

Tetrahedral correlations in ^{80}Zr and ^{98}Zr K. Zborecki,¹ P. Magierski,¹ P.-H. Heenen,² and N. Schunck^{3,4}¹*Faculty of Physics, Warsaw University of Technology, ul. Koszykowa 75, PL-00-662 Warsaw, Poland*²*Service de Physique Nucléaire Théorique, U.L.B.-C.P. 229, B-1050 Brussels, Belgium*³*Institute of Theoretical Physics, ul. Hoza 69, PL-00-631 Warsaw, Poland*⁴*University of Surrey, Guildford GU2 7XH, United Kingdom*

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Axial octupole and tetrahedral correlations in ^{80}Zr and ^{98}Zr have been investigated using the generator coordinate method, applied to a basis generated by Skyrme Hartree-Fock+BCS calculations. We focus on the possible presence of states with tetrahedral symmetry and their stability with respect to octupole vibrations. We show that pairing significantly reduces the stability of the tetrahedral configuration and that a shallow mean-field tetrahedral minimum coexists with an axial octupole minimum. The contributions to the correlation energies coming from the tetrahedral degree of freedom and octupole axial deformation are discussed.

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The possible tetrahedral instability of finite many-fermion systems has been predicted in Ref. [1]. Recently, using the similar arguments, it has been conjectured that the intrinsic ground- or a low-lying isomeric state of some nuclei may possess a tetrahedral deformation [2,3]. This kind of symmetry is rather common in molecules and metallic clusters [4], where the mutual geometric arrangement of the ions determines the shape of the system. In atomic nuclei, the situation is more complicated and only sufficiently large shell effects can generate deformed configurations. Although there is convincing theoretical evidence for the presence of tetrahedral states in nuclear systems, they have not been confirmed experimentally.

Tetrahedral shapes are invariant with respect to the transformations of the point group T_d^D . In nuclei, they are realized at first-order through nonaxial octupole deformations of the nuclear density corresponding to the intrinsic octupole moment $Q_{32} \propto r^3(Y_{32} + Y_{3-2})$. The key argument in favor of the stability of tetrahedral shapes is a direct consequence of the theory of point groups. The group T_d^D possesses two two- and one four-dimensional irreducible representation (irrep). The unusual (in the context of nuclear structure) family of fourfold degenerate levels lead to a bunching of single-particle states resulting in rather large shell gaps and increased stability of specific configurations [2,3,5].

Among the predicted “tetrahedral magic” numbers are the $Z = 40$ proton and $N = 40, 56-58$ neutron numbers [3]. The Zr isotopes with 40 and 58 neutrons are thus predicted to be doubly-magic with respect to this symmetry. However, these nuclei may also exhibit other types of octupole deformations: the coupling between the neutron $d_{5/2}$ and $h_{11/2}$ orbitals and the proton $p_{3/2}$ and $g_{9/2}$ orbitals can lead to both axial and nonaxial octupole correlations [6]. Moreover, octupole deformations are in competition with the quadrupole mode that may obscure the signature of the tetrahedral symmetry. Although experimental data are rather poor for ^{80}Zr , the rotational band built on the ground state suggests the presence of a large quadrupole deformation [7]. The evolution of shapes for the Zr isotopes above the closed-shell nucleus ^{90}Zr is rather complex. The low-energy spectrum of ^{96}Zr exhibits

a pattern typical of a spherical nucleus, whereas $^{100-104}\text{Zr}$ have very large quadrupole deformations in their ground state together with coexisting low-lying oblate and spherical minima [8]. ^{98}Zr lies at the border between these two regions and exhibits a transitional character, as demonstrated both experimentally [9] and theoretically [8,10,11]. In particular, the large experimental $E0$ transition between the first excited 0^+ state and the ground state suggests a strong mixing between coexisting shapes. This nucleus appears thus to be particularly rich in terms of the different deformation modes that are in competition: spherical, oblate, prolate, tetrahedral, and axial-octupole shapes.

The purpose of the present article is to analyze for the first time the role of tetrahedral configurations in the collective excitations of these nuclei. It is organized as follows. First, we investigate the competition between axial and tetrahedral octupole shapes using the Skyrme Hartree-Fock+BCS (HFBCS) approach to probe the potential energy landscape in the octupole directions. We then explore dynamical effects beyond mean-field, parity restoration, and quantum fluctuations to determine whether states with large tetrahedral correlations are present at low excitation energy and thus whether there is a possibility to identify them experimentally. This analysis, performed using the generator coordinate method [12](GCM), aims at paving the way to a more comprehensive quantum treatment of all quadrupole and octupole degrees of freedom of the nuclear surface at the same time. The method has already been applied to the study of the excitation modes of the superdeformed Hg and Pb isotopes [13].

