

SPONTANEOUS FISSION OF SUPERHEAVY NUCLEI IN A MACROSCOPIC-MICROSCOPIC MODEL

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A systematic study of spontaneous fission half-lives of superheavy nuclei in the framework of the macroscopic-microscopic method was performed. The macroscopic-microscopic calculations of the half-lives consist in determining the collective potential energy V which splits into microscopic and smooth average macroscopic parts as well as into a nucleus mass tensor of the nucleus undergoing the fission process. The microscopic part of the energy is calculated using the single-particle Woods-Saxon potential with a *universal* set of parameters. Two models of the residual pairing interaction were studied. In the first approach we used monopole pairing (with constant matrix elements G). In the second approximation the pairing matrix elements were calculated with δ -force and are state dependent. As the macroscopic part of collective energy we examined four different macroscopic models of nuclear energy: Myers - Swiatecki liquid drop, Droplet expansion, Yukawa-plus-Exponential and the Lublin-Strasbourg Drop (*LSD*) model. The analysis covers a wide range of even-even superheavy nuclei from $Z = 100$ to $Z = 126$. The calculations of spontaneous fission half-lives (T_{sf}) were performed by means of a *WKB* approximation, in the multi-dimensional dynamical-programming method (*MDP*) within parameters describe the shape of nuclei. The studies offer an opportunity of a comprehensive approach to a very interesting group of exotic heavier nuclei, which are currently investigated by experimenters.

1. Introduction

The region of superheavy nuclei is one of the most intensely studied ones in recent years. The authors of papers recently published [1 - 3] that overcome the barrier of the island of stability placed in the vicinity of the magic number $Z = 114$.

It is believed that experiments in the near future will focus on nuclei in the neighborhood of $Z = 112 - 122$ and $N \sim 170 - 190$. Nevertheless, experimental evidence is still far from complete. Therefore, in preparing the experimental setups theoretical estimations are mainly used.

The aim of this work is the evaluation of the properties of superheavy nuclei using different macroscopic-microscopic models and a critical analysis of the results. Comparisons of these properties for different models allow for easier determination of identifying the interesting areas of superheavy nuclei.

According to the Strutinsky [4] model, the collective potential energy V is split into a shell δE_{shell} , the pairing correction parts, δE_{pair} and the smooth average background energy E_{smooth} (macroscopic part).

The shell correction energy [5] depends on the form of the single-particle potential used and we believe that the deformed Woods-Saxon potential with universal parameters [6] guarantees good behavior of the fission barrier with deformation.

Literature offers many models of smooth energy. More popular ones include the drop model [7], droplet model [8], the so called Folded-Yukawa with an exponential model [9] and the Lublin-Strasbourg Drop model (*LSD-drop*) [10]. The latter model (i.e. *LSD-drop*) is a revised and improved nuclear liquid drop, in which the corresponding parameter of the extended classical energy formula was adjusted to the currently known nuclear masses and fission barriers heights.

2. Theory

2.1. Nuclear Shape Parameterisation

The shape of the nucleus is defined by the surface Σ :

$$\Sigma: f(r, \theta, \phi) = 0 \quad (1)$$

There are many multi-parameter descriptions of nuclear shapes in literature. One of the most recognised and comprehensive is the expansion of the radius R into spherical harmonics:

$$R(\theta, \phi, \hat{\alpha}) = R_0 \left[1 + \sum_{\lambda \geq 2} \sum_{\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\theta, \phi) \right] \quad (2)$$

In above equation $R_0 = r_0 A^{1/3}$ is the radius of the spherical nucleus with an atomic number A and $\hat{\alpha}$ denotes the full set of deformation parameters. For the axial shapes only Eq. 2 simplifies to:

$$R(\theta, \hat{\beta}) = R_0 \left[1 + \sum_{\lambda \geq 2} \beta_{\lambda} Y_{\lambda 0}(\theta) \right] \quad (3)$$

The β -expansion defined by Eq. (3) is usually limited to the low order coefficients: β_2 (quadrupole), β_3 (octupole) and β_4 (hexadecapole) degrees of freedom. However, for significantly elongated and mass-asymmetric shapes, it is necessary to have liberty to choose higher order multiples. In our code the upper limit on the multiples is $\lambda_{\max} = 9$.

