Potential Energy Surfaces of Actinide Nuclei from a Multidimensional Constrained Covariant Density Functional Theory: Barrier Heights and Saddle Point Shapes (Postprint)

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Abstract

For the first time the potential energy surfaces of actinide nuclei in the (20, 22, 30) deformation space are obtained from a multi-dimensional constrained covariant density functional theory. With this newly developed theory we are able to explore the importance of the triaxial and octupole shapes simultaneously along the whole fission path. It is found that besides the octupole deformation, the triaxiality also plays an important role upon the second fission barriers. The outer barrier as well as the inner barrier are lowered by the triaxial deformation compared with axially symmetric results. This lowering effect for the reflection asymmetric outer barrier is 0.5 1 MeV, accounting for 10 20% of the barrier height. With the inclusion of the triaxial deformation, a good agreement with the data for the outer barriers of actinide nuclei is achieved.

Full Text

Preamble

Potential Energy Surfaces of Actinide Nuclei from a Multidimensional Constraint Covariant Density Functional Theory: Barrier Heights and Saddle Point Shapes

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For the first time, potential energy surfaces of actinide nuclei in the (, ,) deformation space have been obtained from a multi-dimensional constrained covariant density functional theory. This newly developed theory enables us to explore simultaneously the importance of triaxial and octupole shapes along the entire fission path. We find that, besides octupole deformation, triaxiality also plays an important role in determining the second fission barriers. Both the outer and inner barriers are lowered by triaxial deformation compared with axially symmetric results. This lowering effect for the reflection-asymmetric outer barrier amounts to 0.5–1 MeV, accounting for 10–20% of the barrier height. With the inclusion of triaxial deformation, good agreement with experimental data for the outer barriers of actinide nuclei is achieved.

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Since the first interpretation of nuclear fission as a barrier penetration phenomenon [1], theoretical description of this process has remained a challenging task. For instance, studying fission requires extremely accurate information about fission barriers; a difference of just 1 MeV in the barrier height can lead to several orders of magnitude difference in the fission half-life. This is particularly crucial for exploring the island of stability of superheavy nuclei (SHN) [2–4], where accurate predictions of fission barriers are increasingly essential [5–8].

Currently, three types of models are employed for calculating fission barriers. For a long period, the majority of work has been based on macroscopic-microscopic (MM) models [5, 9–11]. These models utilize the Strutinsky shell correction method, enabling rapid calculations of multi-dimensional potential energy surfaces (PES) that incorporate most important shape degrees of freedom. Even today, MM models remain an important candidate for large-scale fission barrier calculations based on multi-dimensional PES analysis [10]. In recent years, the rapid development of density functional theories (DFT) has made fully self-consistent fission barrier calculations possible [12–15]. There are two main reasons for applying DFT to fission studies. First, many new functional forms and effective interactions have been proposed with significantly improved performance for both excited-state and ground-state calculations [16–20], and fission barrier calculations help in developing these DFTs. Second, DFT can include many more shape degrees of freedom self-consistently; for example, the symmetry-unrestricted Skyrme-Hartree-Fock-Bogoliubov model has been applied to fission studies [21]. Besides these two approaches, methods also exist that aim to combine the advantages of MM and self-consistent models, such as the extended Thomas-Fermi method [22].

The double-humped fission barriers of actinide nuclei serve as a benchmark for the predictive power of theoretical models [13, 23–25]. Various shape degrees of freedom play important and distinct roles in the formation and height determination of inner and outer barriers. For example, MM model calculations have long shown that the inner fission barrier is typically lowered when triaxial deformation is allowed, while reflection-asymmetric (RA) shapes are favored for the outer barrier [26, 27]. These points were later confirmed in non-relativistic [24] and relativistic [15, 28] density functional calculations, respectively. Consequently, it has become customary to consider only triaxial and reflection-symmetric (RS) shapes for the inner barrier, and axially symmetric and RA shapes for the outer one [5, 29, 30]. However, as pointed out in Ref. [31], "there is no reason for a fissioning actinide nucleus not to penetrate all symmetry-breaking shapes on its way from the first (triaxial) to the second (mass-asymmetric) saddle." Non-axial octupole deformations have been considered in both MM models [32] and non-relativistic Hartree-Fock theories [33], yet a multi-dimensional PES structure including both triaxial and RA shape degrees of freedom has not been explored within the covariant DFT framework. In this paper, we investigate the influence of triaxiality and octupole shape on PESs from the ground state to the fission configuration when both shape degrees of freedom are included simultaneously. This requires breaking not only as many self-consistent symmetries as possible but also implementing multi-dimensional constraints [34].

To calculate potential energy surfaces and fission barriers, we employ covariant density functional theory (CDFT) [17, 19, 20, 35, 36]. By breaking both axial [37, 38] and reflection symmetries [39], we have developed multi-dimensional constrained CDFTs where the functional can take one of four forms: meson-exchange or point-coupling nucleon interactions combined with either non-linear or density-dependent couplings [40]. Unless specified otherwise, this work uses the point-coupling nucleon interaction with non-linear self-energy terms and the PC-PK1 parameter set [41].

