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**MACROSCOPIC-MICROSCOPIC ENERGY OF
ROTATING NUCLEI IN THE FUSION-LIKE
DEFORMATION VALLEY**

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Rapport Interne SUBATECH 98-12

Macroscopic-microscopic energy of rotating nuclei in the fusion-like deformation valley

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Abstract

The macroscopic-microscopic energy of rotating nuclei moving in the fusion-like deformation valley has been determined within a generalized liquid drop model including the nuclear proximity energy, the two-center shell model and the Strutinsky method. The l -dependent potential barriers of the ^{84}Zr , ^{132}Ce , ^{152}Dy and ^{192}Hg nuclei have been determined. A first minimum having a pure microscopic origin and lodging the normally deformed states progressively disappears with increasing angular momenta. The microscopic and macroscopic energies contribute to generate a second minimum where superdeformed states may survive. It becomes progressively the lowest one at intermediate spins. At still higher angular momenta, the minimum moves towards the foot of the external fission barrier leading to macroscopic hyperdeformed quasi-molecular states.

PACS: 21.10.-k; 21.60.Cs; 21.60.Ev; 24.75.+i; 25.70.Jj

Keywords: highly deformed rotating nuclei, two-center shell model, generalized liquid drop model, quasi-molecular nuclear shapes.

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1 Introduction

The question of the behaviour of a nucleus with respect to rotation remains a basic problem. Starting from an initial spherical nucleus, most of the theoretical studies [1–3] predict a maximal angular momentum against fission of around 80–90 $\hbar$ while Neegard and Pashkevich [4] and us [5] obtained respectively around 110 $\hbar$ and 125 $\hbar$, for medium nuclei. Experimentally, the only way to transfer such high angular momenta is to form these rotating nuclei in heavy-ion collisions via fusion of a projectile with a target.

At $l \sim 140 \hbar$, formation and fast fission of semi-equilibrated fused systems have been observed [6]. In 1986, the γ decay of superdeformed (SD) rotational states has been detected in Dy [7] and, now, around 200 superdeformed bands have been found, mostly in the $A=80, 130, 150$ and 190 mass regions. Only a few of these rotational bands have been firmly linked [8–10] to the normal deformed (ND) states they decay into and, consequently, spins and excitation energies are not fully known for most of these SD bands. The assigned highest spin value for the SD states is around 70 $\hbar$. The presence of identical bands, the SD band feeding [11] at the highest spins and their sudden decay-out at low spins [12] (around spin 25 $\hbar$ and 10 $\hbar$ in the mass 150 and 190 regions) are still poorly understood. Experiments at still higher incident energies [13–15] have suggested the survival of hyperdeformed (HD) rotating nuclei. A first attempt to determine the maximal spin had led to around 95 $\hbar$ in Dy [13]. Subsequent experiments have led also to some ridge structures but not to definitive identification of discrete rotational bands [16–18].

The two remaining problems are the determination of the spin range for which super and hyperdeformed nuclei exist and the knowledge of the shapes of these systems formed in heavy ion reactions. Theoretically, the super and hyperdeformed states are essentially explained from a well already existing for non rotating nuclei and within the Strutinsky shell correction method added to the liquid drop model [19] and the Hartree-Fock-Bogoliubov method [20,21]. For the actinide nuclei, hyperdeformed Th and, recently, U [22] isomers have been effectively observed at $l=0$ in addition to the superdeformed fission isomers. This is not the case for other non rotating nuclei in the intermediate mass range. Geometrically, the spheroid configurations are often selected to calculate the shell effects and the ratios 1.5, 2, 2.5 and 3 of the axes are put forward. This implicitly assumes the complete loss of memory of the entrance channel and neglects the neck degree of freedom. On the other side, rotating hyperdeformed light Hg nuclei looking like two partly overlapping spheres have been obtained in extended cranked Nilsson-Strutinsky calculations with a Woods-Saxon potential and a finite range liquid drop model [23]. Rotating states in Yb have also been described as mass asymmetric nuclear molecules [24]. Furthermore, it has been shown that the density distribution at the third

hyperdeformed minimum of the ^{232}Th nucleus resembles a di-nucleus [25].

