Fission barriers and asymmetric ground states in the relativistic
mean field theory

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Abstract

The symmetric and asymmetric fission path for $^{240}$Pu, $^{232}$Th, and $^{226}$Ra is investigated within the relativistic mean-field model. Standard parametrizations which are well fitted to nuclear ground state properties are found to deliver reasonable qualitative and quantitative features of fission, comparable to similar nonrelativistic calculations. Furthermore, stable octupole deformations in the ground states of Radium isotopes are investigated. They are found in a series of isotopes, qualitatively in agreement with nonrelativistic models. But the quantitative details differ amongst the models and between the various relativistic parametrizations.

I. INTRODUCTION

Nuclear fission has been the challenge to develop microscopic theories of nuclear collective motion. Only a subtle interplay of collective deformations and changing microscopic
shell structure can explain the quantitative details like tunneling times and fragment mass distributions [1]. One of the most decisive features to pin down the contributions from the shell effects is the occurrence of multiple–humped barriers [2]. The macroscopic–microscopic method, based on a phenomenologically fitted shell model plus Strutinsky shell corrections [3], allowed quite early extensive investigations of the various landscapes of collective Potential Energy Surfaces (PES), see e. g. [1,4–7]. Since the early seventies, fully selfconsistent mean–field models have been available for nuclei. These are the nonrelativistic Hartree–Fock models with the Skyrme force [8,9] or the Gogny force [10]. At about the same time competitive relativistic mean–field models for nuclear structure were proposed [11,12]. Although much more elaborate, selfconsistent mean–field calculations of the PES for nuclear fission appeared rather soon for the Skyrme–Hartree–Fock models [13] and later for the Gogny force [14], it was only recently that PES for fission have been calculated with the relativistic mean–field model [15]. These calculations have shown that well adjusted parametrizations for the relativistic mean–field model, see e. g. [16,17], deliver reasonable fission barriers comparable to those of nonrelativistic calculations. A variation of the parametrization, in particular with respect to the effective mass, has shown that the requirement to reproduce reasonable fission barriers excludes many variants and only the standard best–fit forces with the typically very low effective nucleon mass remain. It is the aim of this paper to extend the investigations of [15] to asymmetric fission and to study a larger variety of actinides. We confine the considerations to the two parametrizations NL1 from [16] and PL–40 from [18] which have proven to provide reasonable fission barriers [15]. In addition, we consider the parametrization NL–SH which is claimed to be better adjusted with respect to isovector properties [19]. As a second objective of this paper, we exploit the asymmetric degree of freedom in our calculations to investigate the possibility of stable octupole deformations in the ground states of Radium isotopes which, again, have been investigated first in the macroscopic–microscopic method [4,7].

The paper is outlined as follows: In section [II] we give a short account of the model, its parameters and further ingredients. In section [III] we present results for the PES for
symmetric and asymmetric fission of $^{240}$Pu, $^{232}$Th, and $^{226}$Ra. And in section IV, we discuss the stable octupole deformations in the ground states of Radium isotopes.

**II. THEORETICAL BACKGROUND**

The relativistic mean-field model is meanwhile a standard in nuclear physics, for detailed reviews see [20,21,17]. Thus there is not much to explain. But for completeness we specify here the Lagrangian of the model. It reads

$$\mathcal{L}_{\text{RMF}} = \mathcal{L}_{\text{free nucleon}} + \mathcal{L}_{\text{free meson}} + \mathcal{L}_{\text{lin coupl}} + \mathcal{L}_{\text{nonlin coupl}}$$

$$\mathcal{L}_{\text{free nucleon}} = \overline{\Psi} (i\gamma_\mu \partial^\mu - m_n) \Psi$$

$$\mathcal{L}_{\text{free meson}} = \frac{1}{2} \left( \partial_\mu \Phi \partial^\mu \Phi - m^2_\sigma \Phi^2 \right) - \frac{1}{2} \left( \frac{1}{2} G_{\mu\nu} G^{\mu\nu} - m_\omega^2 V_\mu V^\mu \right)$$

$$- \frac{1}{2} \left( \frac{1}{2} \tilde{B}_{\mu\nu} \cdot \tilde{B}^{\mu\nu} - m^2_\mu \tilde{R}_\mu \cdot \tilde{R}^{\mu} \right) - \frac{1}{4} F_{\mu\nu} F^{\mu\nu}$$

$$\mathcal{L}_{\text{lin coupl}} = - g_\sigma \overline{\Psi} \Phi \Psi - g_\omega V_\mu \overline{\Psi} \gamma^\mu \Psi - g_\rho \overline{\tilde{R}}_\mu \overline{\tilde{R}}^\rho \gamma^{\mu} \Psi$$

$$- e A_\mu \overline{\Psi} \frac{1 + m_\gamma}{2} \gamma^{\mu} \Psi$$

$$\mathcal{L}_{\text{nonlin coupl}} = \frac{1}{2} m^2_\sigma \Phi^2 - U(\Phi)$$

where $\Psi$ is the nucleon field, $\Phi$ the scalar-isoscalar field, $V_\mu$ the vector-isoscalar field, $\tilde{R}_\mu$ the vector-isovector field, and $A_\mu$ the photon field. The corresponding force tensors are

$$G_{\mu\nu} = \partial_\mu V_\nu - \partial_\nu V_\mu , \quad \tilde{B}_{\mu\nu} = \partial_\mu \tilde{R}_\nu - \partial_\nu \tilde{R}_\mu , \quad F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu .$$

