
ELSEVIER

Computer Physics Communications 120 (1999) 57–70

Computer Physics Communications

www.elsevier.nl/locate/cpc

BARRIER code: calculation of fission barriers

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Received 24 October 1998

Abstract

Average values of various nuclear properties are only explained on average by the liquid drop model (where the average might be taken over particle number or, alternatively, over deformation). To reproduce other aspects of nuclear structure, such as ground state spins and energy spectra, it was found elsewhere that a different description is necessary. In this regard, we calculated single particle energies as function of the deformation parameters of an axially deformed Woods–Saxon potential, as input to the shell correction calculations. To obtain the total nuclear energy, it is also necessary to add a pairing energy in order to take into consideration the short range nuclear interactions, which are not taken into account in the mean field approximation. Many works found in the literature deal with potential energy surface and calculated mass by using the Strutinsky method. Bjornholm and Lynn pointed out the impact caused by an adequate description of parametrization in each calculation. In particular, many details in the description of fission processes like fission isomers and angular distribution are sensitive to the choice of the parametrization. Some previous works pointed out the advantages of Cassini ovaloid parametrization for very deformed shape calculations. The numerical code BARRIER, proposed and used in this work, calculates the potential energy surface in the Strutinsky semi-microscopical approach using the Cassini ovaloid shape parametrization for the nuclear potential.

PACS: 24.75.+i; 25.85.–w; 21.60.Cs

Keywords: Fission barrier; Nuclear deformation; Liquid-drop model; Independent-particle model; Nuclear energy levels; Woods–Saxon potential; Cassini ovaloids

PROGRAM SUMMARY

Title of program: BARRIER

Catalogue identifier: ADKF

Program Summary URL:
http://www.cpc.cs.qub.ac.uk/cpc/summaries/ADKF

Program obtainable from: CPC Program Library, Queen's University of Belfast, N. Ireland

Computer for which the program is designed and others on which it is operable:
Computers: Micro-computer with Intel 80386+80387, Intel 80486+80487, and Pentium Intel 150; *Installations:* Linear Accelerator Laboratory, Physics Institute, University of São de Paulo, São Paulo, Brazil

0010-4655/99/$ - see front matter
PII S0010-4655(99)00199-X

Operating systems under which the program has been tested: MS-DOS 6.00, Windows 95 and Windows NT 4.0

Programming language used: Fortran-77 as implemented in Microsoft Fortran 4.0

Memory required to execute with typical data: 8 Mbytes of RAM memory and 100 Mb of Hard disk memory

No. of bits in a word: 16

No. of bytes in distributed program, including test data, etc.: 155912

Distribution format: uuencoded compressed tar file

Keywords: Fission barrier, nuclear deformation, liquid-drop model, independent-particle model, nuclear energy levels, Woods–Saxon potential, Cassini ovaloids

Nature of physical problem
Average values of various nuclear properties are only explained on average by the liquid drop model (where the average might be taken over particle number or, alternatively, over deformation). To reproduce other aspects of nuclear structure, such as ground state spins and energy spectra, it was found elsewhere that a different description was necessary. In this regard, we calculated single particle energies as functions of the deformation parameters of an axially deformed Woods–Saxon potential, as input to the shell correction calculations. To obtain the total nuclear energy, it is also necessary to add a pairing energy in order to take into consideration the short range nuclear interactions, which are not taken into account in the mean field approximation. Many works found in the literature deal with potential energy surface and calculated mass by using the Strutinsky method. Bjornholm and Lynn pointed out the impact caused by an adequate description of parametrization in each calculation. In particular, many details in the description of fission processes, such as fission isomers and angular distribution, are sensitive to the choice of parametrization. Some previous works pointed out the advantages of Cassini ovaloid parametrization for very deformed shape calculations. The numerical code BARRIER, proposed and used in this work, calculates the potential energy surface in the Strutinsky semi-microscopical approach using the Cassini ovaloid shape parametrization for the nuclear potential.

Method of solution
The Cassini ovaloid shape parametrization is used for nuclear average field description. The Woods–Saxon level scheme is obtained at any point of the deformation space. The single-particle level scheme is used to calculate the shell model and pairing corrections to the liquid drop energy in the Strutinsky approach. The BCS method is used in pairing correction calculations, using the 42 levels near the Fermi level. The standard Liquid Drop Model expressions are adopted to calculate the smooth part of the total potential energy.

Restrictions on the complexity of the problem
The use of the standard Liquid Drop Model expressions does not allow the use of the code in calculations with nuclei far from the β-stability line. The implemented parametrization does not contain the γ-nonaxial degrees of freedom. The n–p residual interaction and the exact conservation of partial number of particles is not considered in the usual BCS method implemented in the code.

Typical running time
Depends on the choice for calculations. For a particular set of deformations the running time is approximately 10 seconds.