To investigate the variation of the energy of nuclei as a function of several shape degrees of freedom, the Hartree-Fock (HF) equations have been solved by discretization on a three-dimensional mesh in coordinate space [14]. Contrary to the usual way of solving mean-field equations in a truncated oscillator basis, this technique has the advantage that it allows description of nuclear configurations with any kind of shape with the same, high, numerical accuracy. In particular, this method has been used to describe nuclei from their spherical

ground state up to fission with an accuracy of a few tenths of keV on energy differences [14,15].

Because studying a nucleus as a function of several shape degrees of freedom is computationally a heavy task, we have imposed a symmetry condition that simplifies the problem while retaining the main degrees of freedom relevant for a study of tetrahedral shapes. The mean-field density is required to be symmetric with respect to two mutually perpendicular planes. Such a constraint reduces the complexity of the problem four times but still allows study of the variation of the nuclear energy as a function of all octupole degrees of freedom, although odd- m and even- m modes cannot be treated simultaneously [13]. The coupling between multipole moments with even and odd m -values is beyond the scope of our study, which is focused on the tetrahedral mode. Note that deformations corresponding to all multipole moments with even- m values, in particular triaxial quadrupole deformations are automatically taken into account by our method.

We have performed a full set of calculations with two parametrizations of the Skyrme interaction: SIII, which was used in previous studies of the Zr isotopes with the same method [11,16], and SLy4 [17]. The results that we present in details correspond to the SIII force. Both forces predict very similar behavior of the energy as a function of octupole degrees of freedom around the spherical configuration. However, their predictions for the energy as a function of the axial quadrupole moment are qualitatively different. The main difference between both forces is that, at the mean-field level of approximation, the ^{80}Zr ground state obtained with SLy4 is spherical and the deformed configuration is excited by 3–4 MeV, whereas for SIII the two configurations are almost degenerate. Also the spherical configuration of ^{98}Zr forms a local minimum with respect to the quadrupole deformation for SLy4 force, whereas it turns out to be unstable for SIII.

The pairing interaction has been treated in the BCS approximation including the Lipkin-Nogami (LN) correction [18]. A zero-range density-dependent pairing interaction has been used:

$$V_{\text{pair}} = \frac{1}{2} g_i (1 - P_\sigma) \delta(\mathbf{r} - \mathbf{r}') \left[1 - \frac{\rho(\mathbf{r})}{\rho_0} \right], \quad (1)$$

where $i = n, p$ for neutrons and protons, respectively. As in previous applications, we set $\rho_0 = 0.16 \text{ fm}^{-3}$.

The strengths of the pairing force for both nuclei are listed in Table I together with pairing gaps $\bar{\Delta}_i$ calculated as an average over the single-particle states within a 5-MeV window around the Fermi level. These values reproduce the “experimental” pairing gaps Δ , extracted from the odd-even mass staggering using a three-point filter from Ref. [19]. Because there are large uncertainties in the experimental gaps, especially around ^{80}Zr , we have also performed calculations with reduced pairing

TABLE I. The pairing strengths g_i used for calculations and the averaged pairing gap in the ground state.

SIII	g_p (MeV fm ³)	g_n (MeV fm ³)	$\bar{\Delta}_p$ (MeV)	$\bar{\Delta}_n$ (MeV)
^{80}Zr	1100	1300	1.048	1.415
^{98}Zr	1050	725	0.912	0.655

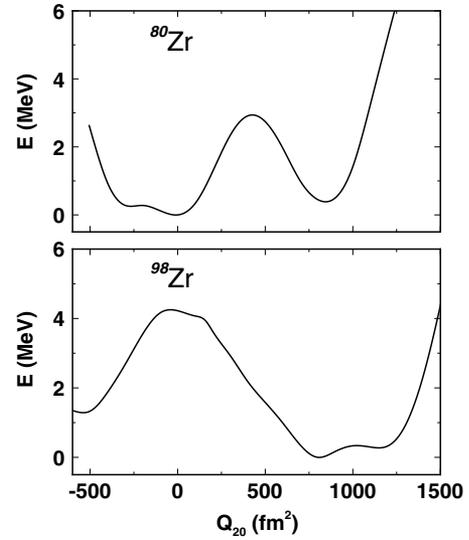


FIG. 1. Variation of the energy as a function of the quadrupole Q_{20} moment calculated in the HFBCS approach.

strengths, in particular with the values used in Ref. [20] that give gaps twice smaller than the “experimental” ones.

