Algorithm and numerical modelling of macroscopic barriers for fission

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Abstract

A practical computing algorithm has been developed for calculating the macroscopic energy of nuclei. Four different models of the macroscopic energy are examined and their influence on the results is discussed.

The results of the calculations are presented in the form of curves to illustrate how the different macroscopic models influence on the spontaneous fission energy barriers of super-heavy nuclei.

1. Introduction

For the first time, the charged liquid-drop model was successfuly applied about 70 years ago [1]. Brilliant employment of the nuclear drop concept was used to explain the nuclear fission phenomenon [2].

Since then, many papers have been devoted to the nuclear model formalism and its improvements. Since then those times, various new terms in the corresponding energy expressions have been proposed.

The contemporary expressions commonly used for the nuclear energy are given by the liquid drop model [3], the droplet expansion [4], the folded-Yukawa plus exponential approximation [5] and recently developed the Lublin-Strasbourg drop (LSD) [6]. The LSD model represents the revised and improved version of the charged liquid drop formula, in which the parameters were adjusted to the known masses and isotopes.

Although, in the above mentioned formulae, the various new terms have been proposed, but the basic concept of the charged liquid drop which could deform and fission remained valid.

The formulae from [3-6] have been used to construct a universal computing algorithm, written in FORTRAN 77, allowing to calculate the nuclear liquid drop energy in different, popular in literature models.

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It is well known that the smooth part of the nuclear energy, represented by the various drop models considerably influences on the spontaneous fission half-lives (T_{sf}) [7-8].

The code introduced in our publication is a very important unit of programme to obtain the estimations of spontaneous fission (T_{sf}) as well as the α-decay half-life times of the heavy and super-heavy nuclei within the macroscopic-microscopic model [9-12].

2. Theory

2.1. Nuclear shape parametrisation

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

$$\sum : f(r,\theta,\varphi) = 0 . \tag{1}$$

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

$$R(\theta,\varphi,\hat{\alpha}) = R_0[1 + \sum_{\lambda \geq 2}\sum_{\mu} \alpha_{\lambda\mu} Y_{\lambda\mu}(\theta,\varphi)]. \tag{2}$$

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

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

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. But for strongly elongated and mass-asymmetric shapes, it is necessary to have a freedom of choosing higher order multipoles. In our code the upper limit on the multipoles is $\lambda_{max} = 9$.

2.2. Various nuclear liquid-drop models.

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

$$E_{LD}(\hat{\beta}) = E_0^C (B_C(\hat{\beta}) - 1) + E_0^S (B_S(\hat{\beta}) - 1) . \tag{4}$$

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

$$B_S = \frac{1}{4\pi R_0^2} \oint_S dS , \tag{5}$$

$$B_C = \frac{1}{32\pi^2 R_0^5} \oint_V W(r)dV \tag{6}$$

here *W(r)* denote the Coulomb potential:

$$W(r) = \oint_V \frac{dr'}{|\vec{r} - \vec{r}'|} . \tag{7}$$

The improved version of 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 the nucleus surface.

The macroscopic energy can expressed in that model as:

$$E_{DROPLET}\left(\hat{\beta}\right) = b_S\left(B_S\left(\hat{\beta}\right)-1\right) + b_{CUR}\left(B_{CUR}\left(\hat{\beta}\right)-1\right) + b_C\left(B_C\left(\hat{\beta}\right)-1\right) + \\ b_R\left(B_R\left(\hat{\beta}\right)-1\right) + b_w\left(B_W\left(\hat{\beta}\right)-1\right). \tag{8}$$

The free parameters included in this Equation (b_i, i=s, c, 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, cur, r, w) depend on nuclei shapes only. Two of them i.e. the relative surface energy B_S and the relative Coulomb energy B_C are defined as in the liquid drop model (Eqs. 5, 6).