The $U(\Phi)$ is the nonlinear functional for the scalar field. We consider two variants, first the standard nonlinear functional

$$U(\Phi) = \frac{1}{2} m^2_\sigma \Phi^2 + \frac{1}{3} b_2 \Phi^3 + \frac{1}{4} b_3 \Phi^4 ,$$

and second, the stabilized nonlinear functional [18]

$$U(\Phi) = \frac{1}{2} m^2_\sigma \Phi^2$$

$$+ \Delta m \left\{ \frac{\delta \Phi^2}{2} \left[ \log \left( 1 + \left( \frac{\Phi - \Phi_0}{\delta \Phi} \right)^2 \right) \right] - \log \left( 1 + \left( \frac{\Phi_0}{\delta \Phi} \right)^2 \right) \right\}$$

$$+ \Phi_0 \Phi \left( 1 + \left( \frac{\Phi_0}{\delta \Phi} \right)^2 \right)^{-1} .$$
The stabilized functional is necessary whenever the shell fluctuations are likely to produce large peaks in the the scalar density. This happens in light nuclei [18] and at large deformations [22]. There is a large variety of parametrizations around in the literature, see [17]. We will discuss here three different sets: NL1 and NL–SH within the standard nonlinear model (1) and PL–40 within the stabilized variant (2). The parameters are listed in Table I and II. The sets NL1 and PL–40 are obtained from a fit to ground state properties of spherical nuclei, as explained in [16] for NL1 and [18] for PL–40. These fits take care of the nuclear charge form factor in terms of the diffraction radius and a surface thickness. The set NL–SH has been obtained also from a fit, but biased more on a smaller isovector parameter and employing only the r.m.s. radii as global information in the nuclear shape. It is claimed that this set is more appropriate for exotic nuclei due its smaller, and thus more realistic, isovector strength [19]. It is to be remarked, however, that the fit of NL–SH includes less information on the nuclear shape because only the overall extension in terms of the r.m.s. radius was employed whereas NL1 and PL–40 carry some extra information on the surface thickness and thus have probably more reliable surface properties. The parameters of the model, as given in Table I and II, serve to specify the used models in detail. More insight into the physical properties of the model is provided by listing the parameters of symmetric nuclear matter. This is done in Table III where we also provide the results for the comparable nonrelativistic models and the experimental data. The most reliable data are the binding energy and equilibrium density, which are well reproduced by all sets. The incompressibility is less well known and accordingly there is somewhat more variation amongst the forces. Where the effective mass is concerned, it is to be noted that the definitions differ. The relativistic models have a much lower \(m^*/m\) throughout. But the relevant quantity for nuclear structure calculations are the single particle level densities at the Fermi surface, and these turn out to be comparable amongst nonrelativistic and relativistic sets [23]. The differences in the symmetry energy cannot be explained away. The relativistic models have a tendency to overestimate it. The force NL–SH has a more realistic value because particular attention was paid to this observable during the fit. It is to be noted that the symmetry
energy determines mainly the position of the isovector giant resonances. It is yet an open question how it affects the isotopic trends in the nuclear ground states.

All three parametrizations are designed to determine an appropriate nuclear mean–field. They need to be completed by a recipe to define the occupation of states. We have used pairing in the constant gap approach with \[ \Delta = 11.2 \text{ MeV}/\sqrt{A}. \]

This is, admittedly, a rather rough estimate. Varying pairing recipes can change the fission barriers by about \( \pm 1 \text{ MeV} \) \[25\]. There are uncertainties in a similar order of magnitude in other parts of the treatment, see below. We can thus live with that level of approach for pairing in the present stage.

Finally, we take into account a correction for the spurious centre–of–mass motion. The standard nonlinear sets NL1 and NL–SH used the estimate

\[ E_{\text{cm}} = \frac{3}{4} \cdot 41 A^{-1/3} \text{ MeV} \quad (3) \]

whereas PL–40 used a microscopically calculated \[ E_{\text{cm}} = \langle \hat{P}_{\text{cm}}^2 \rangle/(2Am_n) \]. The microscopic evaluation is a bit tedious in non–spherical codes. The estimate \[3\] is a fair replacement, particularly in heavy nuclei as studied here. Admittedly, the centre–of–mass correction alone is somewhat incomplete. It suffices only for spherical nuclei. Deformed nuclei would require a rotational projection as well, and collective dynamics like fission, is only complete if also the (collective) vibrational zero–point energies are carefully accounted for. This is a very demanding task. In particular, it requires access to the appropriate collective cranking masses which are not yet available. And a proper implementaion of cranking in the relativistic framework will be a much more demanding task than in nonrelativstic mean–field models because the full Fermi sea of occupied antinucleon states needs to be kept projected out. This inhibits, \( e. \ g. \), the efficient linear response techniques on the grid \[26,27\]. We therefore dismiss these details for the moment. An estimate for all the effects from collective zero–point energies can be taken from the two–centre shell model \[28\]: the
first barrier is lowered by 0.5 MeV and the second barrier by 2 MeV. This is thus the uncertainty in our present calculations. It is about the same order of magnitude as the uncertainty from other parts of the model, e. g. the simple pairing recipe. In that sense, the present level of approach is well equilibrated with respect to precision. However, when comparing with other models, we will have to examine which zero–point energies had been included there and counter–correct properly.

Besides the energy, we will consider several multipole moments

\[ \hat{Q}_\ell = \sum_i r_i^\ell Y_\ell^0(\Omega_i) \]

as observables characterizing the shapes of the nuclei and the electrical dipole moment

\[ \hat{D} = e \frac{NZ}{A} \left( \frac{1}{2} \sum_{i \in \text{prot.}} z_i - \frac{1}{N} \sum_{i \in \text{neut.}} z_i \right). \]

For historical reasons we also display the cartesian quadrupole moment

\[ \hat{Q} = \sqrt{\frac{16\pi}{5}} \hat{Q}_2. \]

There are, in principle, two different sets of multipole moments to be considered in a relativistic model, one computed with the scalar density and another one computed with the vector density (the electrical dipole, of course, is uniquely related to the vector–isovector density). The differences are very small in the present relativistic mean–field model \[29\]. Thus any choice is possible. We are using here the multipole moments from the isoscalar–vector density. Another observable deduced from the isoscalar–vector density is the mass of the heavy fragment

\[ A_h = \int_{z < z_{\text{neck}}} \mathrm{d}V \rho_0(\vec{r}) \quad \text{for} \quad \langle \hat{Q}_3 \rangle > 0. \]

It can be computed only for large deformations when the fragments start to develop visibly.