In previous works [5,26,27] the macroscopic energy of a rotating nucleus moving in the fusion-like deformation valley has been determined within a generalized liquid drop model taking into account the proximity forces when the neck is formed and partially the dependence of the nuclear radius on the mass. In this peculiar deformation path, which corresponds at least to the entrance channel in heavy ion reactions, the fusion [28] but also the fission barrier heights are compatible with experimental data and the Businaro-Gallone point is reproduced [29]. The deformation barrier is a scission barrier and the top corresponds to two separated nuclei maintained in unstable equilibrium by the balance between the repulsive Coulomb forces and the attractive nuclear proximity forces. The curvature at the barrier top of the potential barrier is important and the moment of inertia of the two separated spheres is high. Consequently, the potential energy minimum corresponding to a compact and creviced one-body shape survives even at very high angular momenta. Its origin is essentially macroscopic and hyperdeformed minima are predicted in the whole mass range. Their geometric characteristics are in agreement with the ones possibly observed in Dy. With decreasing spins, the minimum moves to intermediate positions which give a first idea of the geometric characteristics of the superdeformed rotating nuclei.

The purpose of the present work is to add the microscopic effects all along this fusion-like deformation path which contains, in particular, the two tangent sphere configuration and to determine the spin dependence of the different potential pockets and of their relative energies. It is an important step toward a complete study of fusion reaction starting from symmetric fragments up to asymmetric - cluster-like [30] reactions. The single particle levels have been derived from the two-center shell model and the shell corrections have been calculated with the Strutinsky method [31–34]. This macroscopic-microscopic approach has been applied to the calculation of the l -dependent potential barriers of the ^{84}Zr , ^{132}Ce , ^{152}Dy and ^{192}Hg nuclei.

2 Description of the fusion-like deformation valley

The selected shape sequences must lead from two-separated spheres to one sphere and vice versa by the way of two touching spheres and must describe the formation of a deep neck and its progressive filling while the ends of the shape remain quasi-spherical (Fig. 1). In an attempt to obtain a correspondence with the quadrupolar deformation of the initial nucleus ground state the following approximation has been made: the neck radius a approximates the small semiaxis of the ellipsoid while the distance from the separation plane between the two fragments and the left (or right) hand side end of

the shape approximates the large semiaxis. The correspondence holds especially for small deformations or small distances between the centers of the fragments. The macroscopic liquid drop model energy has been calculated for elliptic lemniscatoids which simulate precisely this deformation valley [5,28] while the microscopic energy has been derived from two harmonic oscillators reproducing the two overlapping sphere configuration. The neck radius a allows to connect the two approaches and, then, the elongation is almost the same in the two cases. The shapes presented here correspond to some extent to β_2 - β_4 deformation used in fission barrier study [35]. The total energy depends only on one deformation parameter and the distance R between the centers of the two spheres has been chosen.

3 Macroscopic energy

For an arbitrary deformed nucleus, the macroscopic total energy is defined as :

$$E = E_V + E_S + E_C + E_N + E_{Rot}. \quad (1)$$

The volume E_V and surface E_S energies are respectively given by:

$$E_V = -15.494(1 - 1.8I^2)A \text{ MeV} \quad (2)$$

$$E_S = 17.9439(1 - 2.6I^2)A^{2/3}(S/4\pi R_0^2) \text{ MeV}. \quad (3)$$

$I = (N - Z)/A$ is the relative neutron excess and S the surface of the deformed system. The effective sharp radius R_0 has been chosen as:

$$R_0 = 1.28A^{1/3} - 0.76 + 0.8A^{-1/3} \text{ fm}. \quad (4)$$

This formula allows to reproduce the increase of the ratio $r_0 = R_0/A^{1/3}$ with the mass; for example, $r_0=1.11$ fm for ^{20}Ne and $r_0=1.18$ fm for ^{240}Pu .