The coefficient B_{CUR} is associated with the average curvature of nucleus surface, B_R is associated with the non-uniform charge distribution, 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 drop model are as follows:

$$B_S = \frac{1}{4\pi R_0^2} \oint_S dS , \tag{9}$$

$$B_C = \frac{1}{32\pi^2 R_0^5} \oint_V W(r)dV , \tag{10}$$

$$B_R = \frac{1575}{64\pi^3 R_0^7} \oint_V [W(r)]^2 dV , \tag{11}$$

$$B_W = \frac{225}{64\pi^3 R_0^6} \oint_V [W(r)]^2 dV , \tag{12}$$

$$B_{CUR} = \frac{1}{8\pi R_0} \oint_S dS . \tag{13}$$

The integration is carried out over the nucleus surface S or over the volume V. The value *W(r)* is proportional to the Coulomb potential (Eq. 7).

The Yukawa – plus – exponential model [5] presented in 1979 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 the relative Coulomb energy E_C in that model:

$$E_Y = -\frac{c_S}{8\pi^2 R_0^2 a^3} \int \frac{e^{-\frac{|r-r'|}{a}}}{|r-r'|} d^3r d^3r' \tag{14}$$

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 known fact that the matter density on the surface of actual nuclei is not changed abruptly, but decreased in accordance with the Yukawa model has been considered in the present model.

The macroscopic nuclear energy according to the curvature dependent LSD model proposed in [6] is given by the formula:

$$E_{LSD}\left(\hat{\beta}\right) = b_S \left(1 - \kappa_S I^2\right) A^{2/3} \left(B_S\left(\hat{\beta}\right) - 1\right) +$$
$$b_{CUR} \left(1 - \kappa_{CUR} I^2\right) A^{1/3} \left(B_{CUR}\left(\hat{\beta}\right) - 1\right) + E_0^C \left(B_C\left(\hat{\beta}\right) - 1\right). \tag{15}$$

Definitions of the curvature B_{CUR}, Coulomb B_C and the 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}. The parameters appearing in Eq. 7 are the following

$$b_V = -15.4920 \text{ MeV},$$
$$\kappa_V = 1.8601,$$
$$b_S = 16.9707 \text{ MeV},$$
$$\kappa_S = 2.2938, \tag{16}$$
$$b_{CUR} = 3.8602 \text{ MeV},$$
$$\kappa_{CUR} = -2.3764.$$

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.

3. Program organization

The program has been prepared in FORTRAN77, but it is also compatible with the previous versions of that language.

The file contains the module of main program ENERGY and several procedures associated with that program.

The whole program may be subdivided into three main blocks:

1. The main program named ENERGY (main) reading the data, opening the required files and calling the procedures LIQDROP, ENZ, YUKAWA, ELSD.
2. Four principal procedures, counting the nucleus energy in the four applied models:
   – LIQDROP – liquid drop model,

- – ENZ – liquid droplet model,
- – YUKAWA –Yukawa + exponential model,
- – ELSD – Lublin-Strasbourg liquid drop model.
3. Auxiliary procedures
   - – QG32 – calculating the integrals using 32-point Gauss-Legendre' formula,
   - – QG16 – ditto, but for 16-point Gauss formula,
   - – QG12 – ditto, but for 12-point Gauss formula,
   - – CEL2 – calculating the elliptical integrals; first and second kind,
   - – BC1 – calculating the constant value B_c in liquid drop model,
   - – FPBC1 – defining the integrand in calculation of B_c,
   - – BS1 – calculating the constant value B_s in liquid drop model,
   - – FPBS1 – defining the integrand in calculation of B_s,
   - – COEF – calculating the remaining factors in liquid drop model,
   - – RSUR – calculating the value of nucleus radius vs. angle θ.

