POTENTIAL ENERGY SURFACES OF THORIUM ISOTOPES IN THE 4D FOURIER PARAMETRISATION* **

B. Nerlo-Pomorska, K. Pomorski

Department of Theoretical Physics, Maria Curie Skłodowska University
Radziszewskiego 10, 20-031 Lublin, Poland

J. Bartel

Université de Strasbourg, CNRS IPHC UMR 7178, 67000 Strasbourg, France

C. Schmitt

GANIL, 14000 Caen, France

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The recently developed extremely flexible and rapidly converging Fourier shape parametrisation is used to evaluate the potential energy surfaces of ^{210}Th–^{238}Th even–even isotopes within the macroscopic–microscopic method. A vast sample of 4D landscapes is analysed, searching for absolute and local extrema, ridges and valleys. The expected fission-fragment mass distribution obtained from different Th isotopes at low excitation energy is illustrated by a static analysis of the potential energy landscape. Quadrupole moments in the relevant minima are also evaluated.

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1. Introduction

Potential energy surfaces (PES) describe the energy of nuclei as a function of deformation. They are the necessary starting point for modelling many nuclear properties and reactions, including ground and metastable isomeric states as well as large-scale collective motion such as fission. It has been demonstrated [1] that the quality of the landscape, and thus its predictive power, relies on two essential ingredients, namely the definition of the

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nuclear shape and the number of involved coordinates, and the prescription used to calculate the potential energy. We present here calculations for the isotopic chain of even–even thorium nuclei performed with the macroscopic–microscopic model using the newly developed Fourier parametrisation of nuclear shape [2]. In order to describe the very large variety of shapes a nucleus may undergo, we exploit the recently developed nuclear-shape parametrisation based on a Fourier expansion [2] of the profile function $\rho_{\rm s}^2(z)$ in cylindrical coordinates

$$\frac{\rho_{\rm s}^2(z)}{R_0^2} = \sum_{n=1}^{\infty}\left[a_{2n}\cos\left(\frac{(2n-1)\pi}{2}\,\frac{z-z_{\rm sh}}{z_0}\right) + a_{2n+1}\sin\left(\frac{2n\pi}{2}\,\frac{z-z_{\rm sh}}{z_0}\right)\right] \tag{1.1}$$

that has to vanish at the endpoints of the shape: $\rho_{\rm s}(z_{\rm sh}-z_0)=\rho(z_{\rm sh}+z_0)=0$, a condition which is automatically satisfied by Eq. (1.1). The shift coordinate $z_{\rm sh}$ insures the centre of the nuclear shape to be located at the origin of the coordinate system. The parameters a_2, a_3, a_4 describe elongation, left–right asymmetry, and neck degree of freedom. This parametrisation has shown to be particularly efficient in the context of large-scale collective motion phenomena. Even though the above expansion can be carried to an arbitrary number of dimensions, it turns out that relying on only four deformation parameters (three Fourier plus one non-axiality parameter η to take care of non-axial shapes [2]) allows to cover the whole nuclear chart and to investigate trends as a function of proton (Z) and neutron (N) numbers.

Since the path to fission goes towards smaller a_2 and larger a_4, more physically-intuitive collective coordinates are introduced by:

$$q_2 = \frac{a_2^{(0)}}{a_2} - \frac{a_2}{a_2^{(0)}}\,, \qquad q_3 = a_3\,, \qquad q_4 = a_4 + \sqrt{(q_2/9)^2 + \left(a_4^{(0)}\right)^2}\,, \tag{1.2}$$

where $a_n^{(0)}$ is the value of the coordinate a_n for the spherical shape [2].

2. Results

Our calculation of the nuclear deformation energy is based on the Lublin–Strasbourg Drop (LSD) formula [3] for the macroscopic part, the Strutinsky method [4] and the BCS theory [5] with single-particle levels computed from a Yukawa-folded potential [6], for the microscopic shell corrections and pairing correlations, respectively. A detailed description of the formalism has been presented in Ref. [7], and is thus not repeated here.

The topography of the 4D landscape (with deformation parameters corresponding to elongation, left–right asymmetry, neck formation and non-axiality) has been analysed for 15 even–even thorium ($Z = 90$) isotopes. Six of them are shown in Fig 1. Depending on the specific phenomenon under study, a minimization with respect to one or the other coordinate was carried out. In that process, extrema, ridges and valleys are identified. The presence or absence and the relative depth of various fission valleys are found to be consistent with experimental fission fragment mass or charge distributions. To make more quantitative predictions would require, of course, to go beyond the static picture employed here, and to include dynamical effects. Work in this direction is on our agenda.

