HARTREE-FOCK-BOGOLYUBOV CALCULATIONS FOR NUCLEI WITH TETRAHEDRAL DEFORMATION

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Hartree-Fock-Bogolyubov solutions corresponding to the tetrahedral deformation are found in six tetrahedrally doubly-magic nuclei. Values of the $\beta_{32}$ deformation, depths of the tetrahedral minima, and their energies relative to the co-existing quadrupole minima are determined for several versions of the Skyrme force. Reduction of the tetrahedral deformation energies by pairing correlations is quantitatively analysed. In light nuclei, shallow tetrahedral minima are found to be the lowest in energy, while in heavy nuclei, the minima are deeper but appear at a few MeV of excitation.

1. Introduction

It is known that an increased nuclear binding is caused by the presence of large energy gaps in the single-particle (s.p.) nuclear spectra. The large gaps result in a decreased average density of s.p. levels and influence binding energies through the so-called shell effects. These effects can be further enhanced by high degeneracies of the s.p. levels above and/or below the energy gaps, which results in even larger fluctuations of the average level densities. Such degeneracies, in turn, are consequences of the conservation of certain symmetries in the s.p. Hamiltonian. Ordinary doubly-magic nuclei, for example, are spherically symmetric, i.e. characterized by degeneracies corresponding to the rotational group $O(3)$, and indeed the most strongly bound. Apart from the group of rotations, there exist only two other relevant symmetry groups whose conservation leads to s.p. degeneracies higher than the two-fold Kramers degeneracy. One of them is the point group, $T_d$, of the regular tetrahedron, which yields two-fold and four-fold degenerate s.p. levels. On this
basis, Li and Dudek\cite{1} suggested in 1994 that stable nuclear shapes characterized by the tetrahedral symmetry may exist in Nature.

The lowest-rank multipole deformation which does not violate the $T_d$ symmetry is $\beta_{32}^2$. It represents a shape of a regular tetrahedron with "rounded edges and corners", and is usually called tetrahedral deformation. By using the deformed Woods-Saxon potential, several authors\cite{1,2,3} examined the s.p. energies in function of $\beta_{32}$, and found that, indeed, large energy gaps, sometimes larger than the spherical ones, open up at neutron/proton numbers of $N/Z=16, 20, 32, 40, 56-58, 70, 90-94, 100, 112, 126$ or $136$. They are sometimes referred to as tetrahedral magic numbers. In the vicinity of the tetrahedrally doubly-magic nuclei defined in this way, Strutinsky shell-correction calculations were performed\cite{1,3,4,5}, and energy minima corresponding to the tetrahedral deformation were found in even-even $^{80}\text{Zr}$, $^{106-112}\text{Zr}$, $^{160}\text{Yb}$, $^{222}\text{Rn}$, and $^{242}\text{Fm}$. Similarly, the Hartree-Fock+BCS (HF+BCS) calculations\cite{6}, found tetrahedral solutions in $^{80}\text{Zr}$, and Hartree-Fock-Bogolyubov (HFB) tetrahedral solutions in $^{80}\text{Zr}$ and $^{106-112}\text{Zr}$ were reported in Refs.\cite{7} and\cite{4,5}, respectively.

The present paper reports on the first systematic study of the tetrahedral deformation in various regions of the nuclear chart, carried out by means of self-consistent methods. We focus our study on properties of the tetrahedral minima, mainly their energies and deformations, and analyze their dependence on the Skyrme force parameterizations.

2. HFB calculations

The HFB method was used. Four parameter sets of the Skyrme interaction were taken in the particle-hole channel: SLy4\cite{8}, SkM*\cite{9}, SkP\cite{10}, and SIII\cite{11}. For the description of pairing, procedures of Ref.\cite{12} were followed. The density-dependent delta interaction in the form of

$$ V(\vec{r}_1, \vec{r}_2) = V_0 \left( 1 - \frac{\rho(\vec{r}_1)}{2\rho_0} \right) \delta(\vec{r}_1 - \vec{r}_2) $$

was employed, with the saturation density, $\rho_0=0.16\text{fm}^{-3}$, and strengths of $V_0=-285.88, -233.94, -213.71$, and $-249.04\text{MeV fm}^3$ for SLy4, SkM*, SkP, and SIII, respectively. The densities were constructed out of quasi-particle states with equivalent-spectrum energies\cite{10} up to $60\text{MeV}$. In order to study effects of pairing, the HF calculations were also performed for comparison. Reflection symmetries in two or three perpendicular planes were imposed, correspondingly, when looking for the tetrahedral and quadrupole solutions. The calculations were carried out by using the code HFODD (v2.11k)\cite{13,14,15}, which expands the quasi-particle wave-functions onto the Harmonic-Oscillator basis. Bases of 14 and 16 spherical shells were taken for the Zr and heavier elements, respectively.