The multipole moments serve also as constraints in order to map the whole potential energy surfaces for deformation and fission. They are related to the vector density and thus can be added as a potential–like term in the effective Hamiltonian of the model, i. e.

\[ \hat{H}^C = \hat{H} - \sum_{\ell=1,3} \lambda_\ell \hat{Q}_\ell^D, \]
were $\ell = 2, 3$ serves to implement a constraint on $\langle Q_2 \rangle$ and $\langle Q_3 \rangle$, and $\ell = 1$ is included to fix the centre–of–mass at $\langle z_{\text{cm}} \rangle = 0$. The upper index "D" denotes damped multipole moments. Some damping is required because the mere multipole moments increase rapidly towards the edges of the numerical box which causes several unpleasant numerical instabilities. For example, every nucleus becomes asymptotically unstable with the slightest quadrupole constraint because there arises always one direction where the potential decreases as $-r^2$ with $r \to \infty$. The problem becomes worse with the octupole constraint. The multipole operators thus have to be cut off at large distances from the nucleus. We do this by multiplying them by a Fermi function

$$\hat{C}^D_\ell = \hat{C}_\ell \left[ 1 + \exp \frac{\Delta R - \alpha}{\gamma} \right]^{-1}.$$  

The choice of an appropriate distance $\Delta R$ has to be done with care if many multipoles are involved. We define $\Delta R$ as the distance to an equidensity surface $\rho_0(\vec{r}) = \rho_{\text{sw}}$ of the isovector density $\rho_0$ at some threshold value $\rho_{\text{sw}}$. In practice, we evaluate $\Delta R$ on the grid as

$$\Delta R(\vec{r}_j) = \min \left\{ |\vec{r}_j - \vec{r}_i'| \bigg| \rho_0(\vec{r}_i') \geq \rho_{\text{sw}} \right\} \quad \text{for} \quad \rho_0(\vec{r}_j) \leq \rho_{\text{sw}}$$

$$\Delta R(\vec{r}_j) = - \min \left\{ |\vec{r}_j - \vec{r}_i'| \bigg| \rho_0(\vec{r}_i') < \rho_{\text{sw}} \right\} \quad \text{for} \quad \rho_0(\vec{r}_j) > \rho_{\text{sw}}$$

(5)

where

$$\rho_{\text{sw}} = \frac{\rho_0^{\text{max}}}{10}$$

The factor 1/10 in the definition of $\rho_{\text{sw}}$ has been set by experience. The parameter $\alpha$ is an effective cut–off distance and $\gamma$ is the width of the transitional region; we use here $\alpha = 3 \text{ fm}$ and $\gamma = 0.4 \text{ fm}$.

Finally, we want to make a few remarks on the numerical procedures used: We restrict the calculations to axial symmetry. The wavefunctions are represented on a grid in cylindrical coordinates $r = \sqrt{x^2 + z^2}$ and $z$. The derivatives are handled as matrices on the $r$–grid, or $z$–grid respectively. The matrices are built from a Fourier–definition of the derivatives [30]. We impose no restriction concerning reflection symmetry about the $z = 0$ plane. That is the
new feature of the present calculations compared to earlier work \cite{22,30,31}. We are using a grid spacing of 0.7 fm in each direction and are dealing typically with grid sizes of $25 \times 75$. The solution of the field equations is found by interlaced damped gradient iteration of the nucleon– and meson–field equations \cite{32,30}. The solution for the Coulomb field requires a separate handling of the long range parts which reach far beyond the bounds of the numerical grid; this is done using the techniques of \cite{33}. The iteration includes an iteration of the constraining force as proposed in \cite{34} and implemented in a relativistic context in \cite{22}. The iteration scheme has been extended here to deal with two constraints, which is a straightforward procedure provided the constraining operators are properly damped outside the nuclear density, see Eq. \ref{eq:5}.

III. FISSION OF HEAVY ELEMENTS

First calculations of fission barriers in the actinides were published in \cite{15}. They had shown that the relativistic mean–field model with the parameters NL1 and PL–40 can reproduce approximately the double–humped fission barrier of $^{240}$Pu. The first barrier came out about 4-6 MeV higher than the experimental value. However, it has been shown in the macroscopic–microscopic model \cite{33} as well as in nonrelativistic Hartree–Fock calculations \cite{36} that the first barrier is lowered by about 1-2 MeV if triaxial deformations are allowed. The height of the second barrier was about 4-10 MeV to high in the previous relativistic calculations. That was due to the restriction to symmetric deformation. Here we can now present extended investigations on fission barriers which include also asymmetric shapes and octupole deformations. We will discuss the nuclei $^{240}$Pu, $^{226}$Ra, and $^{232}$Th. And we will compare the PES with those of nonrelativistic calculations.

A. The fission path for $^{240}$Pu

In Fig. \ref{fig:1} we show the PES for asymmetric fission of $^{240}$Pu, computed with the quadrupole constraint only. The octupole deformations have been left free to adjust themselves to the
minimum configuration. More detailed quantitative information on barriers and minima is given in Table IV. The nonrelativistic results with the Gogny force D1s had included an estimate for correction with the collective zero-point energy, see the values in brackets in Table IV. These corrections have been removed for the comparison in Fig. 1. The experimental barriers were obtained by fitting parabolic barriers and minima to the measured tunneling probabilities. The known part of the zero-point energies is given in Table IV and corrected for in Fig. 1. Note that these experimental barriers are indirectly determined and contain an unknown amount of zero-point energies as well as possible contributions from multidimensional tunneling. Thus a comparison must be content with a rough proximity of the values. The energies and deformations at the minima, the ground state and first isomeric state, are very well reproduced by the forces PL–40 and NL1 in comparison to the nonrelativistic results and the data. The deviations are somewhat large for the force NL–SH but still acceptable. The height of the first barrier is comparable amongst all theories and overestimated in relation to the experimental point, even if one corrects for the triaxial deformation. The second barrier is generally better reproduced, in particular the force PL–40 comes very close to the experimental point. In view of the uncertainties on the theoretical as well as on the experimental side, we see a good agreement between the relativistic PES from NL1 and PL–40 with the nonrelativistic results and with the experimental points. The force NL–SH provides also good barrier heights but the deformation of all minima and barrier is systematically shifted to lower values compared to all other results. This is probably due to the higher effective mass of the force NL–SH. The effect of a varying effective nucleon mass was studied in [15]: increasing effective mass softens the barriers and shifts them to smaller deformations.