For one-body shapes, the Coulomb E_C energy is:

$$E_C = 0.6e^2(Z^2/R_0) \times 0.5 \int (V(\theta)/V_0)(R(\theta)/R_0)^3 \sin \theta d\theta, \quad (5)$$

where $V(\theta)$ is the electrostatic potential at the surface and V_0 the surface potential of the sphere. When the two fragments (or the two colliding nuclei)

are separated the Coulomb energy is simply the sum of the self-Coulomb energies and of the Coulomb interaction energy. The surface energy E_S takes only into account the effects of the surface tension forces in a half space and does not include the contribution due to the attractive nuclear forces between the surfaces in regard in the neck or the gap between the fragments. The nuclear proximity energy term E_N allows to take into account these additional surface effects when crevices appear in the deformation path.

$$E_N = 2\gamma \int_{h_{min}}^{h_{max}} \Phi(D/b) 2\pi h dh, \quad (6)$$

where h is the ring radius in the plane perpendicular to the longitudinal deformation axis and D the distance between the infinitesimal surfaces, b is the surface width and Φ is the universal proximity function. The surface parameter γ is given by:

$$\gamma = 0.9517(1 - \kappa_s I^2) \text{ MeV} \cdot \text{fm}^{-2}. \quad (7)$$

In this generalized liquid drop model the surface diffuseness is not considered in the surface energy term and the proximity energy vanishes when there is no neck as for ellipsoids for example.

The rotational energy has been determined within the rigid body ansatz. Indeed, it has been shown that corrective terms arising from the orbital motion and the spin degrees of freedom roughly cancel each other, particularly at large deformations [36,37].

$$E_{Rot} = \frac{\hbar^2 l(l+1)}{2I_{\perp}}. \quad (8)$$

4 Two-center shell model

The study of the deformed nuclei is performed within a fusion-like reaction. Deformed shell models like Nilsson or Woods-Saxon type fail to describe the transition from an initial level scheme of the nucleus to two separate level schemes corresponding to the fragments. Thus a particular feature of our approach is the relation between deformation of the nucleus and a certain reaction channel leading to two separated nuclei. Such a shape evolution can only be described by a two-center shell model [38,31]. We calculated the deformation energy for four nuclei representing the mass regions where superdeformed states have been reported. The corresponding reactions are:

$$^{84}\text{Zr} \leftrightarrow ^{42}\text{Ca} + ^{42}\text{Ca} \quad (9)$$

$$^{132}\text{Ce} \leftrightarrow ^{56}\text{Ni} + ^{56}\text{Zn} \quad (10)$$

$$^{152}\text{Dy} \leftrightarrow ^{76}\text{Ge} + ^{76}\text{Se} \quad (11)$$

$$^{192}\text{Hg} \leftrightarrow ^{96}\text{Zr} + ^{96}\text{Zr}. \quad (12)$$

The starting point for the two-center shell model we are using here is the two-center oscillator potential:

$$\rho(z) = \begin{cases} \frac{1}{2}m_0\omega_z^2(z+z_0)^2 + \frac{1}{2}m_0\omega_\rho^2\rho^2, & z \leq 0 \\ \frac{1}{2}m_0\omega_z^2(z-z_0)^2 + \frac{1}{2}m_0\omega_\rho^2\rho^2, & z > 0 \end{cases} \quad (13)$$

Since we assume spherical fragments the frequencies on ρ and z directions are equal, $\omega_\rho = \omega_z$. The two-center oscillator potential is used to obtain the basis functions by solving:

$$H_0\Psi = E\Psi \quad (14)$$

with H_0 in cylindrical coordinates:

$$H_0 = -\frac{\hbar^2}{2m} \left[\frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \varphi^2} + \frac{\partial^2}{\partial z^2} + \frac{1}{2}m_0\omega_\rho^2\rho^2 + \frac{1}{2}m_0\omega_z^2(z \pm z_0)^2 \right]. \quad (15)$$

The equation is separable. In [39,31] the solution is obtained in terms of hypergeometric functions. We preferred another form for the solutions which involves Laguerre and Hermite functions dependence of the total wave function [40]. The basis corresponds to the following set:

$$\Phi(\varphi) = \frac{1}{\sqrt{2\pi}} e^{im\varphi} \quad (16)$$

$$R_{n_\rho m}(\rho) = \left[\frac{2\alpha_\rho \Gamma(n_\rho + 1)}{\Gamma(n_\rho + |m| + 1)} \right]^{1/2} e^{\frac{\alpha_\rho^2 \rho^2}{2}} (\alpha_\rho \rho)^{|m|} L_{n_\rho}^{|m|}(\alpha_\rho^2 \rho^2) \quad (17)$$