Six nuclei, doubly-magic with respect to the tetrahedral magic numbers, were examined: $^{80}\text{Zr}$, $^{98}\text{Zr}$, $^{110}\text{Zr}$, $^{126}\text{Ba}$, $^{160}\text{Yb}$, and $^{226}\text{Th}$. In all of them, the HF and HFB energy minima corresponding to the tetrahedral shapes were found
with all the examined forces, apart from a few exceptions. The found solutions are characterized by the $\beta_{32}$ deformations ranging from 0.08 to 0.26, and admixtures of $\beta_{40}$ and $\beta_{44}$ deformations in proportions that preserve the tetrahedral symmetry, and with values of $\beta_{40}$ ranging from about 0.01 to 0.07. Deformations of higher multipolarities were found to be negligibly small. As expected for the tetrahedral symmetry, the HF s.p. and HFB quasi-particle spectra are composed of two-fold and four-fold degenerate levels. In the six nuclei in question, spherical, oblate, prolate, and triaxial solutions were also found, depending on the nucleus, as discussed below.

![Graph showing total energy in function of the tetrahedral deformation $\beta_{32}$ in $^{110}$Zr, obtained from the HFB calculations with the SIII force. $\Delta E_{sh}$ denotes the energy difference between the spherical point and the tetrahedral minimum.](image)

Three quantities that characterize the obtained tetrahedral solutions will be examined: the energy difference, $\Delta E_{hq}$, between the tetrahedral ($h$) and lowest quadrupole ($q$) minima, the energy difference, $\Delta E_{sh}$, between the spherical point ($s$) and tetrahedral minimum, and the deformation $\beta_{32}$. $\Delta E_{hq}$ gives an idea of the excitation energy of the tetrahedral states above the ground state. $\Delta E_{sh}$ is important for the following reason. Both from the previous self-consistent studies in $^{80}$Zr\cite{6,7}, as well as from our preliminary results for $^{80,98,110}$Zr, it seems that, at least in the Zr isotopes, there is no energy barrier between the spherical and tetrahedral solutions. Energy in function of $\beta_{32}$ looks rather like the dependence shown in Fig. 1, obtained from the HFB calculations in $^{110}$Zr with the SIII force. One can see that $\Delta E_{sh}$ measures the depth of the tetrahedral minimum against changes in $\beta_{32}$, and thus provides information on whether a stable tetrahedral deformation or rather tetrahedral vibrations about the spherical shape should be expected.

Figure 2 shows the energy minima for selected nuclei and forces as points on the $\beta_{32}$-$E$ plane. In each panel, all the found HFB solutions (plus symbols, upper-case labels) are shown, while the HF solutions (circles, lower-case labels), are given only for the tetrahedral and spherical cases. The labels denote the tetrahedral ($h$, $H$), spherical ($s$, $S$), oblate ($O$), prolate ($P$), and triaxial ($T$) solutions.
One of the principal observations resulting from our calculations is that various Skyrme forces may give significantly different energetical positions of the tetrahedral solutions with respect to the quadrupole minima. This is most pronounced for the SLy4 and SkM* results in $^{80}$Zr (two upmost panels in Fig. 2), which give the
Table 1. Minimum (min) and maximum (max) values of $\Delta E_{hq}$ [MeV], $\Delta E_{sh}$ [MeV], and $\beta_{32}$ from among the results obtained with various Skyrme forces. Results are shown for each nucleus and approximation (HF or HFB) studied here.

| Nucleus | $\Delta E_{hq}$ | $\Delta E_{sh}$ | $\beta_{32}$ |
|---------|-----------------|-----------------|-------------|
|         | HFB | HF | HFB | HF | HFB | HFB | HF | HFB |HF | HFB | HFB |
| $^{80}$Zr | -3 | 3 | 0.1 | 2 | 0.1 | 2 | 0.11 | 0.20 | 0.11 | 0.20 |
| $^{98}$Zr | -1.5 | 2 | 0.3 | 0.7 | 0.04 | 0.5 | 0.14 | 0.16 | 0.09 | 0.20 |
| $^{110}$Zr | -0.4 | 5 | 0.07 | 5 | 0.4 | 2 | 0.08 | 0.23 | 0.14 | 0.21 |
| $^{126}$Ba | 7 | 11 | 3 | 5 | 2 | 2 | 0.17 | 0.26 | 0.22 | 0.22 |
| $^{160}$Yb | 3 | 7 | 3 | 7 | 0.19 | 0.26 | 0.23 | 0.24 |
| $^{226}$Th | 3 | 8 | 0.18 | 0.24 | 0.15 | 0.22 |