For nuclear shape parametrization, we adopt the conventional ansatz used in mean-field calculations: = (3/4 AR) Q , where Q are mass multipole operators. When both axial and reflection symmetries are broken, the nuclear shape remains invariant under reversal of the x and y axes; that is, the intrinsic symmetry group is V , and all shape degrees of freedom with even—including triaxial (0) and octupole (= 3) deformations—are possible. Regardless of the self-consistent symmetries, single-particle wave functions and various densities are expanded in an axially deformed harmonic oscillator basis [38, 42].

To achieve rapid convergence with respect to basis size, more states are included in the elongated direction. Following Warda et al. [43], the basis is truncated according to: n_z/Q_z + (2n_ + |m|)/Q_ N_cut, where n_z, n_ , and m are quantum numbers characterizing each basis state, Q_z = MAX(1, b_z/b), Q_ = MAX(1, b_ /b), and b , b_z, and b_ are oscillator lengths. The calculated binding energy of ^{2} Pu at = 1.3 varies by only about 130 keV and 20 keV when N_cut increases from 16 to 18 and from 18 to 20, respectively, indicating good convergence. This truncation scheme with N_cut = 16 ensures 0.2 MeV accuracy for the deformation range of interest. In the present work, N_cut = 16 (20) is used in triaxial (axial) calculations; more convergence details will be provided in Ref. [40]. The BCS approach is implemented to account for pairing effects. Since BCS calculations with constant pairing gaps cannot adequately describe fission barriers [14], we use a delta force for the pairing interaction with a smooth cutoff [41, 44].

We performed one-dimensional (1-d), two-dimensional (2-d), and three-dimensional (3-d) constrained calculations for the actinide nucleus ^{2} Pu. Figure 1 [Figure 1: see original paper] shows 1-d potential energy curves (PEC) from an oblate shape with -0.2 to fission configurations with beyond 2.0, obtained from calculations imposing different self-consistent symmetries: axial (AS) or triaxial (TS) symmetries combined with reflection-symmetric (RS) or asymmetric cases. The importance of triaxial deformation for the inner barrier and octupole deformation for the outer barrier—emphasized in earlier studies [15, 24, 28]—is clearly evident: triaxial deformation reduces the inner barrier height by more than 2 MeV, yielding better agreement with the empirical value, while RA shapes are favored beyond the fission isomer and substantially lower the outer fission barrier. Additionally, we observe for the first time that the outer barrier is also considerably lowered by about 1 MeV when triaxial deformation is allowed, again improving reproduction of the empirical barrier height. This feature only appears when both axial and reflection symmetries are simultaneously broken.

The instability of the ^{2} Pu PES against triaxial distortion becomes much clearer in Figure 2 [Figure 2: see original paper], which shows 2-d PESs from calculations with and without triaxial deformation. When triaxial deformation is permitted, the binding energy of ^{2} Pu assumes its lowest possible value at each (,) point, yielding non-zero values at some points. This indicates that non-axial solutions are favored over axial ones at these configurations. Triaxial deformation appears primarily in two regions. One region starts from the first saddle point and extends roughly along the axis up to very asymmetric shapes with 1.0. In this region, values are about 0.06–0.12, corresponding to 10°, lowering the energy—especially the inner barrier height—by about 2 MeV. The other region is around the outer barrier, where values are about 0.02–0.03 (2°), gaining about 1 MeV in binding energy at the second saddle point due to triaxiality. In other regions, such as the ground state and fission isomer valleys, only axially symmetric solutions are obtained.

Next, we examine the full 3-d PES of ^{2} Pu obtained from the newly developed multi-dimensional constrained CDFT. For simplicity, Figure 3 [Figure 3: see original paper] shows five typical sections of the 3-d PES in the (,) plane calculated at = 0.3 (ground state region), 0.6 (first saddle point), 0.9 (fission isomer), 1.3 (second saddle point), and 1.6 (beyond outer barrier). Several conclusions can be drawn from these 3-d PESs. First, both the ground state and fission isomer are axially and reflection symmetric, as shown in the 1-d PEC and 2-d PES, but the 3-d PES allows investigation of stability against and deformations. The fission isomer exhibits much greater stiffness than the ground state against both and deformations. Second, while the shape around the inner barrier is triaxial and reflection symmetric, the second saddle point near = 1.3 displays both triaxial and reflection-asymmetric character. Third, triaxial distortion appears only at the tops of fission barriers.

It has been noted that spurious saddle points may arise if only a small number of shape degrees of freedom are constrained [5]. The calculated fission path might jump between valleys, causing discontinuities in lower-dimensional PESs, and in some cases a continuous path may even cross a higher saddle point. While spurious saddle points cannot be completely eliminated, most can be avoided if (1) the obtained fission path remains continuous in both energy and the most important shape degrees of freedom, and (2) results are examined using higher-dimensional calculations. We have carefully checked the full 3-d PES and found that the fission path enters and exits triaxial configurations rather smoothly, with no sudden jumps, suggesting that 1-d (with constrained and , free) and 2-d (with , constrained and free) calculations of fission barriers are well justified for ^{2} Pu. However, continuity in lower-dimensional constraint calculations is a necessary but not sufficient condition for locating the correct saddle point; a definitive conclusion certainly requires multi-dimensional constraint calculations including even higher-multipolarity deformations.