For very large deformations, there is a second branch of solutions visible in Fig. 1. These are strongly favored energetically at large separations because the fragments are less deformed internally. These solutions correspond to the fusion valley in the collective landscape which is distinguished from the fission valley by a smaller hexadecupole moment [36]. The situation is analogous for Radium in Fig. 4.
Table IV also shows the barriers for PL–40 obtained from reflection–symmetric calculations [15]. The asymmetric shapes develop only for larger quadrupole deformations, \( Q_2 > 120 \text{ b} \), such that only the second barrier is affected. But there the effect is dramatic and decisive for the fission process which at the end is dominated by asymmetric fission. We show in Fig. 2 the development of the mass asymmetry \( A_h \) with deformation. The forces PL–40 and NL1 point strongly towards the main peak in the experimental mass distribution, denoted ”St. I”, whereas the nonrelativistic calculations with the Gogny force D1s [36] have their peak at \( A_h = 134 \), just at the maximum ”St. II”. It is furthermore interesting to see that the final mass peak is preformed already at \( Q \approx 200 \text{ b} \) where the two fragments still have a sizeable overlap. It seems as if the mass flow from right to left and back is already strongly inhibited although the geometry does not suggest that. It is most probably a peak in the collective mass distribution which blocks the flow of matter. This point deserves further investigations. But these require first a full solution of the cranking problem along the collective path.

B. The triple–humped fission barrier for \( ^{232}\text{Th} \)

The PES of \( ^{232}\text{Th} \) indicate that there exist strongly stretched stages because they develop a third fission barrier, see e. g. the macroscopic–microscopic analysis of [1]. It is due to strong shell corrections in the outer tail of the second barrier. The third barrier seems to be experimentally supported [11]. It is indicated e. g. by the photofission cross–section [12], or by the asymmetric angular distribution of the light fragment [13]. Fig. 3 shows the PES for asymmetric fission of \( ^{232}\text{Th} \) for the three relativistic parametrizations, compared with the barriers from nonrelativistic calculations and experimentally deduced barriers. The details for the barriers and minima are given in Table V. It is gratifying to see that all three relativistic parametrizations are able to reproduce the third minimum and barrier. There seem to be robust shell effects which appear under widely varying conditions. But beside this robust pattern, there are now more differences visible amongst the parametrizations.
The force NL–SH behaves somewhat strangely. A tendency which was already present in \(^{240}\)Pu, becomes now even more disturbing: the first barrier comes out too low and all minima and barriers are squeezed to lower deformations. The force NL–SH seems to be not too well adapted for the description of fission PES. Two explanations are conceivable: First, the problem can come from the higher effective mass, as it was discussed already in connection with \(^{240}\)Pu, and second, the failure at low \(Q\) may come from the less carefully adjusted surface properties. It was observed in connection with the Skyrme forces that a well–fitted surface tension is required to provide reasonable fission barriers in the actinides \([46]\), and we find in relativistic as well as in nonrelativistic calculations that every parametrization which fits ground state properties including the surface thickness gives comparable and reasonable first barriers. The examples here are the two standard sets, NL1 and PL–40, which are clearly more appropriate. Their overall performance is fair. The second minimum is a bit too bound in all cases. But that is a common disease which is shared with the nonrelativistic models. The two PES of NL1 and PL–40 develop differences with increasing \(Q\). The force NL1 behaves somewhat better at the second minimum and at the third barrier whereas PL–40 is superior at the second barrier. But none of the two is yet ideal. It is a task for future investigations to search for an even better force amongst the more versatile stabilized nonlinear parametrizations of the power–law type \([2]\), \(i. e.\) for a better variant of PL–40. Finally, we want to mention that we again see the fusion valley which is energetically favoured at very large deformations.

**C. Symmetric and asymmetric fission of \(^{226}\)Ra**

The two previous examples, \(^{240}\)Pu and \(^{232}\)Th, preferred asymmetric fission. However, in the region \(84 < Z < 90\) symmetric and asymmetric fission appear with comparable importance, leading to mass yields with typically three peaks: the middle peak from symmetric fission and the two outer peaks corresponding to the light and the heavy fragment from asymmetric fission. These nuclei should display an interesting competition between the
symmetric and asymmetric PES. We will consider here $^{226}$Ra as a typical example for this region of nuclei.

The PES for asymmetric as well as symmetric fission of $^{226}$Ra are shown in Fig. 4. The first surprise is that the ground state of $^{226}$Ra is asymmetric, 2 MeV lower than the nearby symmetric minimum. But the preference of the asymmetric shape at low $Q$ dissapears quickly. The symmetric shape has gained already at the first barrier and the first isomeric minimum is also clearly a symmetric state. Beyond that symmetric and asymmetric PES develop very differently. The second barrier for asymmetric fission is much lower but after the subsequent second minumum, a broad third barrier extends over a wide range of deformations. The second barrier for symmetric fission, on the other hand, is much higher, but a second isomeric minimum and an only shallow third barrier follow. The second symmetric barrier has a further peculiarity: in the range $120 \text{b} < Q < 160 \text{b}$, there are two branches distinguished by the hexadecupole moment. It is interesting to note that the two branches separate at $Q \approx 120 \text{b}$ and merge again at $Q \approx 160 \text{b}$. This can be envisaged in the multidimensional potential energy landscape as having two bifurcation points at these $Q$ for two distinct minimum pathes embracing an island of higher energies. The shapes of the fissioning nucleus for various $Q$ are indicated by half–density contours in Fig. 4. The richness of the various shapes deserves a closer look. We show in Fig. 5 more detailed plots of the density contours along the paths. The features along the symmetric path are particularly remarkable. Note the strong hexadecupole component of the favoured branch at the second barrier. And even more impressive are the long and broad necks for the symmetric configurations at large $Q$. These will give rise to the observed broad fission mass distributions due to the possibility of large fluctuations of the actual neck rupture point [17].

The problem is that Fig. 4 does not trivially suggest a coexistence of symmetric and asymmetric fission. A few further comments are in order:

1. There is only induced fission for $^{226}$Ra at rather substantial excitation energies, e. g. from the reaction $^{226}$Ra(p,f) at 11 MeV [18]; internal excitation reduces the shell effects
and thus favours symmetric shapes.

2. The symmetric second barrier will probably be lowered by allowing triaxial deforma-
tions [5].

3. It is conceivable that fission proceeds first through the asymmetric second barrier and
tunnels then towards the lower symmetric third minimum at large $Q$.

4. PES alone can be misleading; tunneling probabilities are very sensitive to the collective
masses in the tunneling region.