LONG WRITE-UP

1. Shell correction method

The basic idea, advocated by Myers and Swiatecky [1] and Strutinsky [2], is the following: The averaged behavior of nuclear binding energies or masses, as a function of distortion, mass and charge number, is well reproduced by the liquid-drop mass formula. The success of the liquid drop model, as applied to fission theory where large distortion is involved, and for the calculation of nuclear masses, where large numbers of masses are considered, seems to indicate that if shell effects are averaged out by some means, the potential energy surface as a function of deformation and mass number can be well accounted for in this model. The idea is thus that, if we remove the average trend from the single particle and pairing calculations, and replace it by the liquid-drop formula, we shall obtain a much improved energy surface where the local structure is given by the shell model calculations, and the smooth trends are given by the liquid-drop formulae [3],

$$V(N, Z, \beta) = E_{\mathrm{LD}} + E_{\mathrm{shell}} + E_{\mathrm{pair}}\,. \tag{1}$$

The nuclear energy in the basic liquid drop model is characterized by a volume term proportional to the mass number A, a surface energy term proportional to the surface area, and hence to $A^{2/3}$ for a spherical nucleus, and a Coulomb energy term, proportional to $A^{-1/3}$ for a spherical nucleus,

$$E_{\mathrm{LD}} = -c_1 A + c_2 A^{2/3} f(\mathrm{shape}) + \frac{3}{5}\frac{e^2 Z^2}{r_0 A^{1/3}} g(\mathrm{shape}) .$$

As so far as the fission barrier is concerned, the important terms are the surface energy and Coulomb energy terms, and the sum of their contributions to the liquid drop energy relative to the energy of a spherical liquid drop can be written as

$$E_{\mathrm{LD}}(\mathrm{shape}) - E_{\mathrm{LD}}(0) = \{[f(\mathrm{shape} - 1)] + 2\chi[g(\mathrm{shape}) - 1]\}E_s(0) ,$$

where $E_s(0)$, the surface energy of the spherical liquid drop, is equal to $c_2 A^{2/3}$ and χ, the fissility parameter, is defined as the ratio of the Coulomb energy of a spherical drop to $2E_s(0)$,

$$\chi = \frac{3}{5}\frac{e^2}{r_0}\frac{Z^2/A}{2a_2\{1 - \kappa[(N - Z)/A]^2\}} .$$

The fissility parameter, and hence the values of the coefficients a_2 and κ, are crucial in determining the shape dependence of the liquid drop energy and, therefore, of fission barriers.

In this sense, the most useful ways to establish the set of parameters were proposed by Pashkevich [4], Pauli [5] and Myers–Swiatecky [6].

To account for the average properties of a single-particle spectrum, we introduce a smooth function $\tilde{g}(\epsilon, \beta)$. In order to define the function $\tilde{g}$, we introduce the auxiliary function

$$\tilde{G}(\epsilon, \beta) = (\pi^{1/2}\tilde{\gamma})^{-1} \sum_{\nu} \exp\left(- \left\{ \frac{\epsilon - \epsilon_\nu(\beta)}{\tilde{\gamma}} \right\}^2 \right) . \tag{2}$$

The averaging interval $\tilde{\gamma}$ is chosen to be

$$\tilde{\gamma} \approx \hbar\omega_0 \approx 7\text{–}10 \text{ MeV} ,$$

i.e., we represent the intershell distance by $\hbar\omega_0 \approx 41/A^{1/3}$, the shell spacing of a harmonic oscillator spectrum.

Thus, the function $\tilde{G}(\epsilon, \beta)$ is obtained by smearing out the single-particle energies ϵ_ν, over an energy range of the order of $\hbar\omega_0$. It is therefore a smooth function of the energy and does not reflect the existence of shells in the spectrum ϵ_ν.

Care should be taken, so that the local value of the level density is reproduced when the procedure (2) is applied to a uniform level distribution. This is achieved by introducing a curvature correction [7], which contains higher derivatives of the sum defined by (2). Thus, we define the uniform level density as

$$\tilde{g}(\epsilon, \beta) = \tilde{G} - \tfrac{1}{4}\tilde{\gamma}^2\left(\frac{\partial^2 \tilde{G}}{\partial \epsilon^2}\right) + \tfrac{1}{32}\tilde{g}^4\left(\frac{\partial^4 \tilde{G}}{\partial \epsilon^4}\right) - \cdots + a_{2m}\tilde{\gamma}^{2m}\left(\frac{\partial^{2m} \tilde{G}}{\partial \epsilon^{2m}}\right). \tag{3}$$

The last equation may be written as

$$\tilde{g} = \tilde{\gamma}^{-1} \sum_{\nu} \xi\left(\frac{\epsilon - \epsilon_\nu}{\tilde{\gamma}}\right), \tag{4}$$

where the smoothing function is given by

$$\xi(x) = (\pi)^{-1/2} \exp(-x^2) \sum_{k=0,2}^{2m} a_k H_k(x) ,$$

with $H_k(x)$ being the Hermite polynomials, and the coefficients a_k are given by the recurrence relation

$$a_k = -\frac{1}{2k} a_{k-2} ,$$

for $k \geq 2$ and $a_0 = 1$.

It is convenient to introduce another density function, $g_{\rm sh}(\epsilon, \beta)$ in order to describe the local level density of the single-particle spectrum, defined analogously to (2) and (3). As $g_{\rm sh}(\epsilon, \beta)$ shall reflect shell nonuniformities, the smearing interval $\gamma_{\rm sh}$ has to be chosen considerably smaller than $\hbar\omega_0$. On the other hand, $g_{\rm sh}$ should be a continuous function of energy and, therefore, the interval $\gamma_{\rm sh}$ should still contain many levels. In our calculation we have normally used

$$\gamma_{\rm sh} \approx \lambda A^{-2/3} \approx 1\text{–}2 \text{ MeV} .$$

With this choice, $g_{\rm sh}(\epsilon, \beta)$ represents a locally averaged level density, which is a wiggly function of the energy and deformation parameters, oscillating around the "uniform" level density $\tilde{g}(\epsilon, \beta)$.

