A highly relevant field of investigation of nuclei with unusual combinations of the proton and neutron numbers is the search for manifestations of exotic symmetries. In our previous work we reported [1], that of all the various possible non-spherical shape symmetries, tetrahedral and octahedral ones may lead to the largest single-particle shell gaps. Indeed, these can be comparable to, and sometimes even larger than the well-established spherical shell gaps. These properties, far from being restricted to nuclei within a given range of mass or isospin, should in fact be present throughout the nuclear chart. The underlying considerations are based on a very general analysis of the point groups of symmetries of the nuclear mean-fields. They have been confirmed independently via the macroscopic-microscopic method of Strutinsky [1] and the self-consistent Hartree-Fock techniques [2].

The purpose of this Rapid Communication is to support the search for tetrahedral nuclei by providing realistic calculations in some selected study cases.

The neutron-rich Zirconium (Z=40) isotopes provide such an appropriate case. Our previous work predicted that, among others, nucleon numbers $Z = N = 40$ and $Z = N = 70$ correspond to large shell gaps for tetrahedral shapes and thus can be thought of as ‘tetrahedral magic numbers’ [1, 3]. Although the yrast line of the $N = Z = 40$ system $^{80}\text{Zr}$ has been experimentally studied above spins of $10h$ [3], the detailed information concerning in particular the electromagnetic transitions (see below) which is required for probing the tetrahedral symmetry has not yet been achieved. On the neutron-rich side, Zirconium isotopes up to the $N = 70$ system $^{110}\text{Zr}$ have been synthesised using the projectile fission technique at GSI, [4]. The production of such nuclei opens up the possibility of studying their properties via isomeric spectroscopy following projectile fragmentation (e.g. [5]) and projectile-fission (e.g. [6]) or beta-delayed gammaray spectroscopy (e.g. [7]). To date however, such studies have not yet been performed in the very heavy Zirconium isotopes and the most neutron rich $Z = 40$ isotope where information on excited states is available is $^{104}\text{Zr}_{64}$, which was studied as a fragment from spontaneous fission of Cm sources in [8].

In this article we suggest that the heavy Zr isotopes are amongst the best candidates to test the hypothesis of nuclear tetrahedral symmetry: $^{110,112}\text{Zr}$ are indeed predicted by Hartree-Fock calculations to have $T_d^D$-symmetric ground-state configurations, and both non-self-consistent approaches and Hartree-Fock calculations agree on the prediction of low-lying excited $T_d^D$-symmetric minima for a chain of isotopes near $^{110}\text{Zr}$. As outlined above, these nuclei are viable for future experimental study.

In the basis of spherical harmonics, the distance of a point on the nuclear surface relative to the centre of the nucleus can be expressed by

$$ R(\theta, \varphi) = r_0 A^{1/3} c(\alpha) \left[ 1 + \sum_{\lambda, \mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\theta, \varphi) \right], \quad (1) $$

where $\alpha_{\lambda\mu}$ refer to multipole deformations. In Eq. (1), $\alpha = \{\alpha_{\lambda\mu}\}$ represents the complete set of deformations and $c(\alpha)$ accounts for nuclear volume conservation. Several ensembles of deformation parameters $\alpha = \{\alpha_{\lambda\mu}\}$ can generate a geometry characteristic of the group $T_d^D$. The simplest case occurs when all deformations except $\alpha_{32}$ are equal to 0. This simplest form of the tetrahedral deformation is also likely to be favoured in nature since other realizations of the tetrahedral symmetry involve much higher order of multipoles, $\lambda \geq 7$, cf. Ref. [1].

The group $T_d^D$ is characterized by two non-equivalent two-dimensional irreps, and one four-dimensional one. This is an unique feature in nature, since, apart from the spherical symmetry, only the groups $O_d^D$ and $O_d^D$ (the latter, octahedral symmetry is discussed in Ref. [8]) produce single-particle degeneracies higher than 2, cf. Refs. [9, 11]. This high degeneracy pattern, together with a relatively low number of irreps favours the appearance of large shell gaps. In our previous work [1], we reported that such gaps are predicted in a number of different mass regions, and presented various examples of
potential tetrahedral minima.

In the current work, realistic nuclear structure calculations are performed within the standard Woods-Saxon mean-field approach with the universal parameterization. Figure 1 shows the single-particle energies for exotic nuclei with $A \sim 110$ as functions of the lowest order tetrahedral deformation obtained from this Hamiltonian. The most striking result in Fig. 1 is the presence of a large tetrahedral shell gap at $Z = 40$, comparable to the spherical $Z = 50$ gap. Indeed this gap is larger by $\sim 3$ MeV than the spherical one at $Z = 40$.