Altogether, we see that the fission of $^{226}$Ra is an intriguing problem which most probably
requires a fully fledged collective dynamics in at least two degrees of freedom, accounting
for triaxial shapes, computing carefully the corresponding collective mass tensor, and taking
care of temperature effects.

Finally, we compare in Fig. 6 the symmetric PES for the two relativistic forces NL1
and PL–40 and for a more recent fit of a Skyrme force [49]. Table VI complements the
detailed information on the barriers and minima. We see again the same pattern as in
the two previous examples. The two sets NL1 and PL–40 agree with each other and with
comparable nonrelativistic models for low $Q$ including the first barrier and perhaps the
first isomeric minimum. Differences between NL1 and PL–40 develop with deformation.
The nonrelativistic Skyrme force lies in between the two relativistic results showing that
there is no principle difference between a relativistic and a nonrelativistic treatment. The
differences of various parametrizations within a class of models are larger. For example,
the force "Skyrme M*", used in the previous figures, fails to reproduce the third barrier in
$^{226}$Ra. An alternative and more recent Skyrme force from [49] properly manages to deliver
the third barrier. Thus the third barrier may be used as an additional criterion for selecting
effective forces.
IV. ASYMMETRIC GROUND STATES IN RADIUM ISOTOPES

It is an old question whether there exist nuclei which have a ground state with broken reflection symmetry. Already in the fifties, one has observed in the actinides low–lying bands of excitations with negative parity \cite{50} which hint at asymmetric deformations in the ground state \cite{51}. Calculations within the macroscopici–microscopic method \cite{6,7} as well as nonrelativistic Hartree-Fock calculations with the Skyrme III force \cite{52} or a Gogny force \cite{53} found asymmetric ground states in the region of Ra–Th which are by 1-2 MeV lower than the corresponding symmetric ground states. In this section, we are going to investigate the ground states of the Ra isotopes.

In Fig. 7 we show the PES for octupole deformation of the isotopes of Radium and for the three relativistic parametrizations discussed in this paper. The symmetric ground state lies at $Q_3 = 0$. We see for all three forces that $^{216}$Ra is stable against symmetry–breaking deformation. The softness against octupole deformation increases with additional neutrons up to $^{226}$Ra, which displays the deepest asymmetric minimum with the largest octupole moment of all cases. Above $^{226}$Ra, the PES moves slowly back to smaller octupole deformation. Although the general trends are the same for all three forces, there are differences in detail, e. g., the transition point changes from $N = 220$ for NL1 via $N = 222$ for PL–40 up to $N = 224$ for NL–SH.

The PES of Fig. 7 can be characterized by the octupole moment at equilibrium and the depth of the minimum compared with the energy at $Q_3 = 0$. We compile the information from all isotopes and from all three forces in Fig. 8. The figure clearly shows the quantitative difference between the forces. The force NL1 gives the strongest extra binding, closely followed by PL–40. The force NL–SH has the much softer octupole effects, yielding even a systematically lower octupole moment for the well deformed isotopes. The strength of the octupole effects also determines the transition point from symmetric to asymmetric ground states, the stronger the effect the earlier the transition. The sequence in the lower left part of Fig. 8 reminds one of the sensitivity to the force which was observed in the transition.
from spherical to quadrupole–deformed isotopes of Gadolinium in \cite{59}. The upper right part of the figure also shows the quadrupole moment at equilibrium. It grows steadily with neutron number and increasing distance from the magic number 126. But one can also see that the octupole deformation has a side effect on the quadrupole deformation because there is a jump in $Q$ between those forces which have $Q_3 = 0$ and those with $Q_3 \neq 0$. Finally, in the lower right part of Fig. 8, we show the electrical dipole moment of the ground state. A nonvanishing dipole moment becomes possible because the octupole deformations of protons and neutrons are not exactly the same. The emerging dipole moment seems to be related to the octupole moment. The force NL–SH with the smaller $Q_3$ also has the smaller dipole moment. All dipole moments shown here are negative, i. e., the protons prefer the bottom of the "pear" whereas the neutrons prefer the tip. A counterexample are, however, the nonrelativistic results (see also Tab. VII later on) where the dipole moment has a different sign for most isotopes. But one has to keep in mind that the overall effect is extremely small. In the upper left part of Fig. 8, we have inserted the experimental energies of the band–heads of the lowest odd–parity band. These energies should be closely related to the depth of the octupole minimum. And that is indeed the case, particularly in comparison with the behaviour of the energies for NL1 or PL–40.

We also show in Fig. 8 the results from a macroscopic–microscopic model \cite{54–56}. These confirm that octupole deformations in the ground state are to be expected for several Radium isotopes. But the deformations at equilibrium as well as the transition points differ substantially from the results of the present relativistic mean–field model. It is to be remarked that these quantitative details depend strongly on the single particle spectra near the Fermi energy. It is obvious that the shell model with effective mass $m^*/m = 1$ has a spectrum much different from the mean–field models all having a rather low effective mass and thus a much lower level density near the Fermi energy. It is thus interesting to look also at results from nonrelativistic mean–field models. A comparison for the two isotopes $^{222}$Ra and $^{224}$Ra is given in Tab. VII. Stable octupole deformations are also found for the Skyrme III force as well as the Gogny D1s force. But the quantitative details of the octupole
minimum differ. That is not very surprising in view of the fact that these details depend strongly on the spectral density near the Fermi energy. And those spectral relations change very sensitively with the model and even with a slight change of the parameters of one model. But one should not overinterpret those differences concerning the minima as we will see from the discussion in the last paragraph of this section.

As an illustration, we show in Fig. 9 contour plots of the ground states of the Radium isotopes, all computed with PL–40. One clearly sees the transition to octupole shapes between $^{220}$Ra and $^{222}$Ra as well as the increasing quadrupole deformation. The figures compare very well with the nonrelativistic mean–field results [52] and the macroscopic–microscopic method [74].

