Skyrme-Mean-Field Studies of Heavy Nuclei

\(96 \leq Z \leq 104\)

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Abstract

We use the constrained Skyrme-Hartree-Fock plus pairing approach to calculate the fission barriers of heavy nuclei with \(96 \leq Z \leq 104\) in the actinide and transactinide region. We consider axial- and reflection-symmetric fission paths only. In this region, both single- and double-humped barriers are observed. Life time measurements suggest that there is a deformed sub-shell closure at \(N = 152\) in the considered region. The calculated inner barrier heights are almost the same for a given isotope (isotone) while outer barrier heights decrease with increasing \(N\) (\(Z\)). We have investigated the microscopic origin of the variation of outer barrier heights by using Nilsson level diagrams. We found that the main contribution of variation of outer barriers for a given isotope comes from the pairing correlations which increase with high level density.

Introduction

The fission barrier is a fundamental characteristic of heavy atomic nuclei. Many heavy nuclei decay mainly by spontaneous fission, and it is the fission barriers that are responsible for the lifetimes of those nuclei. On the other hand, the probability of superheavy nucleus formation in a heavy-ion fusion reaction is also directly connected to the height of its fission barrier. Skyrme-Hartree-Fock approach (SHF) is a mean-field approximation with Skyrme force that is widely used in self-consistent nuclear structure calculations since it can successfully reproduce the static properties of nuclei such as binding energies, spin-orbit effects, neutron radii, single-particle levels, estimating super heavy nuclei and fission barriers. The experimentally observed fission half-lives show extra stability at \(N = 152\) for the elements \(Fm\) and \(No\). The deduced values, heights of outer barriers for nuclei around \(Z=100\) with \(N=152\), show a maximum compare with those of neighboring nuclei. This fact was pointed out (B. S. Bhandari and Y. B. Bendardaf) that this may be presumably due to the apparent closure of a deformed sub-shell at \(N=152\). This fact motivates us

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to perform constrained mean-field calculation to obtain fission barriers in this region. In addition, the microscopic origin of the different results has been studied by using Nilsson level diagrams of some selected nuclei because the shape of the fission barrier is highly dependent on the shell structure, which can be understood by investigating the single-particle energy levels.

**Calculation of Fission Barrier using Constrained Hartree-Fock Method**

Theoretically, fission barriers can be calculated using either the macroscopic-microscopic model or microscopic mean-field models. In the latter approach, one selects a few important degrees of freedom for fission, such as quadrupole or higher multipole moments, and draws a fission energy surface using the constrained Hartree-Fock method with the corresponding constraining operators (L. Bonneau and P. Quentin, 2005).

Expressing the energy as a function of quadrupole moment, one can draw an energy surface for deformation. The usual HF solution corresponds to the local minimum in the energy surface. The simplest way to minimize the total energy under the constraint \( q_2 = \langle Q \rangle \) is to add the quadrupole moment operator to the Hamiltonian with a Lagrange multiplier,

\[
H' = H - \lambda \langle Q_{20} \rangle, \tag{1}
\]

\[
\langle Q_{20} \rangle = \int d^3 r \rho (r) (2z^2 - x^2 - y^2), \tag{2}
\]

and minimize \( \langle H' \rangle \). The Lagrange multiplier \( \lambda \) is determined so as to satisfy the condition \( \langle Q \rangle = q_2 \). Besides quadrupole constraint, the deformation energy can also be, in principle, minimized with respect to all multipole moments for proton and neutron separately.

**The Skyrme Effective Interaction**

The effective Skyrme interaction is popular due to its simple expression in terms of the \( J(r_i - r_j) \) interaction. Most of the parameter sets of the Skyrme interaction available in the literature are obtained by fitting Hartree-Fock results to experimental data on the ground state properties. Skyrme interaction can be written as a potential

\[
V = \Sigma_{i \leq j} v_{ii} + \Sigma_{i \leq j \neq k} v_{ijk}, \tag{3}
\]
with a two-body part $u_{ij}$, and three-body part $u_{ijk}$. The three-body force is also a zero-range interaction:

$$u_{ijk} = t_3 \delta(r_i - r_j) \delta(r_i - r_k)$$  \hspace{1cm} (4)