tetrahedral minima of about 3 MeV below and above the lowest quadrupole state, respectively. The extremal values of $\Delta E_{hq}$ predicted by various forces for each nucleus studied here are collected in Table 1. They do not depend much on whether pairing is included or not. The differences between the maximum and minimum values are of the order of a few MeV. One can see, nevertheless, that $\Delta E_{hq}$ is lowest in $^{98}$Zr isotopes, where some forces even predict the tetrahedral solution to be the ground state. Values of $\Delta E_{hq}$ are particularly large, not smaller than 7 MeV, in $^{126}$Ba and rather moderate, even about 3 MeV, in $^{160}$Yb and $^{226}$Th.

Further important point is that the depths of the tetrahedral minima, $\Delta E_{sh}$, are reduced by pairing. This can be seen from the comparison of the HF and HFB results for $^{110}$Zr and $^{126}$Ba (four central panels in Fig. 2). The reductions may be as significant as from 3 to 1 MeV in $^{110}$Zr with SkM*, while for SkP the inclusion of pairing suppresses the tetrahedral minimum in $^{110}$Zr altogether. The decrease in $\Delta E_{sh}$ is mainly due to the lowering of the energy at the spherical point, i.e., the pairing influences the spherical state more than the tetrahedral one. This is so because the s.p. energy gaps at the Fermi level are bigger in the latter case, as already discussed in the Introduction. In $^{80}$Zr with SIII, for instance, pairing vanishes at the tetrahedral minimum, and remains non-zero at the spherical point. Predictions concerning the destructive role of pairing strongly depend on the details of the method, as well. The HF+BCS and HFB calculations for $^{80}$Zr, both using the SIII force, yielded $\Delta E_{sh}$ of 0.7 MeV and several tens of keV, respectively. The corresponding result of our calculations is about 2 MeV.

In the current analysis, we also obtain differences in predictions of various Skyrme forces as to the values of $\Delta E_{sh}$, both with and without pairing. In the HFB results for $^{110}$Zr, for example, $\Delta E_{sh}$ varies from about 0.4 for SLy4 to 2 MeV for SIII, not counting SkP. The HF and HFB results for other studied nuclei are summarized in Table 1. In $^{226}$Th, no spherical solutions, and in $^{160}$Yb no spherical HFB solutions were found, so that the corresponding values of $\Delta E_{sh}$ could not be calculated. In $^{126}$Ba, the tetrahedral HFB solution was obtained with only one force, SkM*. However, the HF results exhibit a clear trend that $\Delta E_{sh}$ increases...
with the mass number. It can be as small as a few tens of keV in Zr isotopes, and as large as 7 MeV for $^{160}$Yb with SkM*. The problem of stability of the tetrahedral minima can be even more complicated because of a possible softness of the nuclei in question against the octupole deformations other than $\beta_{32}$.7.

The four Skyrme forces used in our study also give somewhat different values of the $\beta_{32}$ deformation, see Table 1. The inclusion of pairing slightly reduces these values, along with $\Delta E_{sh}$. Heavier isotopes have larger values of $\beta_{32}$.

3. Summary

Hartree-Fock-Bogolyubov solutions corresponding to the tetrahedral deformation were found in six tetrahedrally doubly-magic nuclei: $^{80}$Zr, $^{98}$Zr, $^{110}$Zr, $^{126}$Ba, $^{160}$Yb, and $^{226}$Th. Results with four Skyrme forces, SLy4, SkM*, SIII, and SkP, sometimes significantly differ in the values of $\beta_{32}$, depths of the tetrahedral minima, and their energies with respect to the co-existing quadrupole solutions. The inclusion of pairing reduces the depths, or even suppresses the existence of the tetrahedral minima.

In Zr isotopes, the tetrahedral minima are rather shallow, but some forces predict them as the lowest in energy. In $^{126}$Ba, they are not lower than 7 MeV above the quadrupole solutions, but in $^{160}$Yb and $^{226}$Th that minimum distance is reduced to 3 MeV. Tetrahedral minima in $^{126}$Ba, $^{160}$Yb, and $^{226}$Th are estimated to be deeper than in the Zr isotopes.

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