ROLE OF NON-AXIAL SHAPES IN THE SADDLE-POINT ENERGY OF HEAVIEST NUCLEI

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(Received May 31, 2010)

The role of non-axial shapes in the saddle-point energy of heaviest nuclei is studied in a multidimensional deformation space. The main attention is given to the effect of the high-multipolarity, $\lambda = 6$, non-axial deformations, which is studied for the first time. The analysis is performed within a macroscopic–microscopic approach. Generally, a 10-dimensional deformation space is used in the analysis, but some tests are done in even 13 dimensions. A large number of about 300 even–even heavy and superheavy nuclei with proton number $98 \leq Z \leq 126$ and neutron number $134 \leq N \leq 192$ is considered. It is found that the inclusion of the non-axial shapes of the multipolarity $\lambda = 6$ lowers the saddle-point energy relatively little, by up to about 0.4 MeV. Together with earlier results on the effect of the quadrupole ($\lambda = 2$) and hexadecapole ($\lambda = 4$) shapes, this indicates for the convergence of the effect to zero, with increasing λ. As the ground-state shapes of the considered nuclei are axially symmetric, the discussion also concerns the height of the fission barrier. The heights of our barriers are compared with experimental ones and also with those of other authors.

PACS numbers: 21.60.–n, 24.75.+i, 27.90.+b

1. Introduction

One of the most important quantities in the studies of heaviest nuclei, being intensively done in recent years (*cf. e.g.*, [1–4]), is the cross-section σ for their synthesis. It gives us a knowledge which nuclei, and with how large effort, can be presently synthesized. In theoretical investigations of

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this quantity (*e.g.*, [5–11]), a basic role is played by the height of the (static) fission barrier $B_{\mathrm{f}}^{\mathrm{st}}$. This motivates the intensive studies of the barrier, being recently performed (*e.g.*, [12–26]). A big sensitivity of σ to $B_{\mathrm{f}}^{\mathrm{st}}$ stresses a need for as accurate calculations of $B_{\mathrm{f}}^{\mathrm{st}}$ as possible. Really, a change of $B_{\mathrm{f}}^{\mathrm{st}}$ by 1 MeV may result in a change of σ by about one to two orders of magnitude [6, 11]. The basic role in reaching this accuracy is played by the deformation space admitted in the calculations of $B_{\mathrm{f}}^{\mathrm{st}}$. In particular, one should include non-axial deformations of the nuclei.

It was shown in our previous studies that the inclusion of the quadrupole (the multipolarity $\lambda = 2$) non-axial shapes may lower the barriers by up to more than 2 MeV [27] and the inclusion of the hexadecapole ($\lambda = 4$) non-axial deformations may reduce them by up to about 1.5 MeV [28].

The objective of this paper is to learn the effect of non-axial shapes of still higher multipolarity, $\lambda = 6$, not studied earlier. In particular, one would like to see, if there is a convergence to zero of the effect with increasing λ. A large region of heavy and superheavy nuclei with proton number $98 \leq Z \leq 126$ and neutron number $134 \leq N \leq 192$ is considered.

2. Method of the analysis

The analysis is done within a macroscopic–microscopic approach. The Yukawa-plus-exponential model [29] is taken for the macroscopic part of the energy and the Strutinski shell correction, based on the Woods–Saxon single-particle potential [30], is used for its microscopic part. Pairing interaction, with the isotopic-dependent strength of the monopole type, is treated within the BCS approximation. Details of the approach are specified in [31].

Especially important in the analysis is the choice of a sufficiently large deformation space. Such a space is used in our study. In particular, besides the quadrupole (multipolarity $\lambda = 2$) non-axial shapes, it includes a general (if one assumes the reflection symmetry of a nucleus with respect to all three planes of the intrinsic coordinate system) non-axial shapes of multipolarity $\lambda = 4$ [32] and 6. The space is specified by the following expression for the nuclear radius $R(\vartheta, \varphi)$ (in the intrinsic frame of reference) in terms of spherical harmonics $Y_{\lambda\mu}$:

$$\begin{aligned} R(\vartheta,\varphi) = R_0\Big\{1 \; &+ \; \beta_2\left[\cos\gamma_2 \mathrm{Y}_{20} + \sin\gamma_2 \mathrm{Y}_{22}^{(+)}\right] \\ &+ \; a_{40}\mathrm{Y}_{40} + \sqrt{2}\left(a_{42}\mathrm{Y}_{42}^{(+)} + a_{44}\mathrm{Y}_{44}^{(+)}\right) \\ &+ \; a_{60}\mathrm{Y}_{60} + \sqrt{2}\left(a_{62}\mathrm{Y}_{62}^{(+)} + a_{64}\mathrm{Y}_{64}^{(+)} + a_{66}\mathrm{Y}_{66}^{(+)}\right) \\ &+ \; \beta_8\mathrm{Y}_{80} \\ &+ \; \beta_3\mathrm{Y}_{30} + \beta_5\mathrm{Y}_{50} + \beta_7\mathrm{Y}_{70}\Big\}\,, \end{aligned} \tag{1}$$