It provides a simple phenomenological representation of many-body effects, and describes the way in which the interaction between two nucleons is influenced by the presence of others. The standard form of the Skyrme interaction has the following form:

$$V_{\text{Skyrme}} = t_0 (1 + x_0 P_o) \delta(r_i - r_j)$$  \hspace{1cm} (5)

$$+ \frac{1}{2} t_1 (1 + x_1 P^2_o) [P_{12}^2 \delta(r_i - r_j) + \delta(r_i - r_k) P_{12}^2]$$

$$+ t_2 (1 + x_2 P^2_o) P_{12} \delta(r_i - r_j) P_{12}$$

$$+ \frac{1}{6} t_3 (1 + x_3 P^2_o) \rho^{\alpha}(r_i) \delta(r_i - r_j) + \delta(r_i - r_k) (\sigma_i + \sigma_j) \times P_{12}$$

$P_o = \frac{1}{2} (1 + \sigma_1 \cdot \sigma_2)$ is the spin exchange operator,

$\sigma$ is the vector of Pauli spin matrices.

The expectation value of the total energy of a nucleus whose wave function is represented by a Slater determinant $\Phi$ is

$$\mathcal{E} = \langle \Phi | T + V_{\text{Skyrme}} | \Phi \rangle = \int \mathcal{H}(r) d^3r.$$  \hspace{1cm} (6)

For the Skyrme interaction the energy density $H(r)$ is an algebraic function of the nucleon densities $\rho_n (r_p)$, the kinetic energy densities $\mathcal{E}_n (\mathcal{E}_p)$, and spin- densities $\mathcal{J}_n (\mathcal{J}_p)$. These quantities in turn depend on the single-particle states $\Phi_i$ defining the Slater determinant wave function $\Phi$,

$$\rho(r) = \sum_i |\Phi_i(r)|^2, \quad \mathcal{E}_n (\mathcal{E}_p) = \int \mathcal{H}_n (\mathcal{H}_p) d^3r$$

$$\mathcal{J}_n (\mathcal{J}_p) = \int \mathcal{J}_n (\mathcal{J}_p) d^3r.$$  \hspace{1cm} (7)

The sums in Equation (7) are taken over occupied proton (neutron) single-particle states to get the proton (neutron) densities.

The Hartree-Fock equations

$$\left(-\nabla^2 + u(r)\right) \Phi_i(r) = \epsilon_i \Phi_i(r)$$  \hspace{1cm} (8)
are obtained by varying Equation (6) with respect to the single-particle states $\phi_i$ and have the form of a local equation, with an effective mass $m^*(r)$.

It is well known that in a nuclear system the structure dependence of the effective interaction is crucially important. One of the basic problems in determining the barrier height using the Skyrme-Hartree-Fock method is the choosing of the effective interaction to be used. $(SkM^*)$ is a modification of a previous force, SkM, modified to account for the fission barrier in $^{240}Pu$. It has rather good surface properties which make it well suited for the description of very elongated nuclear shapes as encountered during the fission process. $SLy4$ is also the most widely used Skyrme parametrization which was fitted to the equation of state of pure neutron matter as well as doubly magic nuclei, and therefore represents a good candidate for calculation of neutron rich systems. The parametre set $SkM^*$ has very similar properties to that of $SLy4$, but the only difference is the surface coefficient for nuclear matter properties which is important for describing the shape of nuclei at large deformation. We select the $SkM^*$ and also $SLy4$ and $SLy6$ parameter sets to compare the effect of interaction.

Selection of Pairing Strength

Table 1 Pairing strengths $V_n$ for the neutrons and $V_p$ for the protons for the mean-field forces used in this study. $m^*/m$ is the effective mass in the infinite nuclear matter.

<table>
<thead>
<tr>
<th>Force</th>
<th>$m^*/m$</th>
<th>$V_n$(MeV)</th>
<th>$V_p$(MeV)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$SkM^*$</td>
<td>0.79</td>
<td>910</td>
<td>1410</td>
</tr>
<tr>
<td>$SLy4$</td>
<td>0.70</td>
<td>965</td>
<td>1425</td>
</tr>
<tr>
<td>$SLy6$</td>
<td>0.69</td>
<td>970</td>
<td>1470</td>
</tr>
</tbody>
</table>

The pairing correlation is treated within the BCS approximation using an effective density-dependent zero-range delta pairing force:
where $V_0$ is the pairing strength, chosen to be different for proton and neutron and $\rho_0$ is the saturation density. We use the same pairing scheme for all calculations. In this work pairing gaps are adjusted to reproduce the empirical pairing gaps of $^{238}$U, that is, $\Delta_n = 0.67$ MeV and $\Delta_p = 1.16$ MeV obtained from the three point formula of nuclear mass.