The procedures BC1, BS1 and a part of procedure COEF, liquid droplet coefficients and other required coefficients for the remaining macroscopic nucleus models are presented below:

```
C*************************** BS1 ***************************
FUNCTION BS1(CMALE)
   COMMON /DEF/ BET1,BET2,BET3,BET4,BET5,BET6,BET7,BET8,BET9
C
C      BS1 CALCULATES CONSTANT BS
C
   EXTERNAL FPBS1
   XG=1.
   IF(ABS(BET3)+ABS(BET5)+ABS(BET7)+ABS(BET9).EQ.0.) XG=0.
   XD=-1.
   UM1=(XG-XD)*0.5
   CALL QG32(XD,UM1,FPBS1,RA)
   CALL QG32(UM1,XG,FPBS1,RB)
   RES=RA+RB
   BS1=RES*CMALE**2
   IF(XG.EQ.1.) BS1=BS1*0.5
C
   RETURN
   END


C*************************** BC1 ***************************
FUNCTION BC1(CMALE)
C
```

```
C     BC1 CALCULATES CONSTANT BC
C     CALLED FROM INTRO
C
      COMMON /DEF/ BETA1,BETA2,BETA3,BETA4,BETA5,BETA6,BETA7,
     *         BETA8,BETA9
      EXTERNAL FPBC1
      DATA PI /3.14159265/
      XG=PI
      IF(ABS(BETA3)+ABS(BETA5)+ABS(BETA7)+ABS(BETA9).EQ.0.) XG=PI/2.
C
      CALL QG16(0.,XG,FPBC1,RES)
      BC1=RES*3./4./PI*CMALE**5
      IF(XG.EQ.PI) BC1=BC1*0.5
C
      RETURN
      END


C
C.....EVALUATION OF THE LIQUID DROPLET PARAMETERS.....................
C
      CALL QG16(-1.,1.,RIG,W)
      BJ=0.375*W
      CALL QG16P(-1.,1.,CUR,W)
      BK=0.25*W
      IF(I.EQ.2) RETURN
      CALL QG12(-1.,1.,WDS,W)
      BP=3./(8.*PI)*W
      BV=6.*BC*BS-5.*BP
      CALL QG12(-1.,1.,WSDS,W)
      BQ=9./(32.*PI**2)*W
      BW=25.*BQ-60.*BC*BP+36.*BC**2*BS
      CALL QG12(-1.,1.,WBM,W)
      BM=315./(544.*PI*PI)*W
      BR=85.*BM-84.*BC**2
      RETURN
      END
```

The application of Gauss procedures for integration with various numbers of knot points should be emphasized, owing to its impact on computation time. The procedures have been tested in order to maintain the error of obtained macroscopic nucleus energy $\delta \leq 0.001$MeV in the whole range of applied deformations β_λ.

The application of the basic procedures used for energy values calculations in various models has been illustrated by means of the following code fragment.

```
C
   DO 105 IJ=1,NJ
   IN = IN0 + (IJ - 1) * 2
   IA = IN + IZ
   A = IA
C
C    WRITE (IJ+31,103) IZ, IA, NJ
C    WRITE (IJ+31,104)
C
C   ************** YUKAWA *********************
C
   CALL YUKMOD(Z,A,OM,BC,YS,YSC,ECOUL,YXMAS0,YDEF)
   YXMAS = YXMAS0 + YDEF
C
C   *************** DROP **********************
C
   CALL LIQDROP(Z,A,BS,BC,DBSURF,DBCOUL)

   DROP = DBCOUL + DBSURF
C
C   ************** DROPLET ********************
C
   DLIQQP=ENZ(Z,A,BS,BK,BC,BV,BW,BR)
   DLIQQK=ENZ(Z,A,1.,1.,1.,1.,1.,1.)
   DLIQQ=DLIQQP - DLIQQK
C
C   ************** DROP LSD********** *********
C
   DDLSD=ELSD(Z,A,BS,BK,BC)
C
C   ********************************************
C
C
   105 CONTINUE
```

Input data

The creation of a text file with the name DATA.INP is required for the input data in the same directory. The input data is organized as NAMELISTE. Refer to the data sequence example presented below:

```
$JADDAT  IZ=100,     IA=260,     NJ=8, $END
$DEFOR  NBET2=24, BETA2D= 0.0, DBETA2=0.05,
        NBET4=12, BETA4D=-0.08, DBETA4=0.04, $END
```

Where

IZ – nucleus atomic number

IA – nucleus mass number

NJ – nucleus isotopic number

NBET2 – number of deformation points β_2

BETA2D – initial deformation value β_2

DBETA2 – deformation change step β_2

NAMELIST $DEFOR encompasses only the deformations to be actually considered in our calculations. Remaining deformations, not specified in the list, will be equal to zero. The macroscopic energies for even – even nuclei, with the atomic number of IŻ and the mass numbers of IA, IA + 2, ... successively are calculated by the program until NJ range is exhausted.