The HFBCS+LN calculations presented in Fig. 1 show the variation of the energy as function of the axial quadrupole moment. For ^{80}Zr , the spherical and deformed configurations are almost degenerate, whereas for ^{98}Zr , the SIII interaction does not predict a spherical minimum. However, calculations with the SLy4 force give a shallow spherical minimum with a depth of 200 keV. These differences between the two parametrizations are due to the transitional character of ^{98}Zr , which makes the study of its quadrupole properties very sensitive to the details of the effective interaction.

To probe the octupole susceptibility of the spherical configurations, we have performed two sets of calculations along the axial octupole path (Q_{32} was kept equal to zero) and the tetrahedral path (Q_{30} was kept equal to zero). In both cases, the quadrupole moment was constrained to zero. The results are shown in Fig. 2. The octupole moments have been expressed through the dimensionless deformation parameters using the relation $\beta_{30} = \langle Q_{30} \rangle / C_0$, $\beta_{32} = \langle Q_{32} \rangle / C_2$, where $C_0 = 3/4\pi A^2 r_0^3$, $C_2 = C_0 / \sqrt{2}$ with $r_0 = 1.2$ fm. For each octupole mode, we have performed calculations with pairing switched off and on. In the HF approximation, the spherical configuration is always unstable with respect to the octupole modes. The energy gained by octupole deformations is around 1 MeV for Y_{30} and is still larger for Y_{32} , around 2 MeV for ^{80}Zr and 3 MeV for ^{98}Zr . This result is consistent with calculations performed within the macroscopic-microscopic method with a Woods-Saxon potential [3]. When pairing correlations are taken into account, the effects of octupole correlations are strongly reduced. For ^{98}Zr the energy gain does not exceed 1 MeV and for ^{80}Zr the octupole minima even disappear completely. Nevertheless the susceptibility toward the Y_{32} mode remains slightly larger than for the axial octupole mode. Note that octupole minima in ^{98}Zr are saddle points. Very similar results concerning the tetrahedral instability of the spherical configuration of ^{80}Zr have been found in Skyrme

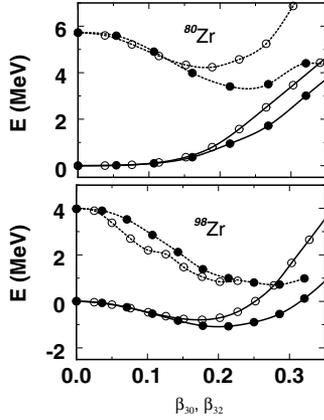


FIG. 2. Energy as function of the octupole moments. The quadrupole deformation has been constrained to zero. The solid and dotted lines denotes the HFBCS results and pure HF results, respectively. Lines with solid and empty circles denote the energy as a function of the Q_{32} and Q_{30} moment, respectively.

HFBCS [21] and HFB [20,22] calculations. The mechanism by which pairing correlations makes the tetrahedral minimum weaker is rather simple. In these nuclei, the single-particle gaps are not large in the spherical configuration and are increased almost twice by tetrahedral deformations. As a result, shell effects favor the creation of a tetrahedral minimum. However, the pairing interaction is the largest for the spherical configuration and is very small in the tetrahedral minimum, resulting in a flat potential energy curve.

This result shows that a static tetrahedral configuration may appear only as a result of a delicate balance between pairing and shell effects, which makes its prediction strongly dependent on the effective interaction that is used. Moreover should there be a static tetrahedral minimum, it is likely to be shallow and could be destroyed by dynamical correlations. One must also emphasize that our mean-field calculations were performed around the spherical configuration by constraining the quadrupole moment to zero. The octupole minima that are obtained could therefore also be unstable against quadrupole deformations. Yet, dynamical factors may also play in favor of octupole minima. In particular, when octupole correlations are included, the mean-field wave function breaks parity and parity projection brings a correlation energy that favors octupole correlation, especially for negative-parity states. We will study these effects in the next section to determine the stability of a tetrahedral state with respect to correlations beyond a mean-field approach.