$$Z_\nu(z) = \begin{cases} C_\nu \exp\left[-\frac{\alpha_z^2(z+z_0)^2}{2}\right] \mathcal{H}_\nu[-\alpha(z+z_0)] & , z \leq 0 \\ (-1)^{n_z} C_\nu \exp\left[-\frac{\alpha_z^2(z-z_0)^2}{2}\right] \mathcal{H}_\nu[-\alpha(z-z_0)] & , z > 0 \end{cases} \quad (18)$$

where $\alpha_z = \left(\frac{m\omega_z}{\hbar}\right)^{1/2}$ and $\alpha_\rho = \left(\frac{m\omega_\rho}{\hbar}\right)^{1/2}$, $L_n^m(x)$ is the Laguerre polynom and $\mathcal{H}_\nu(x)$ is the Hermite function.

The oscillator energy reads:

$$E_{n_\rho m n_z} = \hbar\omega_\rho[2n_\rho + |m| + 1] + \hbar\omega_z \left(\nu + \frac{1}{2} \right). \quad (19)$$

When the system is deformed, n_z is no more an integer until the two final fragments are obtained. The intermediate values ν and the normalization constants C_ν corresponding to the oscillation on the Oz axis are calculated by imposing the continuity of $Z_\nu(z)$ and dZ_ν/dz on the separation plane. One obtains for intermediate shapes [40]:

$$C_{n_z} = \left[\frac{2}{\alpha_z} j_{\nu\nu z_0} \right]^{-\frac{1}{2}} \quad (20)$$

where:

$$j_{\nu\nu z_0} = \frac{e^{-z_0^2}}{2\Gamma(-\nu)} \left[\nu \mathcal{H}_{\nu-1}(-z_0) \sum_{m=0}^{\infty} \frac{(-1)^m \Gamma\left(\frac{m-\nu}{2}\right) \Psi\left(\frac{m-\nu}{2}\right)}{m!} + \right. \\ \left. \mathcal{H}(-z_0) \sum_{m=0}^{\infty} \frac{(-1)^m \Gamma\left(\frac{m-\nu+1}{2}\right) \Psi\left(\frac{m-\nu+1}{2}\right)}{m!} (-2z_0)^m \right]. \quad (21)$$

In the last equation $\Gamma(x)$ is the gamma function and $\Psi(x)$ is its logarithmic derivative. We cut the sum when terms became less than $0.5 \cdot 10^{-9}$. At this point we have an orthonormalized basis as the eigenfunctions of the two-center symmetric oscillator.

5 Spin-orbit interaction

Shell closures are decided by the spin-orbit $\mathbf{ls}$ and $\mathbf{l}^2$ interactions. The total Hamiltonian of the two-center shell model reads:

$$H = -\frac{\hbar^2}{2m} + V_{osc} + V(\mathbf{ls}) + V(\mathbf{l}^2). \quad (22)$$

When the system is deformed the value of the angular momentum l is no more a good quantum number. Therefore, in order to have an invariant for the spin-orbit interaction during deformation we used $\frac{\nabla V_{osc} \times \mathbf{p}}{m_0 \omega_0^2} \mathbf{s}$ instead of $\mathbf{ls}$ as discussed by [41] and $\left[\frac{\nabla V_{osc} \times \mathbf{p}}{m_0 \omega_0^2} \right]^2$ for $\mathbf{l}^2$. Consequently the $\mathbf{ls}$ and $\mathbf{l}^2$ operators are expressed, in terms of cylindrical operators, as:

$$\mathbf{ls} = \frac{1}{2}(\mathbf{l}_+\mathbf{s}_- + \mathbf{l}_-\mathbf{s}_+ + \mathbf{l}_z\mathbf{s}_z) \quad (23)$$

$$\mathbf{l}^2 = \frac{1}{2}(\mathbf{l}_+\mathbf{l}_- + \mathbf{l}_-\mathbf{l}_+ + \mathbf{l}_z^2) \quad (24)$$

where:

$$\mathbf{l}_+ = -e^{i\varphi} \left(\rho \frac{\partial}{\partial z'} - z' \frac{\partial}{\partial \rho} - i \frac{z'}{\rho} \frac{\partial}{\partial \varphi} \right) \quad (25)$$

$$\mathbf{l}_- = e^{-i\varphi} \left(\rho \frac{\partial}{\partial z'} - z' \frac{\partial}{\partial \rho} + \frac{z'}{\rho} \frac{\partial}{\partial \varphi} \right) \quad (26)$$

$$\mathbf{l}_z = -i \frac{\partial}{\partial \varphi} \quad (27)$$

where

$$z' = \begin{cases} z + z_0, & z \leq 0 \\ z - z_0, & z > 0 \end{cases} \quad (28)$$

$\pm z_0$ are the positions of the two centers on the Oz axis.