With the definition above, the variations in the single-particle level density caused by the shells can be described by the function

$$\delta g(\epsilon, \beta) = g_{\rm sh}(\epsilon, \beta) - \tilde{g}(\epsilon, \beta) . \tag{5}$$

Furthermore, the sum of single-particle energies

$$U = 2 \sum_{\nu} \epsilon_{\nu}(\beta) \tag{6}$$

can be replaced by

$$U = 2 \int_{-\infty}^{\lambda_{\rm sh}(\beta)} \epsilon g_{\rm sh}(\epsilon, \beta)\, d\epsilon . \tag{7}$$

In the limiting case $\gamma_{\rm sh} \to 0$, the integral (7) is the sum of the single particle energies $\epsilon_{\nu}(\beta)$ in Eq. (6). The Fermi energies $\lambda_{\rm sh}(\beta)$ and $\tilde{\lambda}(\beta)$ are determined from the condition that the number of particles (protons or neutrons) is fixed, and that it is the same for both distributions,

$$N = 2 \int_{-\infty}^{\lambda_{\rm sh}(\beta)} g_{\rm sh}(\epsilon, \beta)\, d\epsilon = 2 \int_{-\infty}^{\tilde{\lambda}(\beta)} \tilde{g}_{\rm sh}(\epsilon, \beta)\, d\epsilon . \tag{8}$$

The energy shell corrections can be written as

$$E_{\rm shell} = 2 \left[\int_{-\infty}^{\lambda_{\rm sh}(\beta)} \epsilon g_{\rm sh}(\epsilon, \beta)\, d\epsilon - \int_{-\infty}^{\tilde{\lambda}(\beta)} \epsilon \tilde{g}_{\rm sh}(\epsilon, \beta)\, d\epsilon \right] . \tag{9}$$

1.1. Renormalization in BCS theory

In our calculations, the pairing correlation energy was evaluated as in the commonly used prescriptions of the BCS approach. We have found it very useful to apply the idea of a renormalization based on the extraction of a smooth part, and also to the calculation of the pairing energies [7]. In this way, we evaluated only the essential energy variation gap Δ and the pairing energy due to the shell structure, while the same quantities

for a uniform model distribution of the single particle states are described phenomenologically by means of the smoothed distribution gap parameter $\tilde{\Delta}$. It was found very convenient the use of $\tilde{\Delta}$ as an input parameter, as determining the intensity of the pairing correlations, because the value of $\tilde{\Delta}$ varies relatively not too much throughout the Periodic Table, and it is easy to find a good approximation for it. In fact, the use of the relation

$$\tilde{\Delta} = \frac{12.0}{\sqrt{A}} \text{ MeV}$$

gives a good agreement, throughout the Periodic Table, between the calculated values of the energy gap Δ, in a specific nucleus, and the values experimentally deduced (see also [8]).

We start with the following BCS equation:

$$\frac{2}{G} = \sum_{\alpha=n-n_c}^{n+n_c} [(\epsilon_\alpha - \lambda)^2 + \Delta^2]^{-1/2}, \tag{10}$$

and

$$\frac{2}{G} = \int_{\tilde{\lambda}-\Omega}^{\tilde{\lambda}+\Omega} \frac{\tilde{g}(E)\, dE}{[(E-\tilde{\lambda})^2 + \tilde{\Delta}^2]^{-1/2}} \approx 2\tilde{g}(\tilde{\lambda}) \ln\left(\frac{2\Omega}{\tilde{\Delta}}\right), \tag{11}$$

where the integral is a uniform distribution analogous to the sum (10). In the integral (11), the cutoff energy Ω is related to the number of states $2n_c$, taken into account in the sum (10) by the relation

$$2\Omega = \frac{2n_c}{\tilde{g}(\tilde{\lambda})},$$

where $\tilde{g}(\tilde{\lambda})$ is the average level density at the Fermi energy. The BCS equation must be solved with the constraint that the particle number

$$N = 2\sum_\nu v_\nu^2 \tag{12}$$

is conserved. Here we have

$$v_\nu = \left(\frac{1}{2}\left\{1 - \frac{\epsilon_\nu - \lambda}{[(\epsilon_\nu - \lambda)^2 + \Delta^2]^{1/2}}\right\}\right)^{1/2}.$$

Eq. (12), together with (10), determines the two parameters Δ and λ in terms of the pairing strength and the cutoff parameter n_c.

We define now the energy P of the pairing correlations as the difference between the sums of single-particle energies evaluated with and without the pairing correlations. This quantity is found to be equal to

$$P = \sum (\epsilon_\nu - \lambda)\, \text{sign}[\epsilon_\nu - \lambda_0] - \frac{(\epsilon_\nu - \lambda)^2 + \frac{1}{2}\Delta^2}{[(\epsilon_\nu - \lambda)^2 + \Delta^2]^{1/2}}, \tag{13}$$

analogously to Eq. (9) in [2] where, however, the change of the Fermi energy due to the pairing correlations was ignored. In Eq. (13), λ_0 is the Fermi energy for $\Delta = 0$, i.e., $\lambda_0 = (\epsilon_n + \epsilon_{n+1})/2$. The sum in Eq. (13) converges and no cutoff problem arises.