The adjustment is made for each force separately because the difference in effective mass calls for different pairing strengths in each force. The interaction with small effective mass gives large energy spacing of single particle levels and need larger pairing strengths compare with that of small effective mass. It is found that the absolute value of the pairing strength decreases with increasing effective mass as shown in Table (1). We mainly use $SKM^*$ parametrization, but we also perform the same calculation with different parametrizations shown in Table (1) for some selected nuclei.

**Systematic of Fission Barriers around $N = 152$**

The interesting feature of measured values of spontaneous fission half-lives of heavy nuclei around $Z = 100$ is the appearance of longer half-life (or higher stability) of $^{252}$Fm and $^{252}$No with $N = 152$. This fact motivates us to make a systematic study of variation of fission barriers of nuclei ($96 \leq Z \leq 104$) with $N = 152$ and calculate the potential energy surfaces up to and beyond the second saddle point.

The first and second fission barriers of isotones are calculated first with $N = 152$. The calculated results are plotted in Fig. (2). All curves are shifted in order to get the ground state minimum at the same position. The systematic variation of the outer barrier heights with increasing atomic number $Z$ can be seen in this figure. The double-humped fission barriers are found for lighter nuclides but with different heights. Although the first barriers have similar widths and heights, the locations and heights of their outer barriers differ from each other. In general, the second barrier heights decrease with increasing $Z$. For heaviest isotope, $^{254}$Fm, the height of second barrier is very close to that of ground state minimum. The lower the
second barrier height, the easier the spontaneous fission and consequently shorter lifetime of the corresponding nucleus can be expected.

From this fact, it can be expected that the difference in the lifetimes against spontaneous fission mainly comes from the difference in the second barrier heights. This behaviour can also be predicted by the simple liquid drop model since the fissility parameter varies with the square of the atomic number $Z$. The larger the atomic number $Z$, the larger the fissility parameter becomes and so is the fission probability.

Fig.(2) The comparison of the height of fission barriers for the various doubly even-even transactinium nuclei ($96 \leq Z \leq 104$) with 152 neutrons each.

Next the variation of fission barriers on neutron number is considered for the same elements. Fig. (3) shows the valleys in the potential energy surface of $\text{Cm, Cf, Fm, No and Rf}$ isotopes with neutron number $150, 152$ and $154$. The numerical values of the first barriers, superdeformed minima and second barriers are listed in Table (2).

As in the previous case for $N = 152$ isotones, the first barriers have similar shapes and heights while the second barriers decrease with increasing neutron number. Macroscopically, the fissility parameters reduce
with increasing neutron number for a given isotope. As a result, higher barriers are expected for larger neutron number. In contrast to this simple macroscopic prediction, Fig. (3) shows the lower barriers for larger neutron number.

Table (2). HF+BCS relative energies (in MeV) of the first barrier ($E_A$), of the superdeformed minimum ($E_B$) and of the second barrier ($E_B$) with respect to the energy of the normally deformed minimum for the calculated nuclei