For RS calculations, triaxiality also lowers the fission path by a few MeV beyond the second saddle point, as illustrated by the dotted line in Figure 1 and the local minima with = 0.0 in the = 1.6 sub-figures of Figure 3. However, this effect is relatively unimportant because RA fission remains the most favored path even with triaxiality included.

Guided by features observed in the 1-d, 2-d, and 3-d PESs of ^{2} Pu, we extracted fission barrier heights for even-even actinide nuclei with empirical values recommended in RIPL-3 (see Table XI in [45]), focusing on the influence of triaxial deformation on both fission barriers.

As shown previously, an actinide nucleus assumes triaxial and reflection-symmetric shapes around the inner barrier. Thus, to obtain the inner fission barrier height B_f^i, we can safely perform a one-dimensional constraint calculation with triaxial deformation allowed and reflection symmetry imposed. Figure 4(a) [Figure 4: see original paper] presents the calculated inner barrier heights B_f^i compared with empirical values. Triaxiality lowers the inner barrier heights of these actinide nuclei by 1–4 MeV, as demonstrated in Ref. [15]. Overall, our calculations agree very well with empirical values, except for two thorium isotopes and ^{23} U. For ^{23} Th and ^{232}Th, the calculated inner barrier heights are smaller than empirical values by about 1–2 MeV, depending on whether triaxial deformation is included. In these nuclei, the outer barrier is higher than the inner one, which may introduce uncertainties in empirically determining the inner barrier height that is not the primary barrier [12]. Similar results for ^{23} Th and ^{232}Th were obtained from the Skyrme-Hartree-Fock-Bogoliubov model [12], and a very small inner barrier height was found for ^{232}Th in Ref. [15]. For ^{23} U, the axial calculation yields excellent agreement with the empirical value, but triaxiality reduces the barrier height by about 1.5 MeV, creating a discrepancy similar to that in Ref. [15].

Obtaining the outer fission barrier height B_fˆo is more complicated because additional shape degrees of freedom significantly influence the region around the outer fission barrier. For example, including reflection-asymmetric shapes makes possible two or more competing fission paths in the (,) plane. This occurs in ^{2} ,^{2} Pu and ^{2} ,^{2} ,^{2} Cm in the present study, with a typical example shown in Figure 5 [Figure 5: see original paper] for ^{2} Cm. Both the 1-d E curve and the 2-d E (,) PES exhibit two fission paths: path "I" favors shapes with larger octupole deformations, while path "II" favors less RA shapes. In such nuclei, performing a 1-d constraint calculation to obtain B_fˆo is unreliable. Therefore, we first assume axial symmetry and perform a 2-d calculation in the (,) plane to approximately identify the lowest fission path _lowest( ) and the location of the second saddle point. Then, along this fission path, we perform a 1-d -constraint calculation allowing both triaxial and octupole deformations. At each point, initial deformations are taken as ˆini = 0 and ˆini = _lowest( ). In this 1-d PEC, we can locate the second saddle point and extract the outer barrier height for each nucleus.

The lower panel of Figure 4 [Figure 4: see original paper] shows the outer barrier heights B_fˆo compared with empirical values. For most nuclei investigated, triaxiality lowers the outer barrier by 0.5–1 MeV, accounting for about 10–20% of the barrier height. Our calculations with triaxiality agree well with empirical values, with the only exception being ^{2} Cm. For this nucleus, even the axial calculation yields an outer barrier height smaller than the empirical value. This discrepancy may relate to the existence of two possible fission paths beyond the first barrier, as seen in Figure 5. For path I, which has a lower saddle point from which we extract the outer fission barrier height, the barrier is very wide, while for path II with a higher saddle point, the barrier is relatively narrow. Therefore, the empirical outer fission barrier height may be difficult to extract for two reasons: (i) strong competition must exist between the two fission paths, and (ii) empirical evaluation of outer barrier height typically assumes an anti-parabolic shape with a fixed, smaller width for the second barrier [45].

We also examined the parameter dependence of our results. The lowering effect of triaxiality on the outer fission barrier is observed when using parameter sets other than PC-PK1.

In summary, we have developed a multi-dimensional constrained covariant density functional theory that allows simultaneous study of triaxial and octupole shape importance along the entire fission path. The one-dimensional PEC E , two-dimensional PES E (,), and three-dimensional PES E (, ,) of actinide nuclei are presented and studied in detail. Both triaxiality and reflection asymmetry play crucial roles at and around the second saddle point. The outer barrier, as well as the inner barrier, is lowered by triaxial deformation compared with axially symmetric results. For most nuclei investigated, triaxiality lowers the outer barrier by 0.5–1 MeV, accounting for about 10–20% of the barrier height. The calculated outer barrier heights agree well with empirical values.

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