2.2. Collective energy

Collective energy V is calculated for a given nucleus by the macroscopic--microscopic model developed by Strutinsky [4]. In this model the fission barrier energy is split into two parts: the smooth macroscopic E_{macr} part and the microscopic energy consisting of the shell δE_{shell} and pairing δE_{pair} energies.

$$V = E_{\text{macr}}(\beta) + \delta E_{\text{shell}}(\beta) + \delta E_{\text{pair}}(\beta, \Delta) \quad (4)$$

The smooth part of energy E_{macr} includes various nuclear drop models. In this study we tested the Myers - Swiatecki drop model [7], the droplet model [8], the Folded - Yukawa plus exponential model [9] and the Lublin-Strasbourg drop model (LSD) [10].

The latest and most promising LSD model constitutes a revised and improved version of the nuclear liquid drop, in which the corresponding parameters of the extended classical energy formula were adjusted to the currently known nuclear masses and fission barrier heights.

The shell energy correction δE_{shell} depends on the form of the single-particle potential. There is a common belief that the deformed Woods-Saxon potential with a universal set of parameters [6] reflects the proper behavior of the fission barrier as a function of the deformation.

Pairing energy δE_{pair} is the third component of total energy. Two residual pairing interaction models were examined. In the first approach we used the monopole pairing (with constant matrix elements $\langle \nu \bar{\nu} | \hat{V}_{\text{pair}} | \mu \bar{\mu} \rangle = \text{const}$). In the second approximation, the pairing matrix elements were calculated with the δ force [11].

2.3. Various nuclear liquid-drop models.

If we normalize the energy to zero at spherical shape [8], the formulae for liquid drop model [3] comprising the surface and Coulomb energy can be written:

$$E_{LD}(\hat{\beta}) = E_0^C (B_C(\hat{\beta}) - 1) + E_0^S (B_S(\hat{\beta}) - 1) \quad (5)$$

The numerical value of the parameters E_0^C and E_0^S is taken from a mass formula [3]. The entire deformation dependence is contained in $B_S(\hat{\beta})$ and $B_C(\hat{\beta})$ coefficients. They both can be expressed by two or three dimensional integrals:

$$B_S = \frac{1}{4\pi R_0^2} \oint_S dS \quad (6)$$

$$B_C = \frac{1}{32\pi^2 R_0^5} \oint_V W(r) dV \quad (7)$$

where $W(r)$ denote the Coulomb potential:

$$W(r) = \oint_V \frac{dr'}{|\vec{r} - \vec{r}'|} \quad (8)$$

The improved version of the liquid drop model was proposed by Myers and Świątecki [5] in 1969 as the liquid drop model extension in the form of curvatures and corrections resulting from non - uniform distribution of charges on nucleus surface.

Macroscopic energy can express in that model as:

$$\begin{aligned} E_{\text{DROPLET}}(\hat{\beta}) = & b_S (B_S(\hat{\beta}) - 1) + b_{\text{CUR}} (B_{\text{CUR}}(\hat{\beta}) - 1) + b_C (B_C(\hat{\beta}) - 1) + \\ & + b_R (B_R(\hat{\beta}) - 1) + b_w (B_w(\hat{\beta}) - 1) \end{aligned} \quad (9)$$

The free parameters included in this Equation (b_i , $i = s, c, \text{cur}, r, w$) are determined phenomenologically by their adjustment to nuclear masses, multipolar moments and barriers for fission. The functions B_i ($i = s, c, \text{cur}, r, w$) depend

on shapes of nuclei only. Two of them i.e. relative surface energy B_S and relative Coulomb energy B_C are defined as in the liquid drop model (Eqs. 5, 6).

Coefficients B_{CUR} is associated with the average curvature of nucleus surface, B_R is associated with non-uniform charge distribution, and B_W is used to describe the non-uniformity of charge distribution on the nucleus surface. The explicit equations for function B_i in the liquid droplet model are performed in [8].