The generator coordinate method (GCM) allows at the same time to study the collective dynamics of a nucleus with respect to a collective variable and to restore the symmetries broken in a pure mean-field approach (see Ref. [12] and references therein). It is perfectly suited to our goal, which is to determine a possible influence of the tetrahedral mode on low-lying collective states.

The information given by a mean-field potential energy surface is of a purely static nature and one must go beyond a mean-field approach to study its stability with respect to vibrations in the potential well. In cases where the energy

surface presents several coexisting minima separated by low barriers, the very concept of a mean-field state with a specific deformation may even break down. Correlations beyond mean-field lead then to states that represent a mixture of configurations with different deformations. All these effects are taken into account in the GCM approach.

We limit here the collective space to octupole modes against which ^{80}Zr and ^{98}Zr are very soft. It is clear that a full study of these nuclei would require to include also quadrupole deformations and to mix both octupole modes. Such multidimensional GCM calculations are feasible but represent a heavy task that is beyond the scope of this exploratory article. The purpose of the present GCM calculations is limited to finding out whether there is a chance to have a clear signature of the tetrahedral mode in the low-energy spectrum.

We have taken either Q_{30} or Q_{32} as generator coordinate. The wave functions generated by the constrained mean-field calculations were first projected on particle numbers and parity:

$$E(N, Z, \beta_{3\mu})_{\pm} = \frac{\langle \phi(\beta_{3\mu}) | \hat{H} \hat{P}_{(\pm, N, Z)} | \phi(\beta_{3\mu}) \rangle}{\langle \phi(\beta_{3\mu}) | \hat{P}_{(\pm, N, Z)} | \phi(\beta_{3\mu}) \rangle}, \quad (2)$$

where $|\phi(\beta_{3\mu})\rangle$ are HFBCS wave functions generated with the constraint $\langle \phi(\beta_{3\mu}) | \hat{Q}_{3\mu} | \phi(\beta_{3\mu}) \rangle = C_{\mu} \beta_{3\mu}$. The operator $\hat{P}_{(\pm, N, Z)}$ is the product of operators projecting on $\pi = \pm 1$ parity and on N neutrons and Z protons. The parity-projected energies are shown in the upper part of Fig. 3. As usual after parity restoration [13] the energy minima for positive-parity states are shifted toward smaller octupole deformations compared to the HFBCS minima (see Fig. 2), whereas the negative-parity states have larger deformations. For both nuclei the energy minima for positive parity correspond to very similar β_{30} and β_{32} values. For the negative-parity curve, β_{32} is systematically larger than β_{30} in the minimum. Qualitatively similar results have been obtained with the SLy4 Skyrme parametrization.

The GCM allows to study the stability of the configurations, corresponding to the minima of these energy curves, with respect to large amplitude vibrations. A collective wave function is constructed by mixing the mean-field states corresponding to different values of the octupole moment, after their projection on particle number and parity:

$$|\Psi\rangle = \int f(\beta_{3\mu}) \hat{P}_{(\pm, N, Z)} |\phi(\beta_{3\mu})\rangle d\beta_{3\mu}. \quad (3)$$

The coefficients $f(\beta_{3\mu})$ are determined by minimization of the total energy of the collective wave function $|\Psi\rangle$. The same effective interactions as in the mean-field calculations are used. In practice, the integral is replaced by a discrete summation over $\beta_{3\mu}$, with a number of points large enough to obtain results independent of the discretization [12]. The discretized Hill-Wheeler (HW) equation was solved separately for each collective coordinate Q_{30} and Q_{32} . The collective wave functions [related to $f(\beta_{3\mu})$ by an integral transformation] are plotted in Fig. 3. One can see that these wave functions are spread around the minima of the projected mean-field energy

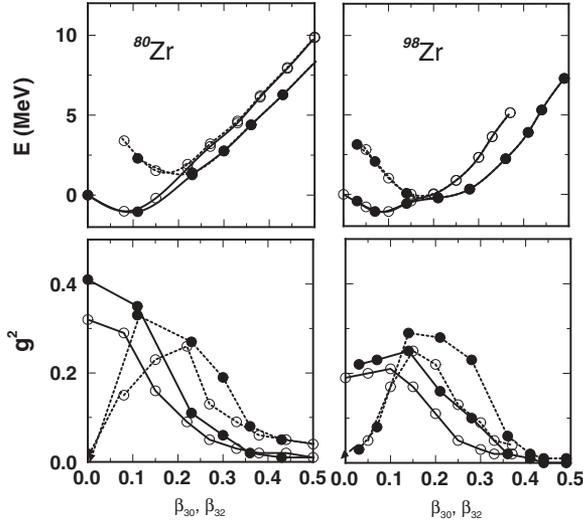


FIG. 3. The parity projected mean-field energy as function of the octupole moments is shown in the upper figures. The solid and dotted lines denote the positive and negative parity results, respectively. Lines with open and filled circles denote the energy as a function of the Q_{30} and Q_{32} moment, respectively. In the lower figure, the square of collective wave functions are shown. The line styles correspond to those in the upper figure.

curves, with a shape typical of a vibration in a one-dimensional energy well.