<table>
<thead>
<tr>
<th>Nucleus</th>
<th>$E_A$</th>
<th>$E_B$</th>
<th>$E_B$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^{248}_{\text{Cm}}$</td>
<td>9.99</td>
<td>1.75</td>
<td>6.99</td>
</tr>
<tr>
<td>$^{248}_{\text{Cm}}$</td>
<td>9.68</td>
<td>1.69</td>
<td>5.91</td>
</tr>
<tr>
<td>$^{248}_{\text{Cm}}$</td>
<td>9.02</td>
<td>48</td>
<td>4.08</td>
</tr>
<tr>
<td>$^{248}_{\text{Cf}}$</td>
<td>10.34</td>
<td>1.33</td>
<td>5.42</td>
</tr>
<tr>
<td>$^{248}_{\text{Cf}}$</td>
<td>10.07</td>
<td>1.24</td>
<td>4.39</td>
</tr>
<tr>
<td>$^{248}_{\text{Cf}}$</td>
<td>9.45</td>
<td>0.89</td>
<td>3.11</td>
</tr>
<tr>
<td>$^{252}_{\text{Fm}}$</td>
<td>10.24</td>
<td>0.58</td>
<td>3.84</td>
</tr>
<tr>
<td>$^{252}_{\text{Fm}}$</td>
<td>10.09</td>
<td>0.62</td>
<td>2.87</td>
</tr>
<tr>
<td>$^{252}_{\text{Fm}}$</td>
<td>9.59</td>
<td>0.26</td>
<td>1.4</td>
</tr>
<tr>
<td>$^{254}_{\text{No}}$</td>
<td>9.74</td>
<td>-0.28</td>
<td>2.07</td>
</tr>
<tr>
<td>$^{254}_{\text{No}}$</td>
<td>9.72</td>
<td>-0.17</td>
<td>1.86</td>
</tr>
<tr>
<td>$^{254}_{\text{No}}$</td>
<td>9.33</td>
<td>-0.45</td>
<td>0.8</td>
</tr>
<tr>
<td>$^{254}_{\text{Rf}}$</td>
<td>8.85</td>
<td>-1.31</td>
<td>0</td>
</tr>
<tr>
<td>$^{254}_{\text{Rf}}$</td>
<td>9</td>
<td>-1.01</td>
<td>0</td>
</tr>
<tr>
<td>$^{254}_{\text{Rf}}$</td>
<td>8.7</td>
<td>-1.21</td>
<td>0</td>
</tr>
</tbody>
</table>

As shown in the Figures(2) and (3), no clear evidence of extra stability at $N = 152$ is found in the calculated results. We confirm this result by using the different parameter set, SLy4, for some selected isotopes. We find the same trend in the variation of outer barriers as in the calculation with SkM* force. The same trend given by different forces
suggests that the variation of the height of the second barrier would be due to detail shell structure of the particular nucleus.

Fig. (3) The comparison of the height of inner and outer barriers for 
\( ^{Cm, Cf, Fm, No and Rf} \) nuclei with \( N = 150, 152, 154 \).
To trace back the microscopic origin of the lowering of the outer barriers, the Nilsson diagrams of $\text{Cf}$ isotopes are plotted as a function of deformation. Fig. (4) and Fig. (5) show the neutron single-particle level diagrams for $\text{Cf}$ isotopes. As shown in these figures, the single-particle level density at corresponding neutron number increases with increasing neutron number. For $^{248}\text{Cf}$, there is a gap at $N = 150$. The smaller gap appears at $N = 152$ for $^{250}\text{Cf}$ and high level density occurs at $N = 154$ for $^{252}\text{Cf}$. Higher level density leads to larger pairing correlation, and in consequence, to a lower fission barrier.

![Fig. (4) Neutron single-particle energies in $^{248}\text{Cf}$ (left) and $^{250}\text{Cf}$ (right) as a function of the quadrupole deformation]
Fig. (5) Neutron single-particle energies in $^{252}$Cf as a function of the quadrupole deformation

**Conclusion**

The potential energy surfaces of the even-even actinide and transactinide nuclei have been studied using self-consistent Skyrme-Hartree-Fock method. Pairing correlation is implemented with BCS approach using density-dependent zero-range pairing scheme. We have computed fission barriers of three isotopic series of Cm, Cf, Fm, No and Rf elements with neutron numbers $^{150,152}$ and $^{154}$. Experimentally, the measured half-lives of Fm and No isotopes suggest extra stability of nuclei with $N = 152$. This is investigated by comparing the outer barrier heights of those isotopes. The calculated results do not show such behaviour at $N = 152$. It is found that the heights of outer barriers decrease with increasing neutron number. It is expected that the outer barrier heights will play a decisive role in the stability of the corresponding nuclei since the inner barriers are found to have similar shapes and heights. The calculated
outer barriers show different trend compared with the values obtained from experimental data. The microscopic origin of the variation of the outer barriers is investigated by using Nilsson level diagrams. We find that for a given isotope, variation of outer barriers come from the level density of the corresponding nucleus. The nucleus with higher level density will have lower barrier due to pairing correlation. The effect of pairing correlation has significant effect on the fission barriers.

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**References**