The Yukawa - plus - exponential model [9] developed in 1979 it is a more universal model of macroscopic energy of nucleus. The following term describing the broadening of nucleus surface is added to the surface energy E_S and relative Coulomb energy E_C in that model:

$$E_Y = -\frac{c_S}{8\pi^2 R_0^2 a^3} \int \frac{e^{-\frac{|r-r'|}{a}}}{|r-r'|} d^3r d^3r' \quad (10)$$

with R_0 constituting the nucleus radius with sharp cut-off of matter density on the surface and a constituting the broadening function range (for $a \rightarrow 0$ this term disappears). The well-known fact that the matter density on the surface of actual nuclei is not changed abruptly, but it decreases in accordance with the Yukawa model was considered in the present model.

The macroscopic nuclear energy according to the curvature dependent LSD model proposed in [10] is provided in the formula bellow:

$$E_{LSD}(\hat{\beta}) = b_S(1 - \kappa_S I^2) A^{\frac{2}{3}} (B_S(\hat{\beta}) - 1) + b_{CUR}(1 - \kappa_{CUR} I^2) A^{\frac{1}{3}} (B_{CUR}(\hat{\beta}) - 1) + E_0^C (B_C(\hat{\beta}) - 1) \quad (11)$$

Definitions of the curvature B_{CUR} , Coulomb B_C and surface B_S coefficients remain the same as in the standard drop model (Coulomb and surface coefficients) or in the Droplet model (curvature coefficient B_{CUR}).

Such a liquid drop formula results in rms mass deviations equal to 0.698-MeV for binding energies of 2766 nuclei with $Z > 8$ and $N > 8$ and rms = 0.88 MeV for 40 fission barrier heights experimentally known [10]. As it was shown in [12], the LSD model seems to be comparable in accuracy to the Thomas - Fermi macroscopic model and can be used as a fast and exact tool for calculation of the properties of the nuclei.

2.4. Pairing model

Two models of residual pairing interaction are studied in our work. The first approach is based on the use of monopole pairing, with constant matrix elements $\langle v\bar{v} | \hat{V}_{pair} | \mu\bar{\mu} \rangle = G$, while in the other approximation the pairing matrix elements are calculated with the δ -force, and they are state dependent [11].

The first approximation of the monopole type leads to the averaging of the superconductive properties of nuclei and reflects the structure of nucleon pairs rather weakly. A more realistic model consists of state-dependent pairing matrix elements $G_{\mu\nu} = \langle v\bar{v} | \hat{V}_{pair} | \mu\bar{\mu} \rangle$, where the pairing interaction \hat{V}_{pair} takes the following form: [13]

$$\hat{V}_{pair} = -V_0 \frac{1 - \sigma_1 * \sigma_2}{4} \delta(\vec{r}_{12}) \quad (12)$$

The following values of pairing strengths V_0 were used [11]:

$$V_0^p = 216 \text{ MeV } fm^3 \text{ and } V_0^n = 218 \text{ MeV } fm^3 \quad (13)$$

for protons and neutrons respectively.

The residual pairing interaction is treated in the BCS and Lipkin-Nogami (LN) approximation. In the case of the Lipkin-Nogami (LN) [14, 15] model the fluctuations of the particle number are reduced by adding the quadratic term $-\lambda_2 (\hat{N} - \langle \hat{N} \rangle)^2$ to the Hamiltonian \hat{H} and by minimizing the average energy with respect to λ_2

The procedure offers the following expression for the newly corrected energy:

$$E_{LN} = E - \lambda_2 \langle \Psi | \Delta \hat{N} | \Psi \rangle \quad (14)$$

where

$$\lambda_2 = \frac{\langle \Psi | (\Delta \hat{N})^2 | \Psi \rangle}{\langle \Psi | (\Delta \hat{N}) | \Psi \rangle}, \quad \Delta \hat{N} = \hat{N} - \langle \Psi | \hat{N} | \Psi \rangle \quad (15)$$

and \hat{N} the number operator and Ψ is the BCS ground state.