The energy gain due to correlations beyond the mean field is shown in Table II. The correlation energy is defined by:

$$E_{\text{corr}} = E(N, Z, \text{spher.}) - E^+, \quad (4)$$

where $E(N, Z, \text{spher.})$ is the energy of the particle number projected spherical configuration obtained in the HFBCS approach and E^+ is the lowest positive-parity energy obtained in the GCM. We calculated also a dynamical deformation associated with the lowest collective eigenstates for both parities defined by:

$$\tilde{\beta}_{3\mu} = \sum_{\beta_{3\mu}} \beta_{3\mu} g_{\pm}^2(\beta_{3\mu}). \quad (5)$$

TABLE II. Results of the GCM calculations. E_{exc} denotes the excitation energy of the first negative-parity collective state with respect to the first positive-parity state. E_{corr} is the correlation energy as defined in Ref. [4] and $\tilde{\beta}_{3\mu}$ refers to the dynamical deformation of Ref. [5].

SIII	E_{exc} (MeV)	E_{corr} (MeV)	π	$\tilde{\beta}_{30}$	$\tilde{\beta}_{32}$
^{80}Zr	0.0	1.499	+1	0.0	0.12
	2.22	—	-1	0.0	0.25
	0.0	1.459	+1	0.13	0.0
	2.52	—	-1	0.23	0.0
^{98}Zr	0.0	1.485	+1	0.0	0.14
	0.784	—	-1	0.0	0.21
	0.0	1.387	+1	0.11	0.0
	1.09	—	-1	0.19	0.0

The correlation energies are very similar for both modes and both nuclei with, however, a slightly larger gain for the Q_{32} mode. This small difference induces also an increase of dynamical deformations with respect to static ones. More significant are the differences obtained for the negative-parity states whose excitations are lower by 300 keV. Qualitatively similar predictions are obtained with the SLy4 interaction.

To check the sensitivity of the GCM results on the magnitude of pairing correlations, we performed calculations with pairing strengths that produce gaps larger or smaller by a factor of 2. Qualitatively, the GCM results are not affected: the changes in the collective wave functions and dynamical deformations are marginal. The correlation energies vary by 10–20%. A doubling of the pairing gap results in approximately twice as large excitation energy for the negative-parity states. We have found also that the results for ^{98}Zr are less sensitive to the pairing strength than those for ^{80}Zr .

We have studied two nuclei, ^{80}Zr and ^{98}Zr , which are doubly magic with respect to the tetrahedral symmetry, to establish whether they may serve as good candidates to obtain experimental evidence of a stable tetrahedral deformation. Our results, based on the mean-field approach, indicate that the spherical configuration of both nuclei is indeed unstable against octupole deformations. The presence of a tetrahedral minimum is the result of a delicate balance between shell effects and pairing. Due to the very shallow energy minima, quantum fluctuations beyond mean field play a significant role. To quantify this role, we performed dynamical calculations using the GCM in two octupole directions, specified by either tetrahedral or axial octupole deformations. The correlation energies associated with the octupole collective modes are large in both cases and lower significantly the energy of the spherical configuration. These results seem to be qualitatively independent of the Skyrme parametrization.

We performed the calculation in such conditions that each mode is clearly separated from the other, constraining in particular the quadrupole deformations to be zero. Under these conditions it turns out that the correlation energies are slightly larger for the tetrahedral mode than for the axial one. Also the tetrahedral vibration has smaller energy than the corresponding energy of axial octupole collective mode. Hence it was shown that, thanks to dynamical effects, the tetrahedral mode is energetically more favorable as compared to the axial octupole mode. However, the possible mixture between these modes cannot be excluded.

In summary, our results suggest that both the axial and tetrahedral type of octupole correlations play an important role in these nuclei, and they possess very similar characteristics.

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