The shell correction in the pairing energy is now determined as

$$E_{\text{pair}} = P - \tilde{P}, \tag{14}$$

where $\tilde{P}$ is the pairing correlation energy for the uniform distribution

$$\tilde{P} = -\tfrac{1}{2}\tilde{g}(\tilde{\lambda})\tilde{\Delta}^2 . \tag{15}$$

1.2. Nuclear shape parametrization

The deformed shape (up to and beyond its separation into two fragments) can be conveniently described by the Cassini ovaloids proposed by Pashkevich, as shown in detail elsewhere [4,10].

Considering only axially symmetric nuclear shapes, the Cassini ovaloids are taken as the first approximation to the nuclear shape. The deviation from the ovaloid shape is given by an expansion into a series of Legendre polynomials. Geometrically, the family of Cassini ovaloids is defined by [11]

$$r^2(z,\epsilon) = \sqrt{(a^4 + 4(cz)^2)} - (c^2 + z^2 - \epsilon^2) . \tag{16}$$

In this equation, r and z are cylindrical coordinates; ϵ is a dimensionless quantity such that $c = \epsilon R_0^2$; c stands for the square distance from the focus of the Cassini ovaloids to the origin of the coordinates; and a is a dimensionless parameter which completely defines the shape, taking into account volume conservation.

In the plane containing the symmetry axis a system of coordinates (R, x), such that the coordinate line R is constant, is defined. This is a Cassini ovaloid where $0 \leq R < \infty$ and $-1 \leq x \leq 1$. The (R, x) coordinates are related to the cylindrical ones (r, z) by the following equations:

$$R(z,r) = \sqrt[4]{[(z^2 + r^2)^2 - 2\epsilon R_0^2 \cdot (z^2 - r^2) + \epsilon^2 R_0^2]} , \tag{17}$$

$$x(z,r) = \frac{\mathrm{sign}(z)}{\sqrt{2}} \left[1 + \frac{z^2 - r^2 - \epsilon R_0^2}{R^2(z,r)}\right]^{1/2} . \tag{18}$$

In this system of coordinates, the basic shape of the nucleus is described by these equations, with R constant, determining thus the Cassini ovaloids. Therefore, the nuclear shape can be defined as a curve $R(x)$ that does not intersect any straight line x = const in more than one point. Then, we expand the function $R(x)$ into multipoles,

$$R(x) = R_0[1 + \sum \beta_m Y_{m0}(x)] . \tag{19}$$

Therefore, the set of parameters (ϵ, β) determines the nuclear shape. The details of this parametrization are given in [4,11]. As an example, we show in Fig. 1 $\{\epsilon, \alpha_4\}$ as a function of $\{\beta_2, \beta_4\}$. As it is clearly seen in this figure, it is difficult to establish an analytical connection between the two sets of parameters. A relation was obtained by a least-square fit of the parameters β_2, β_4 to the shapes described in this work by the Cassini ovaloids. By using this figure it is possible to establish a connection between the two sets of parameters to describe the same nuclear shape, but for more complex shapes more coefficients are needed in the harmonic spherical expansion.

2. Program organization

The code developed to calculate the fission barrier as a function of the deformation uses the single particle energies calculated as in the code CASSINI [12]. In the BARRIER code the shell correction package is composed by the following new routines.

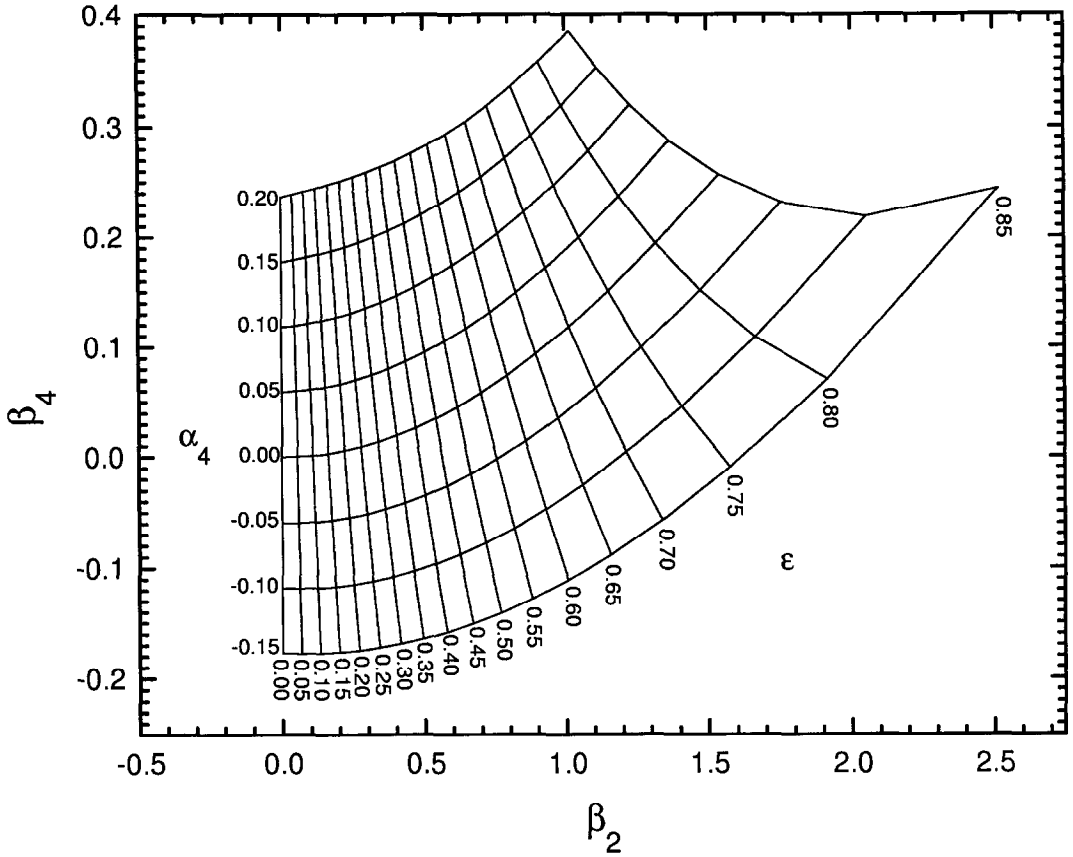

Fig. 1. Parameters (ϵ, α_4) as a function of (β_2, β_4).