2.5. Woods-Saxon potential

The one-body Woods-Saxon Hamiltonian formula consists of the kinetic energy term T , the potential energy V^{WS} , the spin-orbit term V_{so}^{WS} and the Coulomb potential V_{Coul} for protons:

$$H^{WS} = T + V^{WS}(\vec{r};\beta) + V_{so}^{WS}(\vec{r};\beta) + \frac{1}{2}(1 + \sigma_3)V_{Coul}(\vec{r};\beta) \quad (16)$$

In the above equation

$$V^{WS}(\vec{r};\beta) = \frac{V_0 \left[1 \pm \kappa \frac{N-Z}{N+Z} \right]}{1 + \exp \left[\frac{dist(\vec{r};\beta)}{a} \right]}, \quad (17)$$

and

$$V_{so}^{WS}(\vec{r};\beta) = -\lambda \left(V^{WS} \cdot \vec{p} \cdot \vec{s} \right), \quad (18)$$

where $dist(\vec{r};\beta)$ denotes the distance of a point \vec{r} from the surface of the nucleus whereas V_0, κ, a, λ , are adjustable constants.

The Coulomb potential V_{Coul} is assumed to be that of the nuclear charge equal to $(Z-1)e$ and uniformly distributed inside the nuclear surface. In our calculations, we used the Woods-Saxon Hamiltonian formula with the so-called “universal” set of its parameters [6] which were adjusted to the single – particle levels of odd-A nuclei with $A \geq 40$.

2.6. Fission process

Fission is treated as a tunneling through the collective potential energy barrier within the multidimensional deformation parameter space. The spontaneous-fission half-life is inversely proportional to the probability of penetration of the barrier:

$$T_{sf} = \frac{\log 2}{n} \frac{1}{P} \quad (19)$$

Here, n is the number of *assaults* of the nucleus on the fission barrier per unit of time. For the vibration frequency $\hbar\omega_0 = 1 \text{ MeV}$ assumed in our study one can obtain $n = 10^{20.28} \text{ s}^{-1}$. The tunneling probability P in a one-dimensional WKB [] semi-classical approximation is derived using the following formula:

$$P = \left(1 + e^{2S} \right)^{-1} \quad (20)$$

where $S(L)$ is the action integral evaluated along the fission path $L(s)$, which minimizes the reduced action in the multidimensional collective space:

$$S(L) = \int_{s_2}^{s_1} \left\{ \frac{2}{\hbar} B_{eff}(s) [V(s) - E] \right\}^{1/2} ds \quad (21)$$

Effective inertia associated with the fission motion along the path $L(s)$ is

$$B_{eff}(s) = \sum_{k,l} B_{kl}(\{\beta_k\}) \frac{d\beta_k}{ds} \frac{d\beta_l}{ds} \quad (22)$$

where ds denotes the path-length element in the collective space. The integration limits s_1 and s_2 correspond to the classical turning points, determined by the equation $V(s) = E$, where E is the total energy of the nucleus. Collective tensor components B_{kl} are calculated in the adiabatic cranking model [17] and are dependent on collective coordinates.

The dynamic calculation of the T_{sf} means a quest for the trajectory L_{min} which fulfills the principle of stationary action:

$$\delta S(L) = 0 \quad (23)$$

To minimize the action integral we used the multi-dimensional dynamic-programming method (MDP) [18].

3. Results

3.1. Macroscopic models

Parameters of the macroscopic part of the energy of the atomic nuclei are usually fitted to experimental masses of nuclei (small deformations). Only the LSD-drop model [10] takes into account the heights of fission barriers. This leads to the effect of good conformities of each model for small deformations and divergences for deformations leading to the fission. This problem is illustrated in Fig. 1. where as an example, the diagrams for potential barriers for various models were made [12].

It can be seen that fission barriers in the liquid drop model [7] are relatively high and wide. It is especially visible in heavier isotopes. This effect leads to considerably longer spontaneous fission half-lives for heavier isotopes [19].

An interesting behaviour of fission barriers obtained with the droplet model [8] can be observed. For lighter isotopes, the barriers are in agreement with the liquid drop ones while for heavier nuclei a tendency to a large reduction of the height and thickness of the barrier can be noticed. In earlier papers dealing with the spontaneous fission half-lives this tendency was connected with an abrupt reduction of T_{sf} of heavier isotopes [20].

The Yukawa – plus - exponential model offers the macroscopic fission barriers similar to that of the drop model. However, the barrier heights are slightly lower in the case of heavy isotopes. This decrease in barrier heights influences spontaneous fission half-lives T_{sf} : for heavier isotopes T_{sf} becomes considerably longer. A similar effect was observed in this study [21, 22].