where γ_2 and $a_{\lambda\mu}$, $\lambda = 4, 6$, $\mu > 0$, are the non-axiallity parameters. In the case of the consideration of only axially symmetric shapes of a given multipolarity λ, the usual notation β_λ for the parameters $a_{\lambda 0}$, describing these shapes, is used (*i.e.*, $a_{\lambda 0} \equiv \beta_\lambda$ in this case). The odd-multipolarity degrees of freedom, $\beta_3, \beta_5, \beta_7$, appearing in Eq. (1), are used in our study only to show that they do not influence the studied quantities. The dependence of R_0 on the deformation parameters is determined by the volume-conservation condition. The real functions $\mathrm{Y}^{(+)}_{\lambda\mu}$ are defined as:

$$\mathrm{Y}^{(+)}_{\lambda\mu} = \frac{1}{\sqrt{2}} \left[\mathrm{Y}_{\lambda\mu} + (-1)^\mu \mathrm{Y}_{\lambda -\mu} \right] , \qquad \text{for} \quad \mu > 0 \, . \tag{2}$$

A special care is needed in finding the saddle point of a nucleus. A calculation of it in the full space would not be possible for numerical reasons. After making various tests, we have chosen the following procedure. The search is done in two steps. In the first one, it is done in the most important 3-dimensional space: $\{\beta_2, \gamma_2, a_{40}\}$, in which the saddle point is found (by the dynamic-programming method [33]). Then, with established $\beta_2^{\rm sp}, \gamma_2^{\rm sp}, a_{40}^{\rm sp}$, *i.e.* the values of β_2, γ_2 and a_{40} at the saddle point, the energy is minimized in the remaining degrees of freedom: $\{a_{42}, a_{44}, a_{60}, a_{62}, a_{64}, a_{66}, \beta_8\}$. A direct test, done for a few nuclei, in which the first step is done in a still larger, 4-dimensional space, shows that the results remain practically the same. Additionally, another, independent test is done using the so called immersion method (see [25]) in the 5-dimensional space $\{\beta_2, \gamma_2, a_{40}, a_{42}, a_{44}\}$. This test leads again to practically the same results.

3. Results and discussion

3.1. Potential-energy surface

Our study of the potential energy of the considered nuclei shows that this energy is not influenced by the odd-multipolarity deformations β_3, β_5 and β_7. One should stress, however, that this concerns the region of nuclei studied in the present paper, as for a large number of other heavy nuclei (around radium and heavier neutron-deficient ones) these deformations play an important role (see *e.g.*, Ref. [34]). After this test, the potential energy is studied in a smaller, 10-dimensional space.

Fig. 1 shows an example of the potential-energy surface calculated for a superheavy nucleus ^{294}118. This is the heaviest nucleus observed up to now [35]. The energy $E(\beta_2, \gamma_2; a_{40}^{\rm m}, a_{42}^{\rm m}, a_{44}^{\rm m}, a_{60}^{\rm m}, a_{62}^{\rm m}, a_{64}^{\rm m}, a_{66}^{\rm m}, \beta_8^{\rm m})$, calculated in the 10-dimensional space, is projected in the figure on the (β_2, γ_2) plane. This means that it is shown as a function of β_2, γ_2, but at each point (β_2, γ_2), it is minimized in the remaining degrees of freedom; *e.g.*, $a_{40}^{\rm m}$ denotes the