To calculate the total energy of the nucleus, we employ the microscopic-macroscopic method whose realization closely follows that of Refs. 12 and 13. In this approach, the total energy of the nucleus is given by:

$$E = E_{macro} + E_{micro} = \delta E_{shell} + \delta E_{pair},$$

where $E_{macro}$ is the liquid drop energy, here calculated as in Ref. 14; the latter realization includes in particular the nuclear surface-curvature contributions.

The quantum correction $\delta E_{shell}$, accounts for the nuclear shell structure. It is calculated according to the standard Strutinsky prescription 15, and supplemented with the pairing correlation energy, $\delta E_{pair} = E_{pair} - E_{pair=0}$, obtained within the pairing-selfconsistent Hartree-Fock-Bogolyubov (HFB) formalism as in Ref. 16. The $E_{pair}$ term refers to the energy of the system in the presence of pairing, calculated by using the Particle Number Projection (PNP) technique (before variation), and $E_{pair=0}$ is the analogous term obtained by setting the pairing correlations to zero. The average pairing strength constants have been obtained in the usual way by fitting to the known nuclear masses of nuclei in the studied region.

The deformation space used includes $a priori$ all possible $\alpha_{3\mu}$ up to $\lambda = 12$, with $-\lambda \leq \mu \leq +\lambda$. However, the number of multipoles effectively used was significantly reduced since the effect of high-$\lambda$ was found to be negligible (by a direct verification).

The potential energy landscapes of Fig. 2 top, confirm the earlier calculations by 13, 14, 15, 16, all of which predict that at its ground-state, the $^{110}$Zr nucleus has a significant prolate deformation with an axial hexadecapole deformation $\alpha_{40}$ of about 0.10. The calculation for the top frame of Fig. 2 has been performed according to the general procedure discussed above, but the deformation space included only the quadrupole ($\beta_2, \gamma$) and axial hexadecapole $\alpha_{40}$ deformation (in the following we employ the standard Hill-Wheeler parameterization for quadrupole deformations). Beside the prolate ground-state, we note the presence of a very flat oblate pattern together with a small spherical minimum. However, the inclusion of the tetrahedral degree of freedom has a strong impact on this energy landscape. While the prolate minimum remains, the minimum at $\beta_2 = 0$ is lowered in energy by more than 1 MeV and corresponds to a tetrahedral configuration with $\alpha_{32} \sim 0.14$. In the calculations this minimum appears as pure $i.e.$ all other deformations turn out to be zero as the result of the minimization.

The often employed technique of calculations using a mesh of deformation points (as in Fig. 2) has the drawback of taking into account only a very partial projection (usually less than 4 deformations) out of the full deformation space. In order to remove this limitation, we have adopted a strategy based on a dynamical minimization of the total energy: for fixed values of a given deformation parameter (in our case the elongation along the $z$-axis, $\beta_2$), the total energy was minimized with respect to many other deformation variables using the standard Variable Metric Method described in 20. In our calculations the deformation space is composed of the entire set of octupole $\{\alpha_{3\mu}; \mu = 0, 1, 2, 3\}$ and hexadecapole $\{\alpha_{4\mu}; \mu = 0, 1, \ldots, 4\}$ degrees of freedom, in addition to the $\gamma$ angle, i.e. 11 deformation parameters in total. As mentioned above, the effect of higher order multipoles has been investigated and is negligible in the present context.

Figure 3 shows the minimized-energy cross-sections for
the ground-states in several isotopes of Zirconium as function of the quadrupole deformation $\beta_2$. For each isotope three minima appear: one at an elongation of $\beta_2 \sim 0.35 - 0.40$, another one around $\beta_2 \sim -0.25$, and a third one at $\beta_2 \sim 0$. The latter corresponds to a finite tetrahedral deformation of about $\alpha_{32} \sim 0.14$. The curves plotted in Fig. 3 may provide an estimate of the height of the barriers between the tetrahedral minima and the other deformed minima. In the case of $^{110}$Zr, this barrier amounts to up to $\sim 1.5$ MeV with respect to the oblate minimum.

Self-consistent Hartree-Fock-Bogliubov calculations have also been performed for these nuclei, using the SLy4 force \(21\) and the HFODD code (version 2.07) of \(22\), and are reported in Table I. The same energy profiles as shown in Fig. 3 are predicted, with the noticeable exception that the tetrahedral minimum in $^{110}$Zr and $^{112}$Zr lies lower in energy than the now secondary prolate minimum. Both Fig. 3 and Table I show that the influence of the shell effects leading to the tetrahedral symmetry diminishes when going away from the ‘tetrahedral magic gap’ $N = 70$. For the lighter isotopes like $^{104}$Zr and $^{106}$Zr, the tetrahedral minimum lies very high in energy and is extremely shallow.