2.1. Routine FRAQUA

This is the main routine for the shell correction calculations. It only chooses the correct input parameters (G-strength pairing, and particle number) to the routines DELTAU and PAIRING.

Important variables:
- GN, GZ: Strength pairing for neutron and proton.
- DU: Shell corrections + Pairing corrections.

2.2. Routine DENS

It computes the uniform level density and its first and second derivatives for different values of γ and energy. It uses Eq. (4). In this way,

$$\tilde{g}(\epsilon) = \frac{1}{\gamma\sqrt{\pi}} \sum_{\nu} \exp(-x_\nu^2)\left[-\tfrac{1}{6}x_\nu^6 + \tfrac{7}{4}x_\nu^4 - \tfrac{35}{8}x_\nu^2 + \tfrac{35}{16}\right],$$

$$\frac{\partial \tilde{g}}{\partial \epsilon}(\epsilon) = \frac{1}{\gamma^2\sqrt{\pi}} \sum_{\nu} \exp(-x_\nu^2)\left[-\tfrac{1}{3}x_\nu^7 - \tfrac{9}{2}x_\nu^5 + \tfrac{63}{4}x_\nu^3 - \tfrac{105}{8}x_\nu\right],$$

$$\frac{\partial^2 \tilde{g}}{\partial \epsilon^2}(\epsilon) = \frac{1}{\gamma^3\sqrt{\pi}} \sum_{\nu} \exp(-x_\nu^2)\left[-\tfrac{2}{3}x_\nu^8 + \tfrac{34}{3}x_\nu^6 + 54x_\nu u^4 + \tfrac{147}{2}x_\nu^2 - \tfrac{105}{8}\right],$$

where $x_\nu = (\epsilon - \epsilon_\nu)/\gamma$.

Important variables:
- G, GD1, GD2: Uniform level density, and its first and second derivatives.

2.3. Routine EFFNUM

It computes the particle number for a given energy and γ. It is used to compare with the right particle number and to compute in DELTAU the Fermi energy, which satisfies Eq. (8). The uniform level density is used to compute the particle number for a given λ, that is,

$$N = \int_{-\infty}^{\lambda} \tilde{g}(\epsilon)\, d\epsilon\,.$$

Using the above expression (DENS), it is easy to obtain

$$N = 1 + \operatorname{erf}(x) + \frac{\exp(-x^2)}{\sqrt{\pi}}\left(\tfrac{1}{6}x^5 - \tfrac{4}{3}x^3 + \tfrac{19}{8}x\right).$$

In this routine, if $x > 0$ $(\lambda > \epsilon_\nu)$ then $\operatorname{erf}(x) = 1 - P5(x)\cdot\exp(-x^2)$, and

$$N = 2 + \operatorname{erf}(x) + \exp(-x^2)\left[-P5(x) + \frac{1}{\sqrt{\pi}}\left(\tfrac{1}{6}x^5 - \tfrac{4}{3}x^3 + \tfrac{19}{8}x\right)\right].$$

On the contrary, if $x < 0$ $(\lambda < \epsilon_\nu)$ then $\operatorname{erf}(x) = -\operatorname{erf}(|x|)$, and

$$N = \exp(-x^2)\left[P5(|x|) + \frac{1}{\sqrt{\pi}}\left(\tfrac{1}{6}x^5 - \tfrac{4}{3}x^3 + \tfrac{19}{8}x\right)\right].$$

2.4. Function P5

This function computes the error function to be used in EFFNUM and UPOT. This routine uses the approximation 7.1.26 of [5]; thus

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^{\pi} \exp(-t^2)\, dt = 1 - (a_1 t + a_2 t^2 + a_3 t^3 + a_4 t^4 + a_5 t^5)\exp(-t^2)\,,$$

where $a_1 = 0.254829592$, $a_2 = -0.284496736$, $a_3 = 01.421413741$, $a_4 = -1.453152027$, and $a_5 = 1.061405429$. Also $t = 1/(1 + px)$ and $p = 0.3275911$.

Only the polynomial part is computed; therefore, the error function is

$$\operatorname{erf}(x) = 1 - P5(x)\exp(-t^2)\,.$$

2.5. Routine DELTAU

This routine uses Eq. (12) to calculate the Fermi energy. The Fermi energy is used with Eq. (9) to compute the shell correction energy. To this purpose routine UPOT is called,

$$E_{\text{shell}} = 2\left[\sum_{\nu} \epsilon_{\nu}(\beta) - \int_{-\infty}^{\tilde{\lambda}(\beta)} \epsilon \tilde{g}(\epsilon, \beta)\, d\epsilon\right].$$

Important variables:
- FEN: Fermi energy.
- UC: Sum of the single particle energies.
- US: Energy calculated with the uniform level distribution.

