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# INVESTIGATION OF THE INFLUENCE OF THE NUCLEON PAIRING FORCE ON THE OCTUPOLE DEFORMATION OF URANIUM AND THORIUM ISOTOPES IN THE MEAN-FIELD APPROXIMATION

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In the Hartree-Fock-Bogolyubov approximation and the axial symmetry of nuclei with Skyrm forces SkM*, the properties of U with $A$ = 220 – 232 and Th with $A$ = 218 – 230 isotopes were calculated. In addition, the properties of U and Th near the neutron drip line $A$ = 280 – 292 were calculated. Pairing of nucleons in nuclei is described by pairing forces of zero radius of action of a mixed type with different sets of pairing force constants. In our calculations, we used constrained conditions on the parameters of quadrupole $\beta_2$ and octupole $\beta_3$ deformations of nuclei. It is shown that for the considered U isotopes, as well as Th isotopes, the deformation of the $\beta_3$ nuclei strongly depends on the choice of the parameters of the nucleon pairing force.

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## INTRODUCTION

The study of the shape of atomic nuclei is one of the important problems of nuclear physics. The deformation of the shape of atomic nuclei is characterized by the moments of the distribution of the density of nucleons in the nuclei or by the parameters of the deformation of the nuclei. Experimental data indicate the presence of quadrupole moments in a significant part of the known atomic nuclei. Studies of the manifestations of the existence of octupole deformations (pear-shaped shapes) of atomic nuclei are considered in works [1, 2], in which it was shown that nuclei with an octupole deformation of the shape, compared with nuclei with a quadrupole deformation, are represented by small areas $Z$ and $A$.

To describe the properties of large collections of nuclei, microscopic approaches based on the Hartree–Fock–Bogolyubov (HFB) method or on the Hartree–Fock (HF) method [3] with effective forces as well as approaches based on the relativistic theory Hartree–Bogolyubov (RHB) [4] at the present time are widely used. The same approaches for calculating the properties of nuclei with allowance for possible octupole deformation were used in [5–7]. The influence of the choice of parameters of the pairing forces, both on the calculated values of the octupole deformation parameter and on the value of the region of existence nuclei with octupole deformation, is not enough investigated. In spite of the large amount of researches on the manifestations of the octupole deformation of nuclei in the HFB and RHB approaches, the calculations presented in [5–8] demonstrate it.

The purpose of this work is to continue studies [8] of the influence of the choice of pairing force parameters on the value of octupole deformation for nuclei close in $Z$ to radium isotopes. For this, we considered uranium and thorium isotopes in the HFB approximation with the SkM* Skyrme interaction in the range of mass numbers $A$ = 218 – 232, as well as near the neutron drip line of the neutron stability limit with $A$ = 280 – 292.

## CALCULATION METHOD AND MAIN RESULTS

To study the properties of the ground state of even-even isotopes of uranium and thorium based on the HFB method with the effective Skyrme interaction depending on the nucleon density, we used the HFBTHO v2.00d software package [9]. This software package allows solving the system of stationary HFB equations under the assumption of axial symmetry of the shape of the nucleus with conservation or violation of reflection symmetry in the nucleus. The HFBTHO v2.00d software package uses the expansion of single-nucleon wave functions in terms of the wave function basis of an axially deformed harmonic oscillator. In the expansion of single-nucleon wave functions we took into account all the basis wave functions of a harmonic oscillator for which the principal oscillatory quantum number does not exceed $N_0 = 18$. Calculations with an increased dimension of the basis show that the dimension of the basis $N_0 = 18$ is sufficient for the considered region of mass numbers of nuclei. To calculate the matrix elements, we used the quadrature formulas of Gauss–Laguerre and Gauss–Hermit. When the reflection symmetry is broken in the nuclei, the doubled number of nodes of the Gauss-Hermit quadrature formulas are used.