The matrix elements have been calculated as functions of m , $N_\rho = 2n_\rho + |m|$ and n_z in [38], within the basis expressed with help of hypergeometric functions. We give here the matrix elements of $\mathbf{ls}$ and $\mathbf{l}^2$ which do not vanish, as functions of n_ρ , m , and n_z . The spin-orbit potential:

$$V(\mathbf{ls}) = -2\kappa\hbar\omega\mathbf{ls} \quad (29)$$

generates the matrix elements:

$$\begin{aligned} & \langle n'_\rho m' n'_z s' | V(\mathbf{ls}) | n_\rho m n_z s \rangle = \\ & -\kappa\hbar\omega \langle n'_\rho m' n'_z | \mathbf{l}_+ | n_\rho m n_z \rangle \delta_{s's-1} \\ & -\kappa\hbar\omega \langle n'_\rho m' n'_z | \mathbf{l}_- | n_\rho m n_z \rangle \delta_{s's+1} \\ & -2\kappa\hbar\omega \langle n'_\rho m' n'_z | \mathbf{l}_z | n_\rho m n_z \rangle \delta_{s's}. \end{aligned} \quad (30)$$

Since the angular momentum projection m can be either positive or negative, the following expressions are obtained for the two cases: For $m < 0$:

$$\langle n'_\rho m' n'_z | \mathbf{l}_+ | n_\rho m n_z \rangle =$$

$$\begin{aligned}
& \sqrt{n_\rho + 1} \langle n'_z | z' + \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle \delta_{n'_\rho n_\rho + 1} \delta_{m' m + 1} \\
& + \sqrt{n_\rho + |m|} \langle n'_z | z' - \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle \delta_{n'_\rho n_\rho} \delta_{m' m + 1} \\
& \langle n'_\rho m' n'_z | \mathbf{l}_- | n_\rho m n_z \rangle = \\
& \sqrt{n_\rho + |m| + 1} \langle n'_z | z' + \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle \delta_{n'_\rho n_\rho} \delta_{m' m - 1} \\
& + \sqrt{n_\rho} \langle n'_z | z' - \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle \delta_{n'_\rho} \delta_{m' m - 1}
\end{aligned} \tag{31}$$

For $m > 0$ we have:

$$\begin{aligned}
& \langle n'_\rho m' n'_z | \mathbf{l}_+ | n_\rho m n_z \rangle = \\
& -\sqrt{n_\rho + |m| + 1} \langle n'_z | z' + \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle \delta_{n'_\rho n_\rho} \delta_{m' m + 1} \\
& -\sqrt{n_\rho} \langle n'_z | z' - \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle \delta_{n'_\rho n_\rho - 1} \delta_{m' m + 1}
\end{aligned} \tag{32}$$

$$\begin{aligned}
& \langle n'_\rho m' n'_z | \mathbf{l}_- | n_\rho m n_z \rangle = \\
& -\sqrt{n_\rho + |m|} \langle n'_z | z' - \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle \delta_{n'_\rho n_\rho} \delta_{m' m - 1} \\
& -\sqrt{n_\rho + 1} \langle n'_z | z' + \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle \delta_{n'_\rho n_\rho + 1} \delta_{m' m - 1}
\end{aligned} \tag{33}$$

The diagonal term is:

$$\langle n'_\rho m' n'_z | \mathbf{l}_z | n_\rho m n_z \rangle = m \delta_{n'_\rho n_\rho} \delta_{m' m} \delta_{n'_z n_z}. \tag{34}$$