2.6. Routine UPOT

The energy from the uniform level density distribution is calculated in this routine for a given energy by using

$$U_s = \int_{-\infty}^{\tilde{\lambda}(\beta)} \epsilon \tilde{g}(\epsilon, \beta)\, d\epsilon\,.$$

Using the expansion of $\tilde{g}(\epsilon)$ in polynomials it is easy to obtain, for $\epsilon \epsilon_{\nu}$,

$$U_c = \sum_{\nu} \left\{ 2\epsilon_{\nu} + \exp(-x^2)\left[-\epsilon_{\nu} P5(x) + \frac{\epsilon_{\nu}}{\sqrt{\pi}}\left(\tfrac{1}{6}x^5 - \tfrac{4}{3}x^3 + \tfrac{19}{8}x\right) \right.\right.$$
$$\left.\left. -\frac{\gamma}{\sqrt{\pi}}\left(-\tfrac{1}{6}x^6 + \tfrac{5}{4}x^4 - \tfrac{35}{8}x^2 + \tfrac{5}{16}\right)\right]\right\},$$

and, for $\epsilon < \epsilon_{\nu}$,

$$U_c = \sum_{\nu} \left\{ \exp(-x^2)\left[\epsilon_{\nu} P5(|x|) + \frac{\epsilon_{\nu}}{\sqrt{\pi}}\left(\tfrac{1}{6}x^5 - \tfrac{4}{3}x^3 + \tfrac{19}{8}x\right) - \frac{\gamma}{\sqrt{\pi}}\left(-\tfrac{1}{6}x^6 + \tfrac{5}{4}x^4 - \tfrac{35}{8}x^2 + \tfrac{5}{16}\right)\right]\right\},$$

where $x = (\epsilon - \epsilon_{\nu})/\gamma$.

Important variables:
- UPOT: Energy from the uniform level density distribution.

2.7. Routine PAIRING

Pairing correction is computed using Eq. (15), and it calls subroutine SUFQUP to solve the BCS equations in order to obtain the FERMI energy (λ) and the gap parameter (Δ).

Important variables:
- PAR: Pairing energy corrections.
- LAMBDA: Fermi energy.
- GAP: Gap parameter.

2.8. Routine SUFQUP

It solves the BCS equation to obtain the Fermi energy and the gap parameter.

2.9. Routine TARANHA

It organizes the output files of single particle levels near the Fermi level, as a function of selected deformation parameters (typerun=3). The output file format allows us to easily process it with the standard graphics software (Origin, Grapher).

2.10. Routine TABLESP

It performs the organization of output files of single particle level as a function of selected potential parameters (typerun=4).

3. Input cards

BARRIER.INP

INTDAT

IARRAY: If IARRAY = 0, wave functions are not recorded, and if IARRAY = 1 wave functions are recorded.
ISHAPE: If ISHAPE = .true., nuclear shape is plotted.
IPRINT: The number of line printouts for a single particle spectrum (four levels per line).
CASSIN: If CASSIN = .false., beta decomposition is employed as the shape parametrization (default). Otherwise Cassini ovals are employed.
IQUADR: If IQUADR $\neq$ 0, the quadrupole moments associated with the single particle states are calculated.
INCREA: If INCREA = 1, the spin-orbit parameter (λ) and r_{o-so} will be scaled with deformation.
IDECOM: If IDECOM = 1, state decomposition is printed.
MAPAD: If MAPAD = .true., the calculations will be made for any two deformation parameters.
KEYSPE: If KEYSPE > 0, the file SNGLPRT.SPE will be carried out in format DENCOM (DEN97) exactly.
OUTSPE: If OUTSPE = .true., the neutron and proton spectra will be written on file SNGLPRT.SPE and general output in BARRIER.OUT.
TYPERUN: If TYPERUN = 1, the calculation of single particle spectra and deformation energy, will be made for one set of deformations. The possible output files are PASH.DAT, LYNN.DAT, PAULI.DAT, BARRIER.OUT and BARRIER.SPE.

If TYPERUN = 2, the fission barrier will be calculated. The output files are PASH.DAT, LYNN.DAT and PAULI.DAT.

If TYPERUN = 3, the single particle levels near Fermi level as a function of selected deformation parameters are organized in a format that allows us to easily process it with standard graphics software (Origin, Grapher). The output files are ARANHA.DAT and ARANTAB.DAT.

If TYPERUN = 4, the output files of single particle level are organized as a function of selected potential parameters. These files are FERMILEV.DAT and SPTABLE.DAT.

DYNAMC

IZ,IN: Proton and neutron numbers.
ICHOIC: Parameters of the nuclear potential.

ALPHA1...: Deformation parameters (CASSIN is true) (ALPHA1, ALPHA2, ALPHA3, ALPHA4, ALPHA5, ALPHA6 accepted).
EPSIL: Deformation parameter (If CASSIN is true).
VAREPS: If MAPAD = .true., ϵ is varied from EPSIL to END1V with step STEP1V.
VARP1,VARP3,...: Only used when MAPAD = .true.; if VARPi = .true., then ALPHAi is varied with step STEP2V.

4. Output files

BARRIER.OUT: General output.
PASH.DAT, LYNN.DAT, PAULI.DAT: Liquid drop model energies and shell corrections for different liquid drop model formulations as a function of deformation.
SNGLPRT.SPE: Single particle spectra for protons and neutrons.
FERMILEV.DAT: Single particle levels in the neighborhood of the Fermi level.
ARANHA.DAT: Single particle levels near the Fermi level, as a function of selected deformation parameters.
ARANTAB.DAT, SPTABLE.DAT: Output in a convenient format. It allows us to easily process it with standard graphics software (Origin, Grapher).