This software package allows solving the system of HFB equations with constrained conditions on the multipole moments of nuclei, and also allows solving equations without constrained conditions on the deformation moments. In our calculations, we used constrained conditions on the dipole, quadrupole, and octupole deformations of nuclei. In all our calculations, the constrained conditions on the mass dipole moment of the nucleus are: $Q_{10} = 0$. The parameters of the quadrupole and octupole deformations of the nucleon distribution density are determined similarly to [6]:

$$\beta_2 = Q_{20} / \left( \sqrt{\frac{16\pi}{5}} \frac{3}{4\pi} A R_0^2 \right), \quad (1)$$

$$\beta_3 = Q_{30} / \left( \sqrt{\frac{16\pi}{7}} \frac{3}{4\pi} A R_0^3 \right), \quad (2)$$

where $Q_{20}$ and $Q_{30}$ are the mass quadrupole and octupole moments of nuclei as in [6], $A$ is the number of nucleons in the nucleus, and $R_0 = 1.2A^{1/3}$ fm.

In our calculations, we used the Skyrme force parameter sets SkM* [10]. Nucleon pairing is described by zero-range pairing forces that depend on the nucleon density. We used the following form for the pairing forces [9]:

$$\upsilon(\vec{r}_1,\vec{r}_2) = V_\tau \left\{1-\alpha\left[\frac{\rho\left(\vec{R}\right)}{\rho_0}\right]\right\}\delta\left(\vec{r}_1-\vec{r}_2\right), \qquad (3)$$

where $V_\tau$ is the pairing force parameter for neutrons ($\tau = n$) and protons ($\tau = p$), $\alpha$ is the parameter that determines the type of pairing ($\alpha$ = 0, 0.5, 1 – volume, mixed and surface types of pairing, respectively), $\rho_0 = 0.16$ fm$^{-3}$, $\vec{r} = \vec{r}_1 - \vec{r}_2$ is the relative radius-vector and $\vec{R} = (\vec{r}_1 + \vec{r}_2)/2$ radius-vector of the center of mass of interacting nucleons. In the present work, we used only mixed-type pairing forces.

The solutions of the HFB equations corresponding to the most bound state of the nucleus were determined from finding the deepest minimum of the calculated surfaces of the total energies of nuclei $E$ with constrained conditions on the mass parameters of the quadrupole $\beta_2$ and octupole $\beta_3$ deformations. By the binding energy of the nucleus $B$ we will mean $B = -E$. The total energy surfaces of the nuclei were calculated in the range of quadrupole deformation parameters $-0.4 \le \beta_2 \le 1.0$ and octupole deformation $0 \le \beta_3 \le 0.3$.

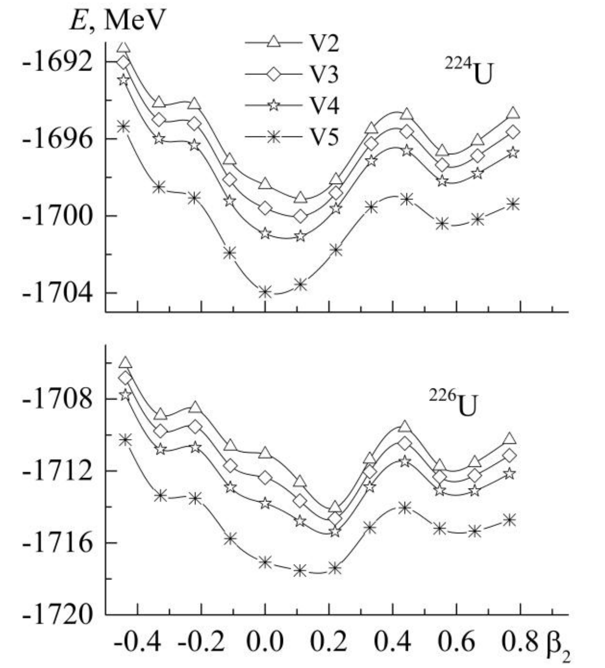


*Fig. 1. Dependence of the total energy E on the value of the quadrupole deformation parameter $\beta_2$ for $^{224,226}$U isotopes in HFB calculations with Skyrme forces SkM* without taking into account the octupole deformation $\beta_3$ with different sets of pairing force parameters*

