin isomers in various nuclei as well as the bands associated with tetrahedral minima (for some quantitative examples cf. preceding sections). One may expect that in some nuclei the band-heads (isomers?) may lie prohibitively high in energy, while in some others [(1-3) MeV above the ground state] they may be much easier to populate. The scales of the energy and of the spin are realistic.

Obviously a possible use of the radioactive beams will be another source of challenges.

To establish an as simple as possible a scenario of reference, let us begin with a model of an *ideal* situation, according to which our hypothetical nuclear configuration is associated with a strong tetrahedral minimum. Suppose that we can neglect any coupling to vibrations (such as *e.g.* the zero-point motion) and/or shape-polarizations that could possibly contaminate the purity of the discussed symmetry. At this limit, both the dipole and the quadrupole electromagnetic transitions are strictly speaking zero and the first allowed ones correspond to $\lambda = 3$ (octupole). Within such an ideal scenario the decay spectra of the tetrahedral nuclei will be composed of *octupole transitions only* while preserving other rules characteristic of the



Fig. 9. Schematic illustration: rotational bands associated with the tetrahedral shapes (right) as well as those associated with the axially-symmetric octupole (pear) shapes (left) are expected to preserve the simplex quantum number and, in the extreme limit, to produce the degenerate parity-doublet bands. The tetrahedral shapes, unlike the pear-shapes, generate vanishing dipole moments. Quadrupole transitions are marked with dashed-, dipole transitions with full-lines; octupole transitions are possible in both cases but are not marked (see the text).

conservation of the simplex quantum number⁴ — at variance with the illustration in Fig. 9. In other words: an extreme beauty of the underlying physical picture consists in the fact that the rotational energy levels satisfying, at least to a leading order, the usual I(I + 1)-rule would be connected through the ($\Delta I = 3$)-octupole transitions rather than through the usual quadrupole ones.

In realistic situations, various deviations from the ideal limit are to be expected. In fact, in Fig. 9 we have chosen to illustrate what we believe is a more likely situation, namely, the presence of a quadrupole polarization and/or a 'residual' quadrupole deformations 'contaminating' the pure symmetry. In such a case the quadrupole transitions accompanying the decay of a tetrahedral nucleus are expected to be weak but most likely dominating the octupole transitions. In contrast, the pear shape nuclei known today have their octupole deformations superposed with the quadrupole ones, and their spectra are characterized by strong quadrupole and dipole transitions at the same time. (One may conjecture that, given the mass of the compared

⁴ Recall that the simplex transformation, say S_y , is by definition equal to the product of the 180° rotation about the \mathcal{O}_y -axis, \mathcal{R}_y , and the inversion \mathcal{I} and we have $S_y = \mathcal{R}_y \mathcal{I}$. In an ideal case of the strong, well defined minimum the energies of the inter-band dipole transitions correspond to half of the related quadrupole intra-band transitions.

nuclei, the quadrupole transitions in tetrahedral nuclei could be at least one order of magnitude weaker than those in the normally deformed octupole ones.)

Another mechanism that is likely to modify the ideal model situation is a possibility that the parity doublet structures are split by a considerable fractions of their energy. Such a mechanism is likely to occur when the tetrahedral minima are not sufficiently deep. As a consequence, instead of having a particularly simple picture as the one in Fig. 9, the bands appearing degenerate will be considerably displaced with respect to one another.

The decay of the lowest energy states corresponding to the tetrahedral minima may be of particular interest. The corresponding energies of excitation with respect to the ground-state varying between numbers slightly over 1 MeV up to a couple of MeV, the internal pair production may provide an extra signal. Given the fact that mean radius expectation values, $\langle r^2 \rangle$, are likely to differ considerably between the tetrahedral excited- and the quadrupole ground-state minima, the E0 transitions connecting those states are likely to be enhanced.

7. Towards first principles: nuclear quantum mechanics

It turns out that the symmetry-induced properties of the nucleonic levels and wave functions, as suggested in this paper, are unprecedented in nuclear structure studies and provide interesting new challenges already at the level of the nuclear quantum mechanics. First of all, an existence of new quantum numbers is predicted. One of them may take three values in the case of the tetrahedral symmetry; the other two, each of which take in turn three values possible, in the case of the octahedral symmetry, *cf.* Table I. These good quantum numbers will replace the well known *signature quantum number* in the case of the parity-preserving octahedral shapes, and the *simplex quantum number* in the case of intrinsic-parity breaking tetrahedral deformation.

In Table I we compare some properties, parameters or observables related to the specificity of the T_d^D (tetrahedral) and O_h^D (octahedral) double point-group symmetries. In particular, it is easy to see that the numbers of symmetry elements in the case of T_d^D or O_h^D exceed by important factors the number of symmetry elements associated with the well known, 'standard', triaxial-symmetry type shapes. There are in, total six, families of the single-particle levels that can be associated with solutions to the O_h^D symmetric Hamiltonian; three of them belong to the positive- and three to the negative-parity and, moreover, one such a family within each set is characterized by the four-fold degeneracy. A similar property holds for the T_d^D -symmetric Hamiltonians except for the parity that is not conserved in this case. The last line in the table shows how many values can the discrete quantum numbers take in relation to the symmetries compared.