5. Example of runtype

BARRIER.INP

```
&INDAT   IARRAY=0     IPRINT=68     CASSIN=.T.    KEYSPE=68
         OUTSPE=.T.   TYPERUN=2     /END
&DYNAMC  IZ=92        IN=147        ICHOIC=2      IENDD=1
         EPSIL=0.1    ALPHA4=-0.16  VAREPS=.T.    VARP4=.T.
         BEG1V=0.1    STEP1V=0.1    END1V=0.3
         BEG2V=-0.1   STEP2V=0.05   END1V=0.1     /END
```

PASH.DAT

```
EPS=.100 a1=.000 a3=.000 a4=-.100 a5=.000 a6=.000 Gn*A=22.5 Gz*A=26.5

VAR:    T         F         F         T         F         F
P(1)  P(2)  Barrier  Sh.Cor  Eldm   dU(N)  dU(P)  dP(N)  dP(P)  BC    BS
.100 -0.100 12.7716  8.3166  4.455  5.867  6.124 -1.719 -1.955 0.997 1.012
.100 -0.050  9.4188  8.1118  1.307  6.445  6.143 -2.200 -2.276 0.999 1.004
.100  0.000  7.2951  7.0752  0.220  5.228  4.029 -1.172 -1.009 0.999 1.002
.100  0.050  6.9310  5.7111  1.220  4.802  2.080 -1.114 -0.057 0.999 1.004
.200 -0.100 11.8028  6.6953  5.107  4.069  5.723 -1.645 -1.451 0.993 1.019
.200 -0.050  5.8105  3.8359  1.975  1.486  4.366 -0.997 -1.019 0.995 1.011
.200  0.000  1.1673  0.3445  0.823 -1.368  2.022  0.157 -0.467 0.996 1.007
.200  0.050 -1.1113 -2.7886  1.677 -2.435 -1.208  0.190  0.666 0.996 1.009
.200  0.100  0.6961 -3.7729  4.469 -2.017 -3.004  0.343  0.905 0.995 1.015
```

6. Some graphic results

In Fig. 2 the potential energy surface of ^{232}Th in the deformation space of ϵ (elongation) and α_4 (hexadecapolar coordinate) is shown. It is possible to see the extremal points of the fission path: equilibrium

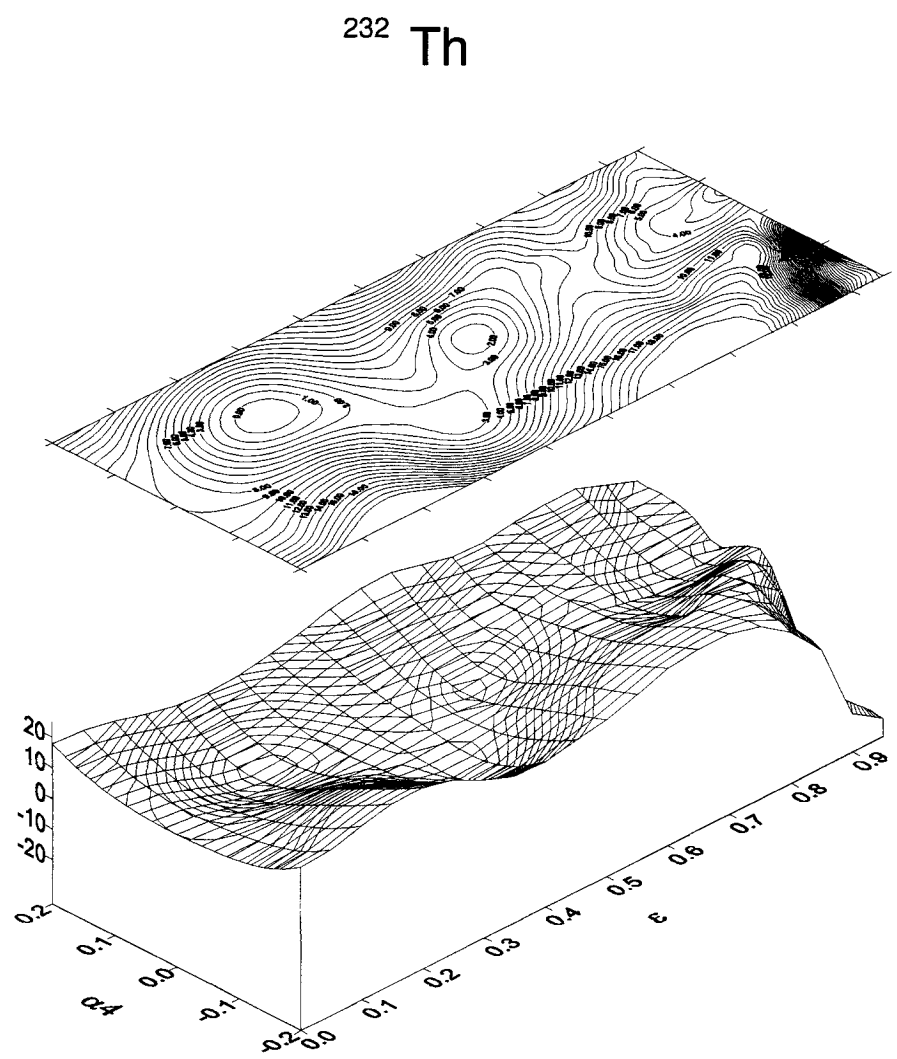

Fig. 2. Calculated fission barrier in the ($\{\epsilon, \alpha_4\}$) plane for ^{232}Th. The contour line separation is 1 MeV.