As an example of calculations with constrained conditions, Fig. 1 shows the dependence curves of the total energy $E$ of the $^{224,226}$U uranium isotopes, calculated with the Skyrme interaction SkM*, on the deformation parameter $\beta_2$ for various sets of pairing forces without taking into account the octupole deformation $\beta_3$. The parameters of the pairing forces V2–V5, which we used in calculations with the Skyrm interaction SkM*, were determined as follows. Parameters of type V2 were considered as reference ones. These V2 parameters are used in the original HFBTHO v2.00d [9] code with Skyrme interaction SkM*. For forces V2, the values of the parameter $V_\tau$ in expression (3) are $V_n$ = -265.25 MeV·fm$^3$, $V_p$ = - 340.0625 MeV·fm$^3$. We obtained the sets of parameters V3, V4, and V5 by multiplying the parameters V2 by 1.025, 1.05, and 1.1, respectively. As can be seen in Fig. 1 in uranium isotopes $^{224,226}$U with different sets of pairing forces, the quadrupole deformation parameter $\beta_2$ in the minima of the surfaces of the total energies of nuclei $E(\beta_2, \beta_3{=}0)$ appreciably depends on the value of the pairing force parameter $V_\tau$. For the other U isotopes from the range $A$ = 220 – 232, the pairing strength parameter also significantly affects $\beta_2$ at the minima of the surfaces of total energies of nuclei $E(\beta_2, \beta_3{=}0)$. The similar results take place for thorium isotopes with $A$ = 218 – 230.

To analyze the influence of the value of the pairing force parameter on the value of the octupole deformation parameter $\beta_3$, it is difficult to use the energy surfaces $E(\beta_2, \beta_3)$, as for the same isotope for different pairing forces, these surfaces can differ significantly in the value of the total energy. For such analysis, it is more convenient to use $\Delta E = E(\beta_2,\beta_3) - E(\beta_2^{'},\beta_3 = 0)$.

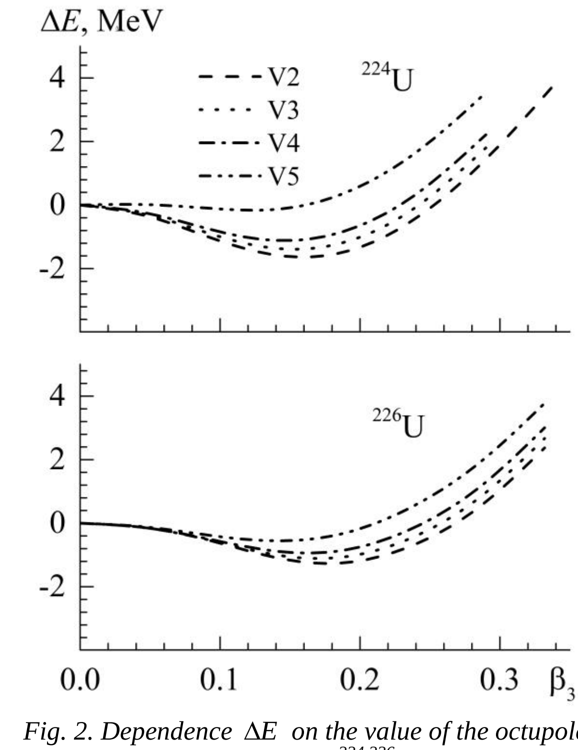


*Fig. 2. Dependence $\Delta E$ on the value of the octupole deformation parameter $\beta_3$ for $^{224,226}$U isotopes in HFB calculations with Skyrme forces SkM* with different sets of pairing force parameters*

Fig. 2 shows the curves of the change in the total energy of uranium isotopes $^{224,226}$U, calculated with the

Skyrme interaction SkM*, on the deformation parameter $\beta_3$ for different sets of pairing forces. In this case, the initial values of $\beta_2$ were set near the minima of the total energies obtained from calculations with constrained conditions on $\beta_2$ (see Fig. 1), and varied during the calculation, providing a minimum of the total energy of the nucleus at a given value of the deformation parameter $\beta_3$. Fig. 2 shows that for $^{224,226}U$ the weakest pairing forces V2 from the forces that we have considered, provide the deepest minimum $\Delta E$. Our calculations showed that this result holds for all the uranium and thorium isotopes we have considered. The increase in the pairing strength in uranium and thorium isotopes leads to the decrease in the depth of the minimum $\Delta E$ in the dependence on $\beta_3$, or to its almost complete disappearance.

For more accurate determination of the minimum value of the total energy of the nucleus after calculations with constrained conditions in the vicinity of the minimum of the dependence $E(\beta_2, \beta_3)$, we performed the calculations without constrained conditions on $\beta_2$ and $\beta_3$. Such calculations were carried out for all uranium and thorium isotopes considered in the work with all variants of the V2–V5 pairing forces. The results of such refined calculations without constrained conditions on $\beta_2$ and $\beta_3$ are shown below in Figs. 3 and 4.