An important aspect associated with the preceding discussion is to find a possibly unambiguous experimental signature of the discussed symmetry. Here we would like to construct a criterion based on the rotational properties of a nucleus with the tetrahedral symmetry. A discussion of other possible experimental signatures can be found in \(3\). We use a generalisation of the rotor hamiltonian often used in molecular physics, cf. e.g. \(23\). We define

\[
\hat{H} = \hat{J}^2 / (2J_0) + h_{32} (\hat{T}_{3,2} + \hat{T}_{3,-2}),
\]

(3)

where the first term which is proportional to the square of the nuclear angular momentum operator assures that the energy vs. spin dependence is approximately quadratic. The second, tensor term, is responsible for the tetrahedral symmetry of the hamiltonian \(3\). The constant $J_0$ represents the effective moment of inertia. By construction, operators $\hat{T}_{3,\pm 2}$ are spherical tensors of rank $\lambda = 3$ with the ‘magnetic’ components $\mu = \pm 2$; they are appropriately symmetrized functions of angular momentum operators \{$I_x, I_y, I_z$\}. The imaginary coefficient $h_{3,2}$ is a parameter of the model. According to the rotor formalism such a parameter must be independent of operators \{$I_x, I_y, I_z$\}, but it may be a scalar function of the spin quantum number $I$. Here we use $h_{3,2} = c_{3,2} / I^2$, with an imaginary constant $c_{3,2}$. This is a convenient parametrisation that allows to keep the third order term dominated by the usual, approximately quadratic energy dependence on spin. In the following we use $c_{3,2} = 0.03$; it turns out that the exact value of this constant has a

FIG. 2: (Color online) Ground-state total energy surfaces in $^{110}$Zr as a function of the quadrupole ($\beta, \gamma$) deformations. Top: minimisation over $\alpha_{40}$ at each ($\beta, \gamma$)-point; bottom: similar to the above but minimized over tetrahedral deformation $\alpha_{32}$. Note that the tetrahedrally-symmetric minimum is lower by more than 1 MeV than the spherical minimum.

FIG. 3: Total energy as function of quadrupole deformation in a chain of Zr isotopes. Negative values of $\beta_2$ correspond to oblate shapes. Each $\beta_2 \sim 0$ minimum correspond to a tetrahedral configuration. (The pairing correlations were included and treated with the help of the PNP technique).

TABLE I: HFB energies (in MeV) for various energy minima in heavy Zr isotopes, relative to the energy of the tetrahedral minimum. Calculations were done with the SLy4 force \(21\).

| Nucleus  | $^{104}$Zr | $^{106}$Zr | $^{108}$Zr | $^{110}$Zr | $^{112}$Zr |
|---------|------------|------------|------------|------------|------------|
| Tetrahedral | +0.00 | +0.00 | +0.00 | +0.00 | +0.00 |
| Spherical | +0.22 | +0.29 | +0.39 | +0.43 | +0.03 |
| Oblate   | -1.57 | -1.52 | -1.10 | +0.07 | +0.30 |
| Prolate  | -2.07 | -1.76 | -0.68 | +0.27 | +1.01 |
very minor influence on the electro-magnetic transition rates, the latter representing the main concern in this part of the discussion.

The solutions of the Schrödinger equation with Hamiltonian \( H \) for an even-even nucleus are characterized by integer spins and thus transform with the help of the irreducible representations of the 'simple' \( T_d \) group (as opposed to the 'double' \( T_d^D \)-group of symmetry that applies for the nucleons (spinors) mentioned earlier). The group \( T_d \) has four irreducible representations, three of them, denoted \( C1, C2 \) and \( C3 \) are one dimensional, the fourth one, \( T1 \), is three-dimensional. Because of the latter, in the strict symmetry limit the rotational spectra must contain three-fold degenerate levels (cf. Fig. 4). However, it is well known that quantum systems manifest zero-point motion oscillations: in the nuclear case the most important oscillations of this type are expected to be of quadrupole nature. We have estimated, using collective model techniques with the Bohr Hamiltonian that the expectation value of the quadrupole deformation in \(^{110}\text{Zr}\) is \( \sim 0.05 \), depending somewhat on the details of the model. To simulate the zero-point motion effect in the following we therefore perform the calculations using a small quadrupole triaxial "contamination" term introducing three moments of inertia \( \tilde{J}_x, \tilde{J}_y \) and \( \tilde{J}_z \) which slightly deviate from \( J_0 \). These are calculated using uniform density ellipsoidal shapes with quadrupole deformations \( \beta = 0.05, \gamma = 30^\circ \) and \( \alpha_{32} = 0.15 \).

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The zero-point motion mechanism simulated in this way has a very small influence on the degeneracy (deviations of the order of 2 keV) but it has a tremendous impact on the electro-magnetic transition probabilities. In particular, at the exact symmetry limit the only transitions allowed are \( E3 \) ones; in the calculations with the zero-point motion effect included, the quadrupole transitions are stronger by 5-6 orders of magnitude and the non-stretched \( B(E2) \)s are usually slightly stronger than the stretched ones.