The barriers for the new LSD model [10] change very weakly with the increasing neutron number N and become only slightly higher and wider.

The studies conducted show that different models for the smooth part of the energy significantly modify the height and the width of the fission barrier and consequently spontaneous fission half life.

Therefore it is important to use the correct model especially for large deformations. It seems that the LSD-drop model is the best.

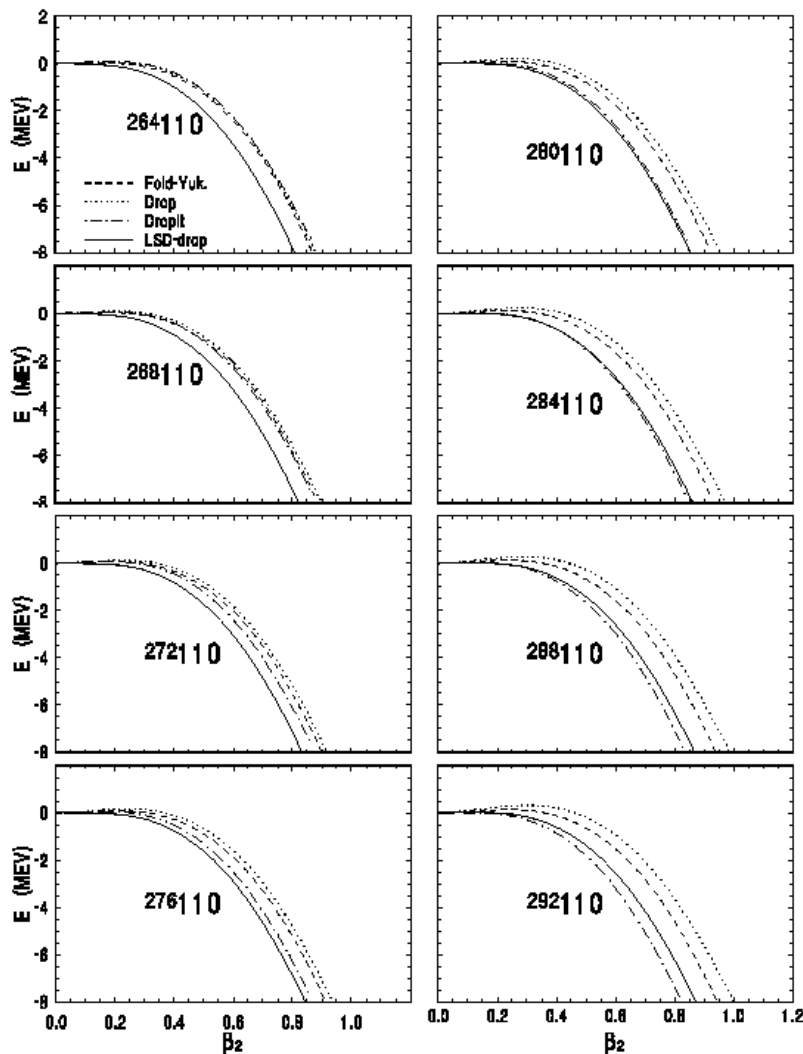


Fig. 1. Diagrams illustrating macroscopic barriers in Drop, Droplet, Folded-Yukawa (Fold-Yuk) and Lublin - Strasbourg (LSD-drop) models for various isotopes of nucleus $Z = 110$.

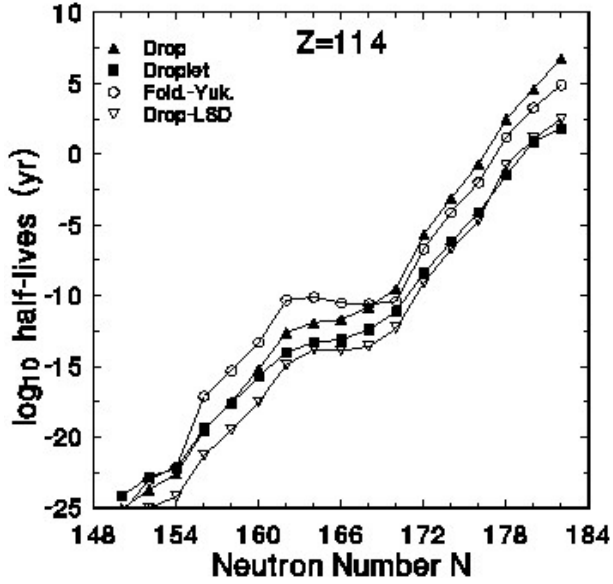


Fig. 2. Spontaneous fission half-lives T_{sf} (in years) for even-even isotopes with the atomic number $Z = 114$ plotted as a function of the neutron number N .