Properties	High Symmetries		'Usual' Symmetries
(or observables)	Tetrahedral	Octahedral	D_2^D ('tri-axial')
No. Sym. Elemts.	48	96	8
Parity	NO	YES	YES
Degeneracies	4,2,2	$\underbrace{4,2,2}_{\pi=+} \underbrace{4,2,2}_{\pi=-}$	$\underbrace{\begin{array}{c}2\\\pi=+\end{array}}^{2}\underbrace{2}_{\pi=-}$
Quantum Numbers	3	$3 + 3 + 2 (\pi = \pm)$	$2 \ (\pi = \pm)$

 $\label{eq:Challenges} Challenges on the level of quantum mechanics (Unprecedented quantum features related to T^D_d and O^D_h nuclear symmetries)$

Another important aspect will need to be considered: the tetrahedrallyor octahedrally-symmetric nuclei, if present in nature, are expected to exhibit the collective rotational properties that are very different from what we have learned by studying the rigid tri-axial rotors. First of all, let us remind the reader that the classical moments of inertia associated with a tetrahedrally-symmetric object are all three equal. As a consequence, the usual way of treating the collective rotation will give the same result as in the case of a rotating rigid *sphere!* (if we accept the rigid-rotation model) or infinity (in the case of the superfluid-rotation models where we impose rotation about a symmetry axis). Yet: a tetrahedrally-deformed nucleus has clearly no symmetry axis, its orientation in space can be very well defined and it is to be expected that the two nuclei which differ in *size* of the tetrahedral deformation will also have non-trivially different rotation-energy spectra.

It then becomes clear that to study such objects we will need to giveup the traditional rotor Hamiltonian expressions that are quadratic in spin: the tetrahedral symmetry can be modeled with the help of polynomial expressions of *at least third order*. But then we are confronted with another beautiful problem both from the mathematics and physics points of view that can be introduced as follows. Consider an even-even nucleus whose rotational spectra are expressed in terms of integer spins (*i.e.* 'boson-type', as opposed to 'fermion-type' half-integer spins, in the case of odd-A nuclei). The corresponding rotor Hamiltonian has therefore the 'usual' tetrahedral group T_d as its symmetry group. At the same time the Schrödinger equation that governs the motion of the nucleons (fermions) in the same nucleus is invariant under the <u>double</u> point group symmetry T_d^D . From the mathematics point of view these two groups are totally different, they have different numbers of groups elements as well as of the equivalence classes and thus of the numbers and types of irreducible representations. In particular: both classical (as opposed to double) point-groups, T_d and O_h , have the same number of *five* irreducible representations, two of them one-dimensional, one two-dimensional, and two three-dimensional. These properties imply an unprecedented degeneracy patterns in terms of the collective rotational spectra: these degeneracy patterns, already exotic, do not resemble at all the exotic degeneracy patterns predicted earlier in the article for the single-nucleonic spectra. (Some mathematical aspects related to quantum mechanical features of highly-symmetric rotating objects are discussed in Ref. [10].)

This brings us to another aspect of the quantum description of the problem: for the first time we will be forced to consider the three-dimensional aspect of the quantum rotation from the start! — no simplifications such as alignments on the 'principal axis' (no such axis can be defined) will be possible.

All these unprecedented quantum mechanisms will (perhaps) not be very easy to establish in experiment. But if confirmed experimentally, the presence of these new symmetries on the subatomic level will strongly influence our present-day understanding of nuclear phenomena.

8. Summary and conclusions

In addition to the general, new quantum mechanics related features summarized in the preceding section, the presented approach involves a new way of thinking about the nuclear stability: it is, for the first time⁵ based on the genuine symmetry considerations, and *not e.g.* on comparing the harmonic oscillator axis-ratios:

a:b:c =ratios of small integers.

Another aspect of novelty consists in going away from the multipole expansion, that has been a standard approach during a long time, for instance when calculating the nuclear potential energy surfaces [$e.g. (\beta, \gamma)$ -plane representation in terms of Y_{20} and Y_{22} multipoles, hexadecapole Y_{40} -deformation etc.]. In this paper we have shown how to construct the point-symmetry oriented bases instead of the spherical harmonic basis, the latter remaining of course an ideal tool for studying the SO(3)-symmetry related properties.

⁵ For a long time, the spherical-symmetry considerations have defined a standard when studying the symmetries in all domains of physics, in particular in relating the problems of degeneracy of levels to the problem of increased stability of the related configurations. Here we return to this very basic quantum mechanical problem in a non-trivially new physical situation generated by the possible occurrence of the tetrahedral and octahedral symmetries in nuclei.

We would like to turn the reader's attention to the fact that if we include the possibility of existence of the tetrahedral and/or octahedral symmetries, an important sub-field of our domain that deals with the Shape Coexistence Phenomena, will contain from now on an impressive number of configurations to study, many of them possibly in one single nucleus (!) These are: Prolate, Spherical, Oblate, Triaxial in various forms, Tetrahedral, Octahedral, 'Triangular' (C_3), Octupole, Superdeformed, Hyperdeformed, and possibly more nuclear shapes and related symmetries.

So far in the nuclear structure physics we were contenting ourselves with the presence of two types of nucleonic level degeneracies: either the (2j+1)-fold degeneracy associated with the nucleonic levels in a sphericallysymmetric potential or the double (spin-up, spin-down) time-reversal degeneracy of Kramers in the case of deformed nuclei. Since we were dealing with these degeneracies for a long time being confronted with them in nearly all microscopic models developed so far, their presence has evolved to a kind of a 'trivial property'. In the problem presented here we deal for the first time with what we would thus call 'non-trivial' degeneracies of the nucleonic levels.

It remains to be seen, as one of important items on the challenge list, whether one will be able to talk about analogies when comparing to the molecular symmetries based on the forces of the infinite range. These are *opposed* to the short range strong-interaction nuclear-forces that, under some specific circumstances related to the nuclear shell structure, may possibly generate the same symmetries. This problem touches upon the very basic issues in nuclear structure physics directly related to the concepts of the mean-field and of spontaneous symmetry breaking.

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