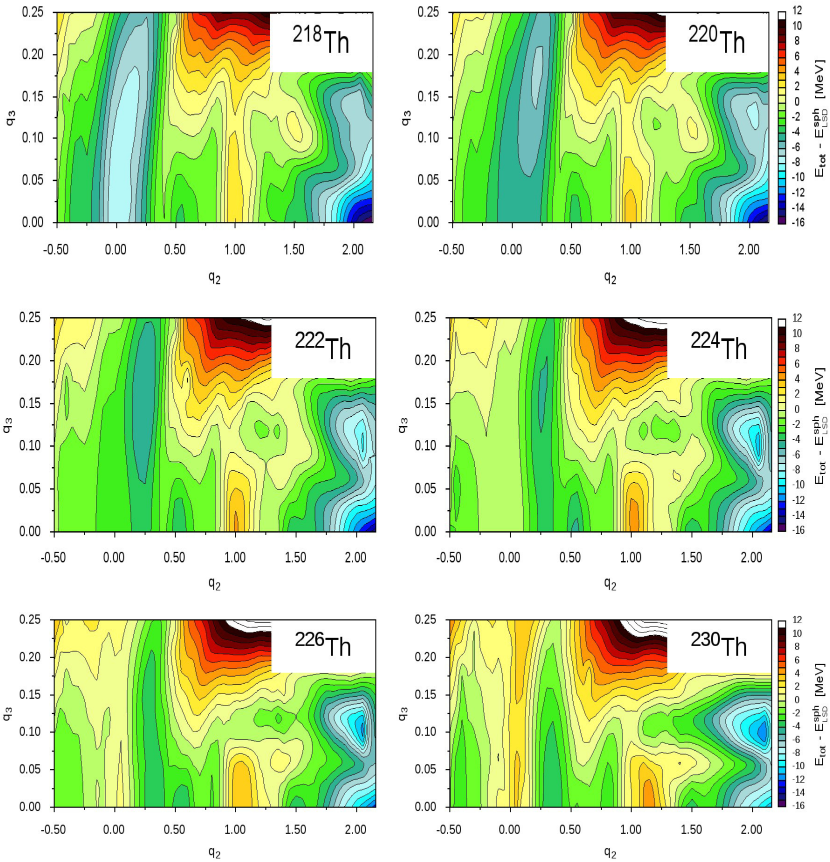

Fig. 1. Potential energy (relative to the spherical LSD energy) landscapes on the (q_2, q_3) plane for 6 even–even isotopes between ^{218}Th–^{230}Th minimised with respect to hexadecapole q_4 and non-axial deformation parameter η.

The calculated fission barriers in the investigated region are quite massive. We have observed, in addition, that the inclusion of shell effects produces local minima which correspond to super-deformed (sd) shapes.

The ground state (gs) of the lightest Th isotopes up to $A = 218$ is found to be spherical. Heavier isotopes are deformed. The evolution of the landscape is interesting to follow: the sd, hd and even ultra-deformed minima appear and disappear as a function of the Th mass. While the landscape is pretty soft for the lightest isotopes, rather pronounced deformed octupole ground states are observed, in particular for ^{220}Th–^{224}Th. There are many other deformed minima. The most deformed superdeformed (sd) isomeric states are certainly worth to be discussed in the context of the debated existence of a third very elongated minimum in the actinide region [8].

The quadrupole moments associated with most pronounced energy minima were evaluated. The corresponding calculated electric quadrupole moments are presented in Fig. 2 for the Th isotopic chain. They agree with the available data for the ground state (gs). Experimental efforts to look for exotic shapes (sd) in this region are strongly encouraged.

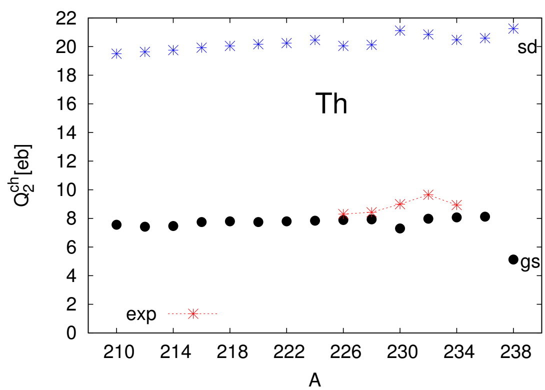

Fig. 2. Electric quadrupole moments $Q_2^{\rm ch}$ for the ground state (gs) and superdeformed (sd) isomeric minima along the Th isotopic chain. Experimental data for the ground state are shown [9].

The above results should be understood as a pilot investigation, aimed at demonstrating the potential and power of the approach. More detailed quantitative studies are in progress.

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