illustration of the effect of different pairing models we show the barriers and spontaneous fission half lives for $Z = 112$ and $Z = 116$ isotopes. The barriers of $Z = 112$ and 116 isotopes are shown in Fig. 2 for both models: $G = \text{const}$ and δ - interaction). Unprojected ($G = \text{const}$ and $\delta + \text{BCS}$) and particle number projected ($G = \text{const} + \text{LN}$ and $\delta + \text{LN}$) methods are taken into account.

One can see that in all pairing models examined barriers height changes are approximately similar together along the neutrons number N .

In the case of δ - pairing interaction, spontaneous fission barriers become higher (the coupling constant V_0 estimated in [11] is probably too high) than in the case of the $G = \text{const}$ model. Our study indicates that model pairing forces weakly influences on the height of fission barriers. The barrier heights shown in Fig. 3 change more smoothly as a function of N in the case of LN projected energies, as compared to the case without projection.

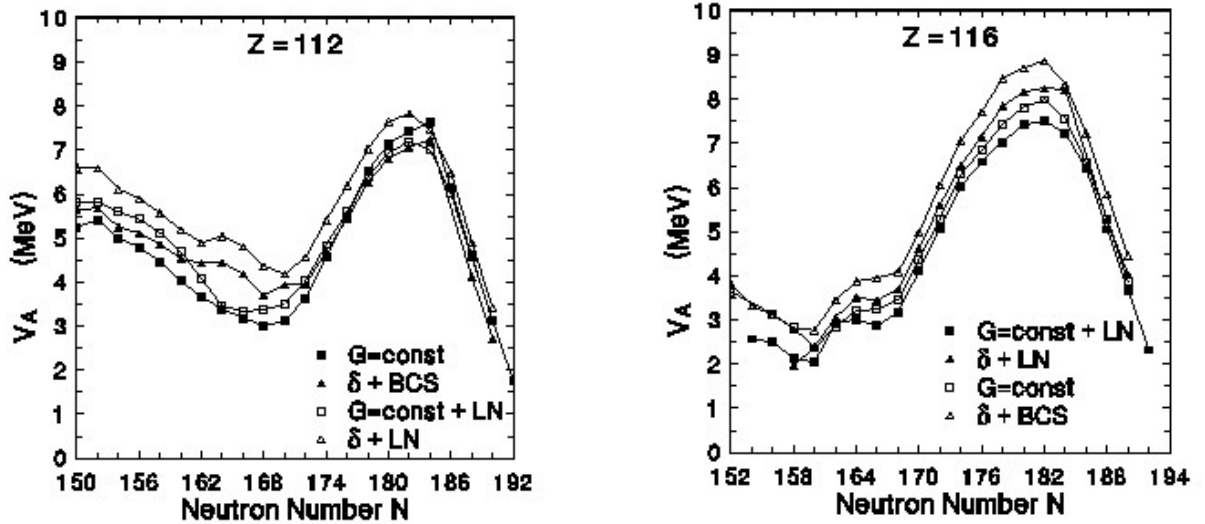


Fig. 3. Barrier height of $Z = 112$ and 116 isotopes for the case of different pairing models.

The spontaneous fission half-lives of the $Z = 112$ and 116 isotopes are shown in Fig. 4. As in the case of fission barriers, the LN projected T_{sf} results are smoother, as compared to the unprojected ones. The most important finding is that different pairing models substantially influence the spontaneous fission half-lives (3-5 orders of magnitude). The differences between the projected and unprojected models are smaller (1 - 2 orders). Projected results are a quite close to the experimental data.

In Fig. 2 the estimates of the spontaneous fission half-lives T_{sf} for isotopes $Z = 114$ are showed. Theoretical results are obtained using the four models for macroscopic energy as referred to above.