The deformation points create a multidimensional lattice (in our example two – dimensional only β_2, β_4) with the initial values constituting (BETA2D and BETA4D) correspondingly and modified every (DBET2, DBET4), with the ranges specified in the variables NBET2 and NBET4.

Organization of the results obtained by means of program

The macroscopic energies for even – even nuclei, with the atomic number of *IZ* and the mass numbers of *IA, IA+2, IA+4,...* successively are calculated by the program until *NJ* range is exhausted.

The deformation points creates a multidimensional lattice (in our example two – dimensional only β_2, β_4) with the initial values constituting (*BETA2D, BETA4D*) correspondingly and modified every (*DBETA2 and DBETA4*), with the ranges specified in the variables *NBET2* and *NBET4*.

The purpose of ENERGY program is to obtain the macroscopic energies of the nuclei for the scope of deformations occurring in the case of nuclear fission. It can be easily stated [9,10] that the quadrupole deformation β_2 responsible for increasingly elongated shape and hexadecapole deformation β_4 responsible for developing of narrowing (necking) leading to the nucleus breaking into two fragments, are the most important deformations in the case of fission.

The role of other kinds of deformations may be also significant, for instance deformation β_3 leading to the unsymmetrical distribution of masses or β_5 and β_6 affecting the value of energy minimum and the thickness of fission barrier [12].

In order to enable general considerations, the program has been adapted to the range of deformations between β_2 and β_9 (refer to Equation 3).

ENERGY program constitutes a part of a wider project performed in order to calculate the lifetimes of nuclei being subject to fission. Refer to studies [8-12]

for the results. Therefore the results are organized in the manner enabling further data processing i.e. in the form of files containing formatted tables containing required numerical data. The files are automatically generated by the program and provided with the name composed of atomic number and extension in the form of neutrons number for the specific isotope e.g. the file with the name 100.154 with the results for the Fermium isotope ($Z = 100$, $N = 154$). Therefore the results can be easily applied for further processing. The block generating the names of needed files is illustrated by means of the following code fragment.

```
C
   DO 110 INJ=1,NJ
   IN0=IA - IZ
   IN=IN0+(INJ-1)*2
   WRITE(CHZ,'(I3.3)') IZ
   WRITE(CHN,'(I3.3)') IN
   OPEN(UNIT=31+INJ,FILE=CHZ//'.'//CHN)
   110 CONTINUE
C
```

Refer to Figure 1 for the example of results fragment for the nucleus $Z=100$, $N=158$. The meaning of the successive columns is as follows:

BET1..BET6 – nucleus deformations,
YUK – energy in YUKAWA-FOLDED model,
DROP – energy in droplet model,
DROPLET – energy in small droplet model,
DLSD – energy in Lublin-Strasbourg Drop (LSD) model.

The results presented below are used for preparation of nucleus macroscopic energy map.

```
*************************************************************************
*                         Z = 100  N = 158                              *
*************************************************************************
* BET1  BET2  BET3  BET4  BET5  BET6    YUK     DROP    DROPLET  DLSD   *
*************************************************************************
*  0.00  0.00  0.00 -0.08  0.00  0.00   1.391   2.089   2.247   1.957  *
*  0.00  0.00  0.00 -0.04  0.00  0.00   0.349   0.523   0.569   0.491  *
*  0.00  0.00  0.00  0.00  0.00  0.00   0.001   0.001   0.010   0.001  *
*  0.00  0.00  0.00  0.04  0.00  0.00   0.349   0.522   0.569   0.492  *
*  0.00  0.00  0.00  0.08  0.00  0.00   1.386   2.068   2.229   1.950  *
*  0.00  0.00  0.00  0.12  0.00  0.00   3.093   4.595   4.936   4.336  *
*  0.00  0.00  0.00  0.16  0.00  0.00   5.447   8.050   8.636   7.605  *
*  0.00  0.00  0.00  0.20  0.00  0.00   8.409  12.362  13.244  11.688  *
*  0.00  0.00  0.00  0.24  0.00  0.00  11.937  17.451  18.669  16.511  *
*  0.00  0.00  0.00  0.28  0.00  0.00  15.982  23.233  24.821  21.995  *
*  0.00  0.00  0.00  0.32  0.00  0.00  20.491  29.623  31.601  28.060  *
*  0.00  0.00  0.00  0.36  0.00  0.00  25.409  36.538  38.915  34.623  *
*  0.00  0.05  0.00 -0.08  0.00  0.00   1.428   2.123   2.273   1.985  *
*  0.00  0.05  0.00 -0.04  0.00  0.00   0.387   0.567   0.605   0.524  *
*  0.00  0.05  0.00  0.00  0.00  0.00   0.037   0.043   0.043   0.031  *
*  0.00  0.05  0.00  0.04  0.00  0.00   0.375   0.546   0.584   0.506  *
*  0.00  0.05  0.00  0.08  0.00  0.00   1.393   2.058   2.203   1.933  *
```