In Fig. 10 we show the relative deviation from the experimental binding energies with and without asymmetric degree of freedom for the three relativistic parametrizations under consideration. The relative error is always very small, generally below 0.5% and for PL–40 even below 0.3%. Nonetheless it is interesting to see the effect of the extra binding through octupole deformation at that scale. The r.m.s. deviation is slightly improved through asymmetric shapes for NL1 and PL–40, but increased for NL–SH which has a bit too much binding anyway. The figure shows also that there is a significant trend with the neutron number in the deviations. The fit could not resolve this isotopic trend in the mismatch. This hints that there is still some open problem in the model concerning isovector properties. It is to be noted, however, that we are discussing deviations at a very fine scale and that the nonrelativistic mean–field models have similar problems [19].

Finally, we show in Figs. 11 and 12 the PES for $^{220}$Ra and $^{222}$Ra in the full $Q–Q_3$ plane. Clearly the octupole deformed minimum in $^{222}$Ra is already announced by the isomeric octupole minimum in $^{220}$Ra. The decision between the minima is related to very small energy changes in a soft energy surface. This is to be related to the typical $1^−$ excitation energies of 0.5 MeV, as can be deduced from the upper left part of Fig. 8. That is a typical case where the minimum alone is not yet conclusive. The true ground state of the system is a coherent superposition of a large neighbourhood around the minimum, not to forget
the rotational and centre–of–mass projection over the continuum of energetically equivalent states. The large fluctuations $\Delta Q$ and $\Delta Q_3$ will add to the ground state deformations for most observables [60], and that can diminish the differences seen in Tab. VII or Fig. 8. One needs first to perform the full collective dynamics in quadrupole and octupole degrees of freedom before comparing models amongst each other and with experimental data. That is a far reaching project which has been accomplished in a few nonrelativistic calculations [61,62] but which is yet a long way to go for the relativistic models. The computation of the various PES, as presented in this paper, is a first step into that direction.

V. CONCLUSIONS

In this paper we have investigated collective deformation paths for actinides in the framework of the relativistic mean–field model. The calculations have been restricted to axial symmetry but allowed for reflection–asymmetric shapes. The quadrupole moment, damped at the edges of the numerical box, has been used as constraining force to generate the fission paths. An additional octupole constraint had been used to map the collective potential energy surface near the ground states of Radium isotopes. Three different parametrizations of the relativistic mean–field model have been employed, NL1 and NL–SH within the standard nonlinear functional for the scalar meson, and PL–40 as one representative for the stabilized nonlinear functional.

We have studied the collective paths for symmetric and asymmetric fission of $^{240}$Pu, $^{232}$Th, and $^{226}$Ra. The relativistic mean–field model was able to reproduce all the essential qualitative features, as e. g. the triple–humped barrier in $^{232}$Th. The two parametrizations NL1 and PL–40 provide also many quantitative details well in agreement with comparable nonrelativistic calculations and with experiment. This holds particularly for the features at lower deformations, e. g. the ground state, the first barrier and the first isomeric minimum. It seems that every mean–field model, which has carefully fitted the nuclear ground state properties including sufficient information on surface properties, behaves reasonably in that
respect. The force NL–SH falls a little bit behind, perhaps due to its larger effective mass and/or its lack of surface information in the fit. Larger differences between the forces develop for larger deformations. This seems to indicate some need for a further selection of the forces, or to say it positively, the chance to discriminate amongst otherwise equivalent forces. In particular the stabilized nonlinear meson functional has still open degrees of freedom for a further fine–tuning.

The outer fission barriers are much lower for asymmetric fission than for symmetric fission in $^{240}$Pu and the (asymmetric) fragment masses from the relativistic calculations agree well with the data. There is an interesting interplay between symmetric and asymmetric fission paths in $^{226}$Ra. Although the symmetric barrier is again much higher, there comes a pronounced third minimum in the symmetric fission path which may counterweight the barrier and thus could serve as explanation for the competition between symmetric and asymmetric fission observed in $^{226}$Ra.

We have furthermore studied the occurrence of stable octupole deformations in the ground states of the Radium isotopes. All three relativistic forces under consideration have produced such isotopes with asymmetric ground states. But the transition point from symmetric to asymmetric shapes is found to depend sensitively on the force. This holds to some extent also for the octupole moment of the deformed ground states. A superficial comparison of the ground state energies with the band head of the low lying odd–parity bands shows that the forces NL1 and PL–40 provide about the right trends.

In both cases, fission paths and octupole deformations, we have only looked at the potential energy surfaces from static deformations. The dynamical aspects, as collective masses and zero–point energy corrections, have not yet been properly accounted for. This was appropriate for the present investigations which aimed to explore first the capability of the relativistic model for the description of fission and other features of actinides. But now we have reached an end where further comparisons need to go into more quantitative detail. This requires as the next important step to implement the cranking scheme for the computation of the appropriate collective masses. And honestly, we see presently no simple
way to perform this task in a relativistic environment. Most probably, one has to perform first a less ambitious step and deduce the collective masses from the generator-coordinate method.

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TABLES

TABLE I. The parameter sets within the standard nonlinear model used in this work. All masses are in MeV and $b_2$ is given in fm$^{-1}$. All other parameters are dimensionless.

|        | $g_\sigma$ | $g_\omega$ | $g_\rho$ | $b_2$ | $b_3$ | $m_\sigma$ | $m_\omega$ | $m_\rho$ | $m_n$   |
|--------|------------|------------|----------|-------|-------|-------------|-------------|----------|---------|
| NL1    | 10.138     | 13.285     | 4.976    | -12.172 | -36.265 | 492.250     | 795.36      | 763.0    | 938.0   |
| NL–SH  | 10.444     | 12.945     | 4.383    | -6.9099 | -15.8337 | 526.059     | 783.0       | 763.0    | 939.0   |

TABLE II. The parameter set PL–40 within the stabilized nonlinear model. $m^2_\infty$ and $\Delta m^2$ are given in fm$^{-2}$, $\delta \Phi$ and $\Phi_0$ are given in fm$^{-1}$. The nucleon mass and the masses of the vector mesons are $m_n = 938.9$ MeV, $m_\omega = 780$ MeV, and $m_\rho = 763$ MeV.

|        | $g_\sigma$ | $g_\omega$ | $g_\rho$ | $m^2_\infty$ | $\Delta m^2$ | $\delta \Phi$ | $\Phi_0$ |
|--------|------------|------------|----------|---------------|---------------|--------------|----------|
| PL–40  | 10.0514    | 12.8861    | 4.81014  | 4.0           | 3.70015       | 0.269688     | -0.111914 |