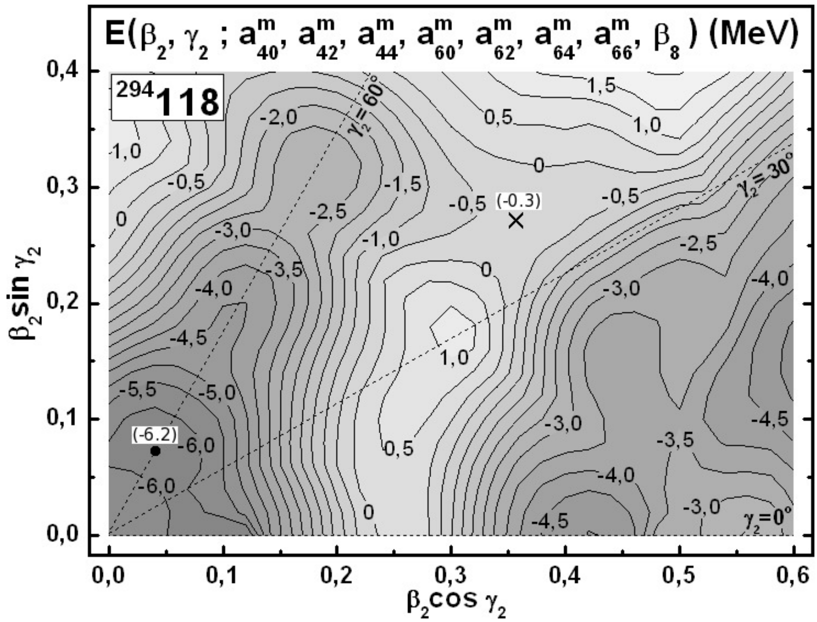

Fig. 1. Contour map of the potential-energy surface of the nucleus $^{294}118$.

value of a_{40}, at which the energy takes its minimum as a function of a_{40}. As usually in the macroscopic–microscopic calculations, the energy is normalized in such a way that its macroscopic part is put equal to zero at the spherical shape of a nucleus. It is seen that the minimum of the energy (ground state) is obtained at an oblate shape ($\gamma_2 = 60°$) and has the value -6.2 MeV. The saddle point is obtained at a non-axial shape of the nucleus with the energy -0.3 MeV. Thus, the fission-barrier height is 5.9 MeV. The parameters of the shape at the saddle point are: $\beta_2^{\rm sp} = 0.444$, $\gamma_2^{\rm sp} = 35.8°$, $a_{40}^{\rm sp} = 0.030$, $a_{42}^{\rm sp} = -0.015$, $a_{44}^{\rm sp} = 0.005$, $a_{60}^{\rm sp} = 0.024$, $a_{62}^{\rm sp} = 0.001$, $a_{64}^{\rm sp} = 0.002$, $a_{66}^{\rm sp} = -0.014$, $\beta_8^{\rm sp} = -0.005$. It is also seen that the quadrupole non-axiallity parameter γ_2 is large, close to the value $\gamma_2 = 30°$, corresponding to the largest non-axiality of the shape. The effect of γ_2 on the saddle-point energy $E^{\rm sp}$ (and the barrier height $B_{\rm f}^{\rm st}$) is about 0.6 MeV, in its absolute value (as can be directly seen in Fig. 3). The hexadecapole and $\lambda = 6$ non-axiallity parameters are small and one should not expect a large effect of them on $E^{\rm sp}$. Really, the effect of each of them is below 0.2 MeV, for this nucleus.

3.2. Role of non-axial shapes of multipolarity 6 of a nucleus in its saddle-point energy

The effect of non-axial shapes of multipolarity $\lambda = 6$ of nuclei on their saddle-point energy, $\delta E^{\mathrm{sp,n6}}$, is illustrated in Fig. 2. The effect is the difference between the energy at the saddle point when the multipolarity-six non-axial deformations are taken into account and when they are not. In the notation given at Fig. 3, it may be written as: $\delta E^{\mathrm{sp,n6}} = E^{\mathrm{sp,n2+n4+n6}} - E^{\mathrm{sp,n2+n4}}$. Fig. 2 gives a contour map of $\delta E^{\mathrm{sp,n6}}$, calculated for the whole investigated region of nuclei. One can see that the effect is rather small, less than 0.4 MeV. Moreover, for quite a large number of the studied nuclei, it is simply zero.

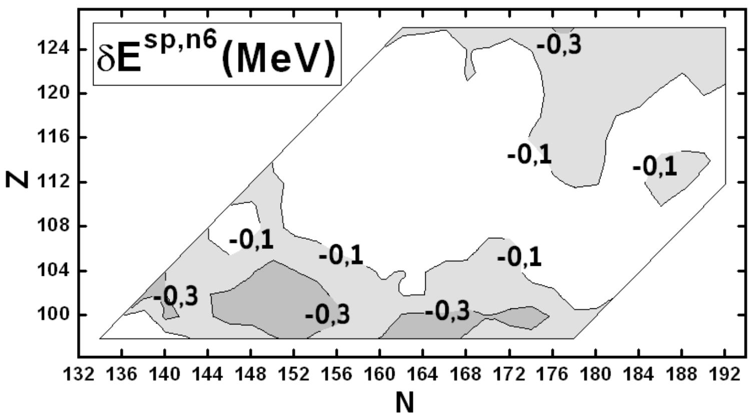

Fig. 2. Contour map of the effect, $\delta E^{\mathrm{sp,n6}}$, of non-axial shapes of multipolarity $\lambda = 6$ of nuclei on their saddle-point energy .