Fig. 1. The example of results obtained by means of ENERGY program for the Fermium isotope

The tables used for determination of fission static barriers for macroscopic energies for four models being used are another type of the results. The energy for a nucleus has been illustrated as the function of quadrupole deformation β_2, with the minimization of all remaining deformation parameters. Refer to Figure 2 for the example of results fragment for the nucleus $Z = 110$ $N = 150$.

```
*************************************************
*            Z = 110    N = 150                 *
*************************************************
*   BET2     YUK     DROP    DROPLET    DLSD     *
*************************************************
*                                               *
*   0.00    0.001    0.001    0.009    0.001     *
*   0.05    0.035    0.040    0.046    0.030     *
*   0.10    0.129    0.146    0.141    0.105     *
*   0.15    0.269    0.307    0.284    0.217     *
*   0.20    0.446    0.511    0.463    0.356     *
*   0.25    0.646    0.747    0.665    0.509     *
*   0.30    0.860    1.003    0.880    0.670     *
*   0.35    1.078    1.272    1.090    0.823     *
*   0.40    1.214    1.417    1.161    0.845     *
*   0.45    1.321    1.546    1.218    0.849     *
*   0.50    1.407    1.663    1.263    0.833     *
*   0.55    1.470    1.766    1.293    0.799     *
*   0.60    1.451    1.776    1.179    0.632     *
*   0.65    1.333    1.664    0.984    0.380     *
*   0.70    1.195    1.549    0.795    0.122     *
*   0.75    0.934    1.320    0.430   -0.298     *
*   0.80    0.619    0.998    0.039   -0.756     *
*   0.85    0.201    0.646   -0.439   -1.303     *
*   0.90   -0.269    0.148   -0.993   -1.928     *
*   0.95   -0.872   -0.359   -1.606   -2.625     *
*   1.00   -1.533   -0.990   -2.274   -3.370     *
*   1.05   -2.265   -1.641   -3.004   -4.199     *
*   1.10   -3.077   -2.359   -3.735   -5.014     *
*   1.15   -3.978   -3.126   -4.550   -5.942     *
*************************************************
```

Fig. 2. Potential barriers obtained in various models of charged droplet for Z=110 isotope

The numerical results enable the comparison of barriers curves for various models and various isotopes of atomic nuclei in an easy and simple manner. The diagrams for potential barriers for various isotopes of $Z = 110$ nucleus have been illustrated in Figure 3.