TABLE III. The nuclear matter properties $E/A \equiv$ binding energy per nucleon, $\rho_0 \equiv$ equilibrium density, $K \equiv$ incompressibility, $m^*/m \equiv$ effective nucleon mass, and $a_4 \equiv$ symmetry energy for the relativistic parametrizations NL1, PL–40, and NL–SH, compared with the two nonrelativistic Hartree–Fock models, and with the deduced experimental data.

|        | $E/A$ [MeV] | $\rho_0$ [fm$^{-3}$] | $K$ [MeV] | $m^*/m$ | $a_4$ [MeV] |
|--------|-------------|----------------------|-----------|---------|-------------|
| PL-40  | -16.17      | 0.152                | 166.1     | 0.58    | 41.7        |
| NL1    | -16.42      | 0.152                | 211.7     | 0.57    | 43.5        |
| NL-SH  | -16.33      | 0.146                | 354.95    | 0.66    | 36.1        |
| Gogny D1s | -16.32      | 0.166                | 216.0     | 0.67    | 30.8        |
| Skyrme M* | -16.01      | 0.161                | 219.2     | 0.786   | 30.0        |
| Exp.   | -15.96      | 0.145                | 240.0     |         |             |
TABLE IV. Quadrupole moment of the protons, binding energy, height of the first ($B_1$) and the second barrier ($B_2$) as well as of the isomeric state ($M_{II}$) for $^{240}$Pu. The parameter sets PL–40, NL1, and NL–SH are compared with nonrelativistic Hartree–Fock calculations using the forces Gogny D1s \[36\] and Skyrme M* \[37\]. For PL–40 we also show the results of a reflection–symmetric calculation \[15\]. The experimental data are taken from \[38\], \[39\], and \[2\]. The values in parentheses are the zero point energies subtracted in those references. The second entry in brackets for the Gogny force D1s gives the lowering of the first barrier due to triaxial deformations.

| set            | $Q_p$[b] | $E_b$[MeV] | $B_1$[MeV] | $M_{II}$[MeV] | $B_2$[MeV] |
|----------------|----------|------------|------------|---------------|------------|
| PL–40          | 11.9     | $-1812.1$  | 9.5        | 0.9           | 6.6        |
| NL1            | 11.7     | $-1811.9$  | 10.8       | 2.9           | 9.4        |
| NL–SH          | 11.1     | $-1818.8$  | 8.4        | 2.0           | 8.5        |
| PL–40, sym     | 11.8     | $-1812.0$  | 9.7        | 1.3           | 8.7        |
| Gogny D1s      |          |            |            | 7.7(+1;+1.7) | 2.6        | 7.5(+1)   |
| Skyrme M*      |          |            |            | 11.7          | 3.6        | 9.1        |
| exp.           | 11.58 ± 0.06 | $-1813.5$  | 5.6 ± 0.2  | 2.4 ± 0.3     | 5.1 ± 0.2  |
|                |          |            |            |               | (+0.5)     |
|                |          |            |            |               | (+0.5)     |
TABLE V. Quadrupole moment of the protons, binding energy, height of the first \((B_1)\), the second \((B_2)\), and the third barrier \((B_3)\), as well as of the isomeric state \((M_{III})\) and the third minimum \((M_{III})\) for \(^{232}\)Th. All energies are given in MeV. The parameter sets PL–40, NL1, and NL–SH are compared with a nonrelativistic Hartree–Fock calculation using the Gogny force D1s \([36]\) and a macroscopic–microscopic calculation (Yukawa–plus–Exponential and Woods–Saxon) \([44]\). The experimental values are from \([45]\), \([39]\), \([2]\), and \([42]\). The values in parentheses are the zero–point energies substracted in those references.

|        | \(Q_p [\text{b}]\) | \(E_b\)     | \(B_1\) | \(M_{III}\) | \(B_2\) | \(M_{III}\) | \(B_3\) |
|--------|-----------------|-------------|---------|-------------|---------|-------------|---------|
| PL–40  | 10.0            | \(-1763.6\) | 5.9     | \(-0.3\)    | 6.7     | 1.7         | 2.8     |
| NL1    | 9.9             | \(-1762.5\) | 7.1     | 1.7         | 9.5     | 5.0         | 7.1     |
| NL–SH  | 8.8             | \(-1769.4\) | 3.5     | 1.4         | 7.3     | 4.4         | 6.3     |
| D1s    |                 |             | \(5.9(+1)\) | 0.8 | \(5.8(+1)\) | 4.2 | 4.3(+1)     |
| YE+WS  |                 |             | 4.8     | 2.1         | 6.4     | 4.2         | 8.3     |
| Exp.\(^1\) & 9.66 & \(-1766.71\) & \(5.8 \pm 0.2\) & \(\ll 4.5\) & 6.2 \(\pm 0.2\) & \(\pm 0.09\) & \((+0.5)\) & \((+0.5)\) |
| Exp.\(^2\) &                 |             | 5.82\(+0.5\) | 2.8 | 6.4\(+0.5\) |
| Exp.\(^2\)(0\(^-\)) &                 |             | 6.2\(+0.5\) | 6.25\(+0.5\) | 6.3\(+0.5\) |

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TABLE VI. Binding energy, height of the first ($B_1$), the second ($B_2$), and the third barrier ($B_3$), as well as the height of the isomeric state ($M_{II}$) and the third minimum ($M_{III}$) for $^{226}$Ra. All energies are in MeV. For each parameter set the upper line shows the results when only reflection–symmetric shapes are considered. For PL–40, NL1, and LD+MO the barrier heights of the reflection–asymmetric solution is given in the lower line. "Skyrme" is a nonrelativistic Hartree–Fock calculation using a recent fit for the skyrme force [49], while LD+MO (liquid drop + modified oscillator) is a macroscopic–microscopic calculation [4].