3.3. Comparison between the effects of non-axial shapes of various multipolarities λ on the saddle-point energy

It is interesting to see how the studied effect depends on the multipolarity λ of the deformations of nuclei at their saddle point. As may be expected, the largest effect comes from the quadrupole ($\lambda = 2$) non-axiallity. It is up to more than 2 MeV for the considered nuclei [27]. For the multipolarity $\lambda = 4$, the non-axial deformations lower the saddle-point energy of the nuclei by up to about 1.5 MeV [28]. As is seen in Fig. 2, non-axial shapes with $\lambda = 6$ decrease the saddle-point energy by up to about 0.4 MeV. Thus, the effect decreases rather fast with the increasing λ, indicating for its convergence to zero.

A detailed illustration of the effect as a function of λ is given in Fig. 3 for isotopes of the element 118. It is seen that this effect strongly depends on the neutron number N. For lighter isotopes (up to $N = 170$), there

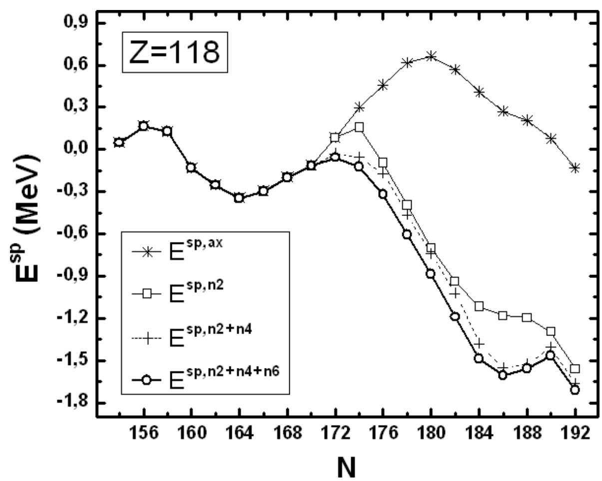

Fig. 3. The saddle-point energy $E^{\rm sp}$ of nuclei in the case of the axial symmetry, $E^{\rm sp,ax}$, after the inclusion of the $\lambda = 2$, $E^{\rm sp,n2}$, also λ=4, $E^{\rm sp,n2+n4}$, and additionally $\lambda = 6$, $E^{\rm sp,n2+n4+n6}$, non-axial shapes, plotted as functions of neutron number N, for the element 118.

is no (or almost no) effect of the non-axiallity for all three multipolarities. For $N > 170$, the effect strongly depends on λ. It is large (up to about 1.5 MeV, in its absolute value) for $\lambda = 2$, it is smaller (up to about 0.4 MeV) for $\lambda = 4$ and still smaller (up to about 0.15 MeV) for $\lambda = 6$, for the considered isotopes of the element 118. Thus, the decrease of the effect with the increasing λ is really quite fast.

3.4. Comparison with experiment and with other calculations

Fig. 4 gives a comparison of our results with experimental ones and also with other theoretical calculations. The experimental values [36] are extracted from measured cross-sections for fission induced in various reactions, with the use of the double-humped-barrier model (see also *e.g.*, Refs. [37,38]). Thus, the results are model dependent. For the comparison with other theoretical calculations, the results of recent studies [22, 25] are taken. The calculations are performed within a macroscopic–microscopic approach (similar as ours), but they still differ from our model by the parametrization of the shape of a nucleus (which is an important difference), single-particle potential, and some other details. The figure presents the results for six even–even nuclei of plutonium, for which the results are available. These are the heights of the inner barrier, which appear to be larger in the evaluations of Ref. [36] than those of the outer ones. One can see in Fig. 4 that the quality of theoretical description is rather much different for dif-