On the basis of the presented diagrams it appears that macroscopic potential barriers significantly differ for various isotopes. The differences in energy may be as high as 2MeV, for the deformation $\beta_2 \approx 1.0$ resulting in significantly diversified lifetimes of atomic nuclei, depending on the applied model [8].
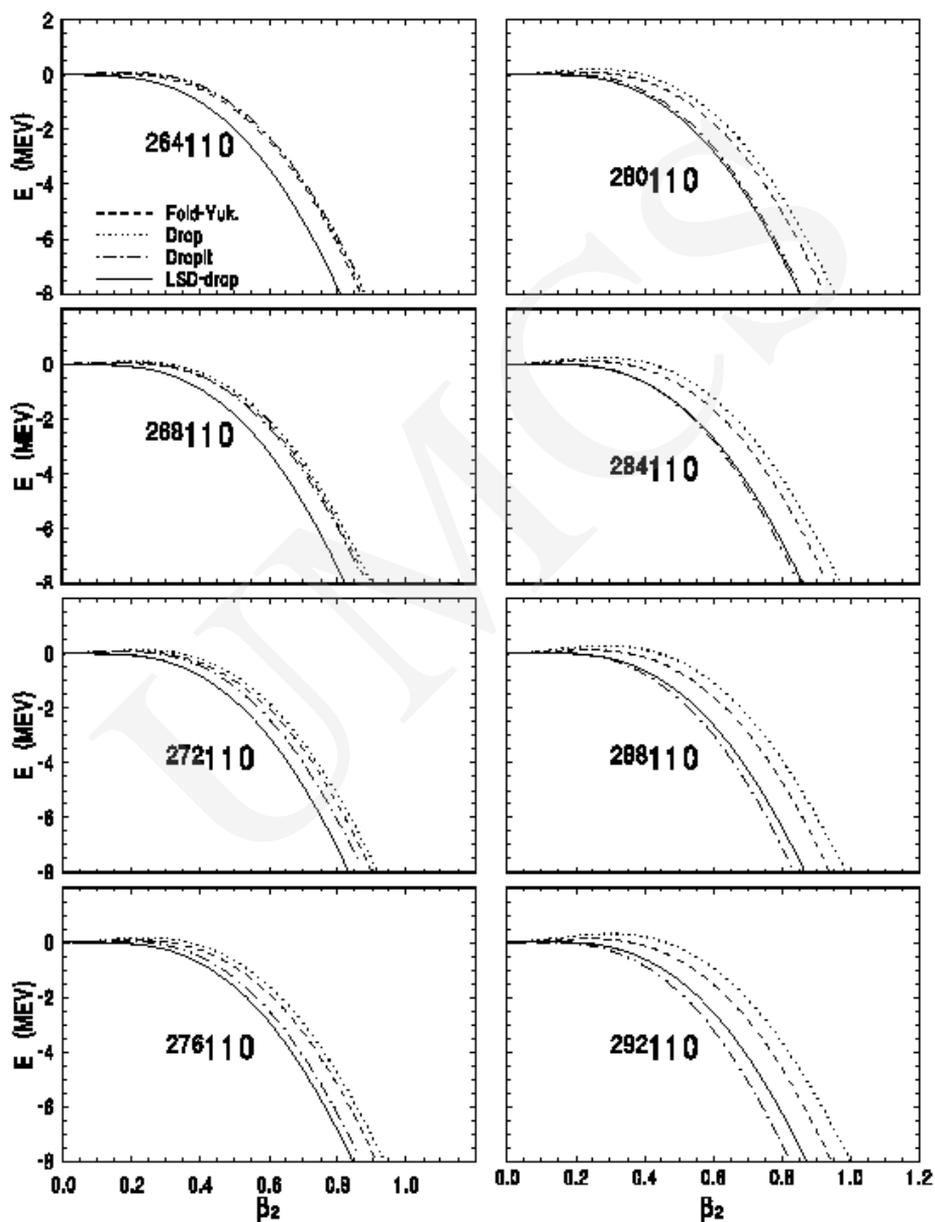
Fig. 3. The diagrams illustrating microscopic barriers in Drop, Droplet, Folded-Yukawa (Fold-Yuk) and Lublin-Strasbourg (LSD-drop) models for various isotopes of nucleus Z = 110

Conclusions

An universal algorithm for calculations of atomic nuclei macroscopic energy has been presented in the present study.

The present algorithm enables the estimation of atomic nuclei potential barriers for four (4) various macroscopic models. Therefore the execution of comparison researches is possible for the models most frequently applied in literature.

The obtained results demonstrate the significant numerical differences, depending on the applied model. The differences in energy may be as high as 2MeV, for the deformations close to the exit point from the barrier ($\beta_2 \approx 1.0$). Therefore the obtained lifetimes for heavy and super-heavy nuclei are significantly modified.

Such results suggest that further intensive efforts are required in order to define the uniform model describing the nucleus energy in the course of fission process.

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