In the adiabatic approximation, the nuclear hamiltonian is a sum of the rotor and the intrinsic energy term (cf. Eq. (4-3) of Ref.[24]) and it follows that the eigenenergies are also sums of two corresponding terms, while the transition rates depend on the electric moments calculated with the help of the intrinsic hamiltonian. The latter were calculated here using an uniform charge distribution with the tetrahedral deformation of 0.15 and small quadrupole deformations cited above. Results in Fig. 4 illustrate only the rotor part of the spectrum. Consequently when reading them one has to bear in mind that the energies of e.g. even-spin sequence and of the odd-spin sequence may be shifted with respect to one another by an amount that needs to be taken from the interpreted measured spectrum. The results of this kind could also be used as a guidance for a band starting at \( I = 3 \) (transitions corresponding to \( I \geq 3 \)) or for the bands with all parities negative.

Moreover, it should be emphasized, that the reduced transition probabilities for \( (I \rightarrow I + 1) \)-transitions are usually some percentage stronger than those for \( (I \rightarrow I - 1) \)-transitions, so that if e.g. the odd-spin sequence is shifted upwards, the inter-band transitions of the type \( 5 \rightarrow 6, 4 \rightarrow 5 \), etc. are to be expected. In short: the information and prediction content of the diagrams of the Fig. 4 type is much richer than what the first-glance reading may suggest.

The partial transition pattern illustrated in Fig. 4 distinguishes clearly between the decay modes of a tetrahedral quantum rotor and the one of an ellipsoidal symmetry. In the latter case, only the stretched \( E2 \)-transitions are present, connecting exclusively the band-members of the same \( D_2 \)-symmetric rotor irreducible-representations, as discussed in Chap. IV of Ref.[24]. But even in the case of a strong triaxial minimum competing (\( \gamma \sim 30^\circ \)) the reduced probabilities for the non-stretched \( E2 \)-transitions are nearly two orders of magnitude weaker compared to the stretched ones. Moreover, they connect only the states of the same \( D_2 \)-symmetry (same common irreps) - while in the case of the \( T_d \)-symmetry, the \( (C_1 \rightarrow C_i) \)-transitions are forbidden, cf. caption to Fig. 4. These differences provide an excellent 'yes-no' criterion, provided that a sufficient number of experimental transitions have been identified.

In the illustration of Fig. 4 we have selected a configuration composed of the lowest lying rotational levels of the same parity with spins \( I \leq 5 \); a more complete analysis will be presented elsewhere.

**In summary:** Low-lying tetrahedral configurations in Zr isotopes with \( 64 \leq N \leq 72 \) are obtained with both

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**FIG. 4:** Color online) Tetrahedral rotor energy spectrum; the irreducible-representation symbols are marked on the right hand-side. Arrows indicate the strongest \( E2 \)-transitions [in units of \( e^2 (fm)^4 \)] depopulating two lowest states of spin \( I=5 \), as an example. Full lines give stretched, dashed lines the non-stretched \( \Delta I = 1 \) transitions. For easier legibility the degenerate \( T1 \) states are marked as split. Observe that the non-zero transitions connect only one-dimensional irrep states among themselves and the three-dimensional irrep states among themselves. In addition, there are no \( E2 \) transitions of the type \( C1 \rightarrow C1, C2 \rightarrow C2 \) nor \( C3 \rightarrow C3 \).
The HFB and Strutinsky techniques. The only noticeable difference between these very different realizations of the mean-field comes from the relative position of the tetrahedral minimum relative to the ground-state. HFB calculations with the SLy4 interaction predict a tetrahedral ground-state in $^{110-112}$Zr. The barrier heights which separate the tetrahedral minima from their prolate counterparts have also been estimated and we emphasize that this region of the nuclear chart is potentially accessible for exploration using isomer and $\beta$-delayed $\gamma$-ray spectroscopy following projectile fission.

The spectral properties expected to accompany the tetrahedral symmetry in nuclei have been briefly discussed in terms of the electro-magnetic transitions in a quantum rotor with tetrahedral symmetry. The predicted decay pattern is very characteristic: it includes a competition between stretched and non-stretched E2-transitions and excludes the possibility of connecting some well defined groups of levels. This decay pattern is clearly distinct from known transition patterns of both the axial or nearly-axial rotors as well as strongly triaxial rotors whose spectra contain principally the E2-transition cascades. Since in the discussed nuclei the tetrahedral-symmetry minima are in competition with the ones of quadrupole type deformation, the electromagnetic decay criteria formulated offer a clear-cut distinction.

We believe that the predicted structure of the nuclear potential energy and the corresponding minima strongly encourages the search for the first experimental evidence of existence of these highly exotic nuclear symmetries.

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