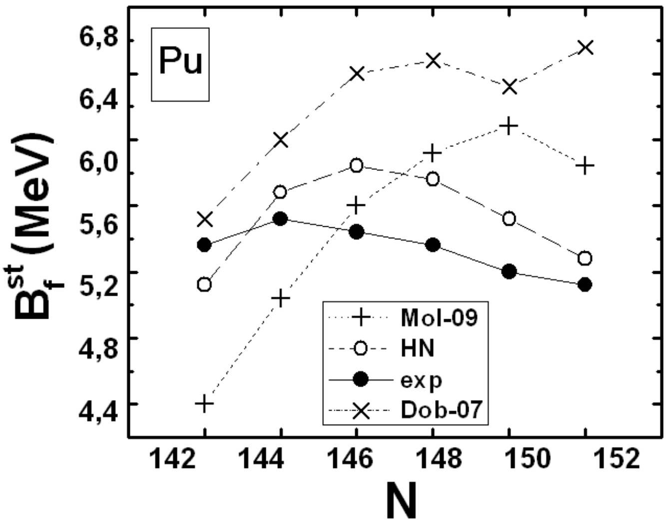

Fig. 4. A comparison of our results (HN) with experimental ones (exp) and also with other theoretical calculations: Dob-07 [22] and Mol-09 [25].

ferent models. The average of the absolute values of the discrepancy for these six Pu nuclei is: 0.35 MeV, 0.78 MeV and 1.10 MeV for the models HN (Heavy Nuclei, our model), Mol-09 [25] and Dob-07 [22], respectively. The same quantity calculated for 18 even–even nuclei of U, Pu, Cm and Cf, for which the experimental values [36] are available, is: 0.34 MeV, 0.97 MeV and 0.90 MeV (only 16 values for these 18 nuclei are available in this study) for the HN, Mol-09 and Dob-07 approaches, respectively. These discrepancies may be compared with the inaccuracy of the experimental values, which is estimated to be ± 0.2 MeV in most cases [37, 38].

It is interesting to see the discrepancy between the theoretical models for superheavy nuclei, far from the region where experimental results are available. The discrepancy is illustrated in Fig. 5 for isotopes of the heaviest element (118) observed up to the present. Two models are considered, as there are no results of Dob-07 [22] for superheavy nuclei. It is seen that the difference between the two models is quite large, up to about 3.5 MeV. This is really much, if one takes into account that a 1 MeV change in the barrier height results in the change of cross-section for the synthesis of a nucleus by about one to two orders of magnitude [6,11], as already mentioned in the Introduction. It would be desirable to recognize the source of this large difference and learn which of these two predictions is more realistic.

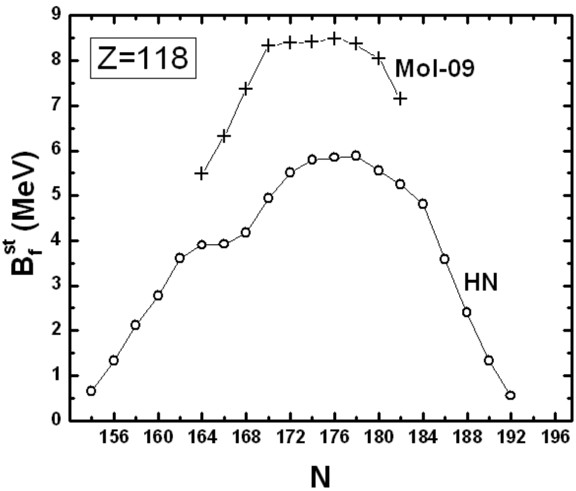

Fig. 5. The discrepancy between two theoretical models for superheavy nuclei, far from the region where experimental results are available.

4. Conclusions

The following conclusions may be drawn from this and our earlier studies:

(1) Non-axial shapes play an important role in the saddle-point energy of heaviest nuclei. The quadrupole ($\lambda = 2$) deformations decrease this energy by up to more than 2 MeV, the hexadecapole ($\lambda = 4$) ones lower it by up to about 1.5 MeV, and the deformations of multipolarity $\lambda = 6$ diminish it by up to about 0.4 MeV, for the considered nuclei.

(2) As the ground-state shapes of the considered nuclei are axially symmetric, the effect also concerns the (static) fission-barrier height $B_{\mathrm{f}}^{\mathrm{st}}$.

(3) The results indicate for the convergence of the effect to zero, with increasing multipolarity λ of the shapes.

(4) Two theoretical results for the barrier height $B_{\mathrm{f}}^{\mathrm{st}}$, which differ by less than 1 MeV in the experimental region ($Z = 92$–98, $N = 140$–154), disagree by up to about 3.5 MeV for superheavy nuclei ($Z = 118$, $N = 164$–182). It would be very interesting to see the reason for such a large increase of the deviation between them with the increase of Z and N, and learn which of them is more realistic.

Support by the Polish Ministry of Science and Higher Education, grant No. 1 P03B 042 30, by Helmholtzinstitute Mainz (HIM), and by the Polish–JINR (Dubna) Cooperation Programme, is gratefully acknowledged.

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