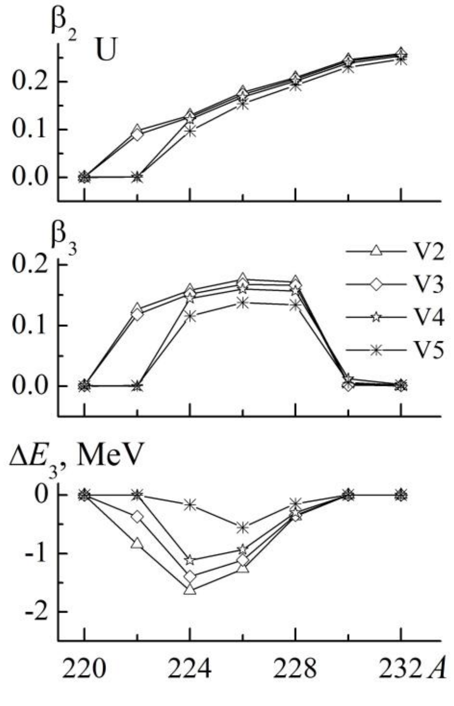


*Fig. 3. Deformation parameters $\beta_2$ and $\beta_3$, as well as octupole energies, calculated with the Skyrme interaction SkM* with different sets of pairing force parameters for U isotopes with A = 220 – 232*

Figs. 3 and 4 show the results of the calculations with Skyrme forces SkM* for the U and Th isotopes of the nuclear deformation parameters $\beta_2$ and $\beta_3$, as well as the value of $\Delta E_3 = E(\beta_2,\beta_3) - E(\beta_2^{'},\beta_3 = 0)$. The energy $\Delta E_3$, which is the contribution to the total energy of the nucleus from taking into account the octupole deformation of the nuclei, we will call the octupole energy of the nucleus. The calculations shown in Figs. 3 and 4, were performed with different sets of pairing force parameters discussed above. As can be seen in Figs. 3 and 4, the choice of the value of the pairing forces significantly affects the values of the deformation parameters $\beta_2$ and $\beta_3$, as well as the value of the octupole energy $\Delta E_3$. The pairing forces V5 for SkM* are so strong that it leads to the disappearance of both the quadrupole and octupole deformations of some uranium and thorium isotopes. The results shown in Figs. 3 and 4 show that the increase in the pairing force leads not only to the decrease or complete disappearance of the quadrupole and octupole deformation of the nuclei, but also, respectively, to the decrease or complete disappearance of the octupole energy. Therefore, in the calculations, it is necessary to control the magnitude of the pairing forces [8] by comparing the calculated pairing energy gaps with their empirical values. In our calculations of the properties of radium isotopes [8], such comparison allows us to give preference for the Skyrme forces SkM* to the pairing forces V2, V3.

We noted above that calculating the properties of large sets of nuclei based on the HFB and RHB approaches [6, 7], the existence of new previously unknown regions of nuclei with octupole deformation was predicted. In particular, such regions of possible existence of nuclei with octupole deformation are predicted in the vicinity of the neutron drip line. In the present work, for uranium and thorium isotopes in the region of nuclei with a large neutron excess in the vicinity of the neutron drip line, we studied the influence of the choice of pairing force parameters on the possibility of octupole deformation manifestation.

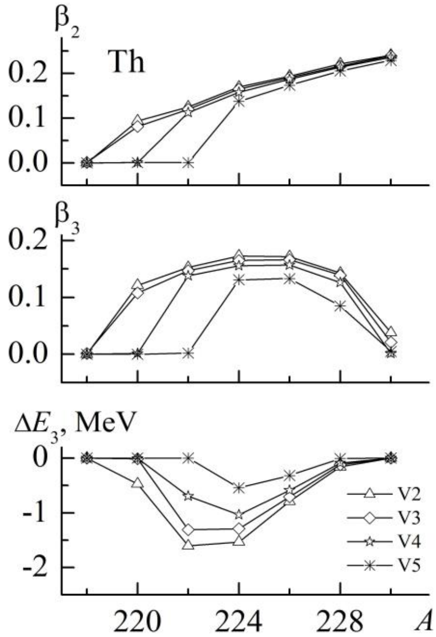


*Fig. 4. The same as in Fig. 3, but Th isotopes with A = 218 – 230*

Fig. 5 shows the results of calculations of $\beta_2$, $\beta_3$ and $\Delta E_3$ of U isotopes for $A = 280 – 292$. The calculation conditions for these nuclei completely coincide with the calculation conditions for the nuclei presented in Figs. 3 and 4.