|        | $E_b$   | $B_1$ | $M_{II}$ | $B_2$ | $M_{III}$ | $B_3$ |
|--------|---------|-------|----------|-------|-----------|-------|
| PL–40  | –1728.8 | 6.2   | 1.7      | 16.1  | 2.4       | 5.9   |
|        |         |       |          |       |           |       |
| NL1    | –1727.7 | 6.7   | 2.9      | 19.6  | 8.2       | 11.8  |
|        |         |       |          |       |           |       |
| Skyrme | –1726.2 | 7.4   | 3.8      | 18.3  | 7.2       | 9.9   |
|        |         |       |          |       |           |       |
| LD+MO  | –1728.8 | 4.3   | 3.4      | 10.4  | 9.2       |       |
TABLE VII. Properties of the intrinsic ground states of $^{222}$Ra and $^{224}$Ra. The results are shown for the parameter sets PL–40, NL1 and NL–SH as well as for nonrelativistic calculations with the Skyrme III \[52\] and the Gogny D1s \[53\] force and for a macroscopic–microscopic calculation (Yukawa–plus–Exponential and Woods–Saxon) \[54\].

|          | $^{222}$Ra |          | $^{224}$Ra |
|----------|------------|----------|------------|
|          | $E_a - E_s$| $Q$      | $Q_3$     | $D$        | $E_a - E_s$| $Q$      | $Q_3$     | $D$        |
|          | [MeV]      | [b]      | [b$^{3/2}$] | [e·fm]    | [MeV]      | [b]      | [b$^{3/2}$] | [e·fm]    |
| PL–40    | $-0.7$     | $14.8$   | $2.4$      | $-0.17$   | $-1.4$     | $16.8$   | $2.9$      | $-0.4$    |
| NL1      | $-1.6$     | $14.9$   | $2.5$      | $-0.19$   | $-2.1$     | $17.0$   | $3.0$      | $-0.47$   |
| NL–SH    | $-0.5$     | $15.3$   | $2.5$      | $-0.17$   |            |          |            |            |
| D1s      | $-1.7$     | $3.0$    | $0.2$      | $-1.5$    | $3.4$      | $-0.06$  |            |            |
| SkyrmeIII| $-0.2$     | $13.0$   | $2.0$      | $0.04$    | $-0.5$     | $11.5$   | $2.2$      |            |
| YE+WS    | $-1.0$     | $10.6$   | $1.9$      | $-0.5$    | $11.5$     | $2.2$    |            |            |
FIGURES

FIG. 1. PES of $^{240}$Pu for the three parametrizations as indicated. Barrier heights obtained in nonrelativistic Hartree–Fock calculations with the Gogny D1s [36] and the Skyrme M* force [37] as well as experimental values from [2] are drawn for comparison. All barrier heights are corrected as described in Table IV.

FIG. 2. Mass of the heavy fragment, $A_h$ as defined in Eq. 4, in the fission of $^{240}$Pu as function of the quadrupole deformation $Q_2$. The right hand side shows an experimental mass distribution which is resolved into two separate mass peaks [40]. The various shapes along the fission path are indicated by the contours of the vector densities at $\rho = 0.07$ fm$^{-3}$.

FIG. 3. PES of $^{232}$Th calculated with different parameter sets as indicated. Barrier heights as obtained in a nonrelativistic Hartree–Fock calculation with the Gogny D1s force [36], in a makroscopic–microscopic calculation [44], and experimental values are drawn for comparison. exp.1 is taken from [2], exp.2 from [42]. All barrier heights are corrected for zero–point energies as described in Table V.

FIG. 4. Potential energy surfaces of $^{226}$Ra, calculated with the parameter set PL–40. The reference point for the energy is the reflection–symmetric ground state. Solutions with asymmetric degrees of freedom are drawn as solid lines and reflection–symmetric solutions are drawn as dashed lines. The nuclear shapes drawn at their corresponding $Q$ are lines of constant vector density at $\rho = 0.07$ fm$^{-3}$. For the ground state and the first barrier only the symmetric shapes are shown.

FIG. 5. Vector densities $\rho_0$ of $^{226}$Ra along the asymmetric and symmetric fission path, calculated with the parameter set PL–40. We show the same densities here as in Figure 4. The contour lines correspond to the densities 0.03, 0.05, 0.07, 0.09, 0.11, 0.13, 0.15, and 0.17 fm$^{-3}$.

FIG. 6. PES for symmetric fission of $^{226}$Ra for the parameter sets PL–40 and NL1. Additionally the result of a nonrelativistic Hartree–Fock calculation using a recent fit for the skyrme force [49] is shown.
FIG. 7. PES for octupole deformation of Radium isotopes for the three parametrizations PL–40, NL1, and NL–SH. The PES are symmetric in $Q_3 < 0$ and $Q_3 > 0$.

FIG. 8. Upper left: energy of the octupole minimum relative to the state with $Q_3 = 0$ in the isotopes of Radium. In addition we show the results of macroscopic–microscopic calculations (Yukawa–plus–Exponential and Woods–Saxon) $^1$ $^{54}$ $^{55}$ $^2$ $^{56}$. The experimental energies of the band–heads of the lowest odd–parity bands are drawn at positive energies and indicated by a "1–" $^{57}$ $^{58}$. The other subplots show octupole (lower left), quadrupole (upper right), and electric dipole moment (lower right) of Radium nuclei in their intrinsic ground state. The deformation parameters $\beta_2$ and $\beta_3$ used in $^{54}$ $^{55}$ were converted to the quadrupole and octupole moments with the approximations $\beta_2 = \sqrt{5\pi/(3AR_0^2)} \cdot Q$ and $\beta_3 = 4\pi/(3AR_0^3) \cdot Q_3$ with a radius of $R_0 = 1.2 A^{1/3}$ fm. The sign of $D$ is shown relative to a positive $Q_3$.

FIG. 9. The vector densities $\rho_0$ of Radium nuclei in their intrinsic ground state, calculated with parameter set PL–40. Contour lines are drawn for the densities 0.03, 0.05, 0.07, 0.09, 0.11, 0.13, 0.15 and 0.17 fm$^{-3}$.

FIG. 10. Relative difference of the binding energy from experimental values $^{39}$ for Radium nuclei. On the left hand side the difference is shown for the symmetric saddle point, on the right hand side for the intrinsic ground state.

FIG. 11. PES in the $Q$–$Q_3$ plane for $^{220}$Ra calculated with the parameter set PL–40. The distance between solid lines is 0.5 MeV and between solid and broken lines 0.25 MeV.

FIG. 12. The same as in figure 11, but for $^{222}$Ra. The intrinsic ground state is denoted by "×", the symmetric saddle point by "•".
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