The data obtained in the liquid drop model are represented by full triangles and the results obtained with the droplet model by squares. The estimates made with the LSD are marked with open triangles. It is seen that the spontaneous fission half-lives differ considerably depending on the model used (1-5 orders of magnitude).

The calculations for the whole region showed that for the liquid drop and folded Yukawa models the results are too large as compared to the experiment, while these for the droplet and LSD models are closer to the measured T_{sf} .

3.2 Influence of pairing forces on fission

Pairing plays an important role in macroscopic-microscopic description of the fission process. We discuss two kinds of pairing models: monopole ($G = \text{const}$) and state dependent (δ -type force). As an

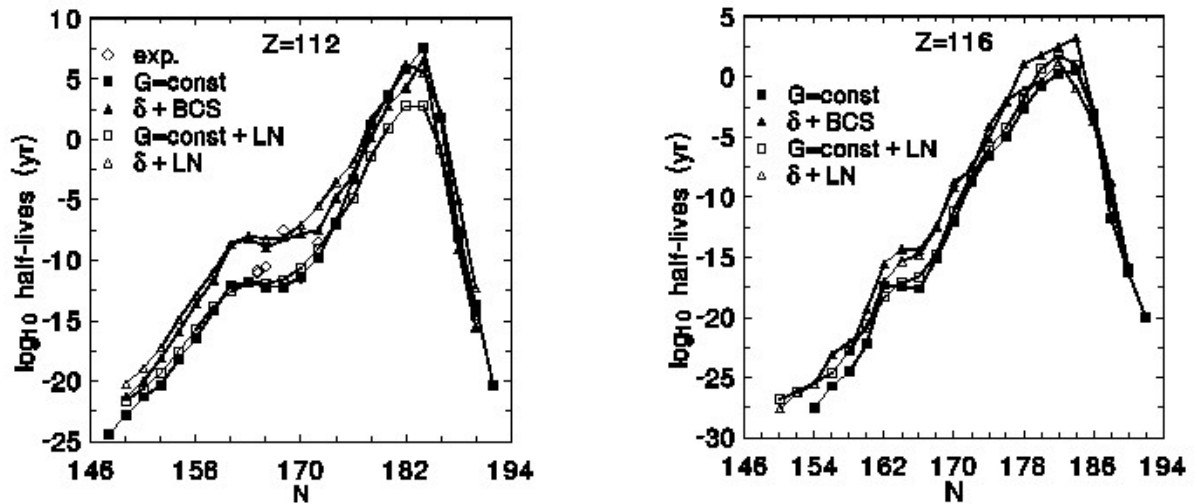


Fig. 4. Spontaneous fission half-lives T_{sf} (in years) for even-even isotopes with atomic number $Z = 112$ and 116 plotted as a function of the neutron number N .

4. Conclusions

Spontaneous fission half lives strongly depended on two main factors: potential energy represented by the collective energy V_{coll} and kinetic energy proportional inversely to the so called collective mass parameter B_{kl} for multipole vibrations.

In our paper in the MM model we examined different forms of collective energy V_{coll} . Our studies show that macroscopic energy influences significantly calculated spontaneous fission half-lives T_{sf} (1 - 5 orders of magnitude).

For the liquid drop and folded Yukawa models the results of T_{sf} are too large as compared to the experiment, while these for the droplet and LSD models are closer to the measured T_{sf} .

The LSD and droplet model seems to be suitable and can be used as a fast and exact tool for calculation of the spontaneous fission half lives T_{sf} .

The different pairing models substantially influence the spontaneous fission half-lives (3 - 5 orders of magnitude).

The fission barriers of the δ -pairing force model are similar to that of the classical pairing, although they are slightly higher.

The differences between the projected and unprojected models are smaller (1 - 2 orders). The state dependent δ -type force, significantly influences the spontaneous fission half lives. At the same time, the isotopic systematic of T_{sf} does not change.

The LN fission barriers are few hundreds of keV lower than the barriers calculated within the BCS approach. Differences between projected and unprojected results of T_{sf} are 1 - 2 orders of magnitude.

Investigations of the pairing interaction and the macroscopic nuclear energy should continue in order to obtain the proper coupling constants and the most appropriate fission barriers and spontaneous fission half lives.

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