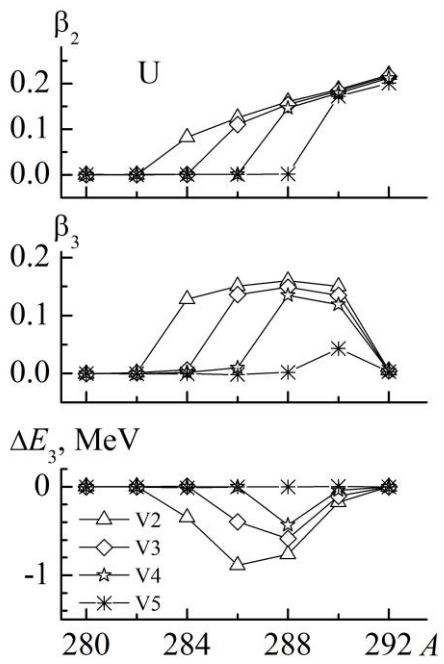


*Fig. 5. The same as in Fig. 3, but for A = 280 – 292*

It can be seen from Fig. 5 that the choice of the parameters of the pairing forces V2 – V5 significantly affects both the values of $\beta_2$, $\beta_3$ and $\Delta E_3$, and the character of their change with increasing mass number *A*. For the range of mass numbers *A* = 280 – 292, it is not possible to estimate the value of the pairing energy gap to select the preferred type of pairing constant $V_\tau$, as it was done in [8] for Ra isotopes, as there are no experimental data on the total energies for nuclei with such a large excess of neutrons. We also performed the calculations of $\beta_2$, $\beta_3$, and Th isotopes for *A* = 280 – 290. Note that for Th isotopes in this range of mass numbers, the character of the change in $\beta_2$, $\beta_3$ and $\Delta E_3$ for the pairing force parameters considered by us is similar to U isotopes.

## CONCLUSIONS

In this work, we performed the calculations in the HFB approximation under the assumption of axial symmetry of nuclei with Skyrme forces SkM* for U isotopes with *A* = 220 – 232 and *A* = 280 – 292, as well as Th isotopes with *A* = 218 – 230 and *A* = 280 – 290. Pairing of nucleons in nuclei is described by density-dependent zero-range pairing forces with different sets of constants that determine the pairing strength. In our calculations, we used the constrained conditions on the parameters of the quadrupole and octupole deformations of the nuclei.

It is shown that for the considered isotopes of uranium and thorium, the octupole deformation of nuclei strongly depends on the choice of parameters of the nucleon pairing force. Overestimated values of the pairing force constants lead to the decrease or complete disappearance of the quadrupole and octupole deformation in the considered nuclei.

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## ДОСЛІДЖЕННЯ ВПЛИВУ СИЛИ СПАРЮВАННЯ НУКЛОНІВ НА ОКТУПОЛЬНУ ДЕФОРМАЦІЮ ІЗОТОПІВ УРАНУ І ТОРІЮ У НАБЛИЖЕННІ СЕРЕДНЬОГО ПОЛЯ

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У наближенні Хартрі-Фока-Боголюбова та аксіальної симетрії ядер із силами Скірма SkM* проведено розрахунки властивостей ізотопів U з A = 220 – 232 і Th з A = 218 – 230. Додатково проведені розрахунки властивостей U і Th біля границі нейтронної стабільності A = 280 – 292. Спарювання нуклонів у ядрах описується силами спарювання нульового радіуса дії змішаного типу з різними наборами констант сил спарювання. У розрахунках використовувалися накладені умови на параметри квадрупольної $\beta_2$ і октупольної $\beta_3$ деформацій ядер. Показано, що для розглянутих ізотопів U, як і ізотопів Th, деформація ядер $\beta_3$ сильно залежить від вибору параметрів сили спарювання нуклонів.