deformation, second minimum and both saddle points. It was used in the calculation of the modified Chepurnov parameters [13] of the nuclear potential, in order to obtain the best results for the single-particle spectrum in the equilibrium deformation. In Fig. 3, the energy surface is presented in the region of the second saddle point of ^{233}Th. The surface is presented on ϵ and α_3 (octupolar coordinate). In this case, as can be seen, the results of the BARRIER code show the existence of mass asymmetry of the external saddle configuration, and a shallow third minimum. Both results (Figs. 2,3) were obtained with the key TYPERUN = 2.

In Fig. 4 the deformation dependence of the neutron single particle levels of ^{237}Pu (TYPERUN = 3), in the region of the second minimum, is presented. This result was used in the study of fission isomer states [14]. This is an example of the use of the BARRIER code for the analysis of superdeformed regions.

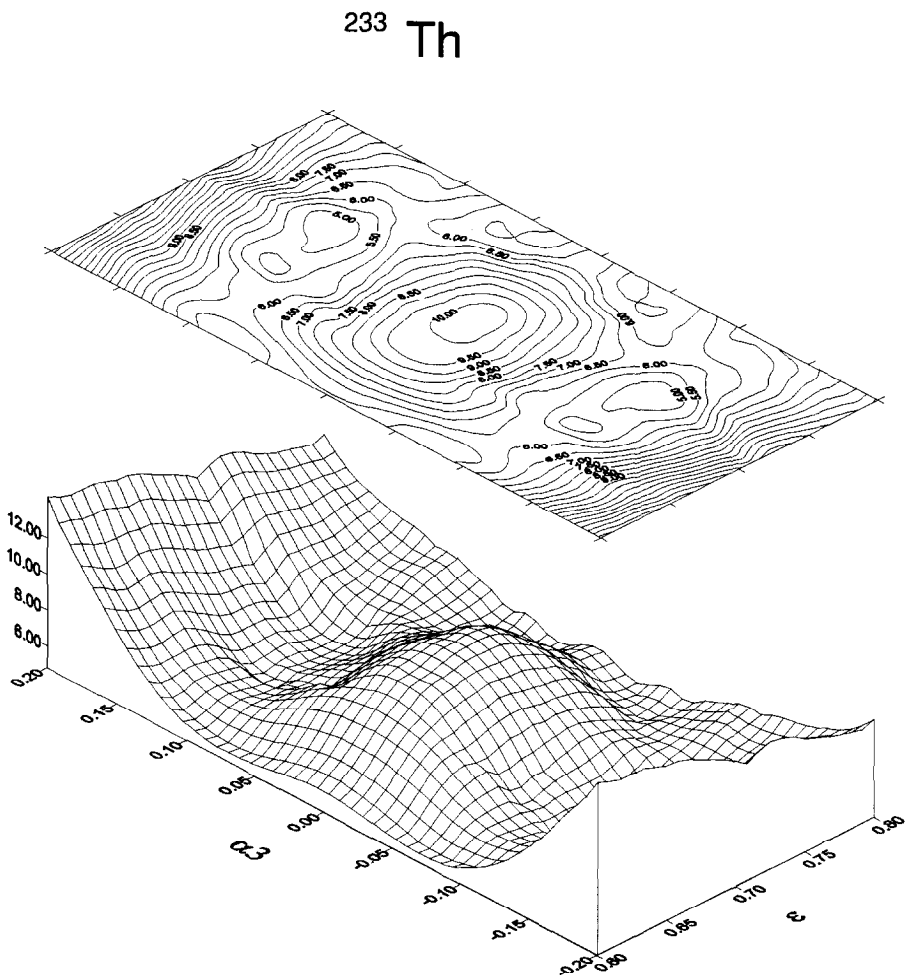

Fig. 3. The potential energy surface of ^{233}Th in terms of the ϵ and α_3 parameters, in the second saddle region. The contour line separation is 0.5 MeV.

Acknowledgements

The authors wish to express their gratitude to the Brazilian FAPESP, CNPq and CLAF for partial support.

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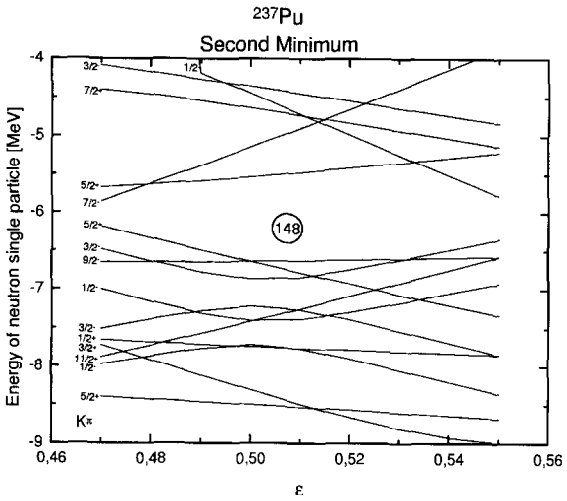

Fig. 4. Single neutron energies calculated in the Woods–Saxon potential as a function of ϵ for ^{237}Pu.

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