The $\mathbf{l}^2$ matrix elements can be easily calculated from:

$$\langle n'_\rho m' n'_z s' | V(\mathbf{l}^2) | n_\rho m n_z s \rangle = -\mu \kappa \hbar \omega \langle n'_\rho m' n'_z s' | \mathbf{l}_+ \mathbf{l}_- + \mathbf{l}_- \mathbf{l}_+ + \mathbf{l}_z^2 | n_\rho m n_z s \rangle \tag{35}$$

and using the completion relation for operators and the relations obtained for $\mathbf{l}_s$ term one can write:

$$\langle n'_\rho m' n'_z | \mathbf{l}_+ \mathbf{l}_- | n_\rho m n_z \rangle = \sum_{''} \langle n'_\rho m' n'_z | \mathbf{l}_+ | n''_\rho m'' n''_z \rangle \langle n''_\rho m'' n''_z | \mathbf{l}_- | n_\rho m n_z \rangle \tag{36}$$

and similarly for $\mathbf{l}_- \mathbf{l}_+$. The $\mathbf{l}_z^2$ term is diagonal and reads:

$$\langle n'_\rho m' n'_z s' | \mathbf{l}_z^2 | n_\rho m n_z s \rangle = m^2 \delta_{n'_\rho n_\rho} \delta_{m' m} \delta_{n'_z n_z} \delta_{s' s}. \tag{37}$$

The z -dependent terms of the matrix elements are:

$$\langle n'_z | z' + \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle = \frac{2\nu_{n_z}}{\alpha^2} C_{\nu'_{n_z}} C_{\nu_{n_z}} j_{\nu'_{n_z} \nu_{n_z} - 1 z_0} [1 + (-1)^{n'_z + n_z + 1}] \quad (38)$$

$$\langle n'_z | z' - \frac{1}{\alpha^2} \frac{\partial}{\partial z'} | n_z \rangle = \frac{1}{\alpha^2} C_{\nu'_{n_z}} C_{\nu_{n_z}} j_{\nu'_{n_z} \nu_{n_z} + 1 z_0} [1 + (-1)^{n'_z + n_z + 1}] \quad (39)$$

where $j_{\nu_1 \nu_2 z_0}$ is the integral:

$$j_{\nu_1 \nu_2 z_0} = \int_0^\infty e^{-(z-z_0)^2} \mathcal{H}_{\nu_1}(z-z_0) \mathcal{H}_{\nu_2}(z-z_0) dz \quad (40)$$

which appears when one calculates the integrals dependent on Hermite functions; its expression is [40]:

$$j_{\nu_1 \nu_2 z_0} = \frac{e^{-z_0^2}}{\nu_1 - \nu_2} [\nu_1 \mathcal{H}_{\nu_1-1}(-z_0) \mathcal{H}_{\nu_2}(-z_0) - \nu_2 \mathcal{H}_{\nu_1}(-z_0) \mathcal{H}_{\nu_2-1}(-z_0)] \quad (41)$$

For $\nu_1 = \nu_2$ one obtains eq. 21 by applying l'Hospital rule.

At this point the matrix for the $\mathbf{l}_s$ and $\mathbf{l}^2$ operators can be constructed directly, by using the above relations. After diagonalization the levels of the deformed system are obtained as a function of the distance between centers.

6 Strength parameters κ and μ

The spin-orbit and $\mathbf{l}^2$ interactions decide the level sequence that can be achieved within the single-particle model. The strength parameters κ and μ are not yet uniquely defined. A first rule is to obtain the correct levels so that the known magic numbers can be reproduced. We calculated the shell effects within the Strutinsky method. At a magic number the correct level scheme must yield a negative minimum for the shell correction energy. In this work a minimum of $E_{shell} = -3.8$ MeV has been found for $Z=50$, for protons coefficients $\kappa_p = 0.0889$ and $\mu_p = 0.664$; for $N=82$ and $\kappa_n = 0.0842$, $\mu_n = 0.868$, the shell correction has a minimum $E_{shell} = -4.11$ MeV, and for $N=126$ one has $E_{shell} = -3.63$ MeV for $\kappa_n = 0.0746$ and $\mu_n = 0.774$. For the separated fragment configurations, the search of strength parameters aimed to find negative minima of the shell corrections for pairs of proton or neutron magic numbers. Thus one finds $E_{shell} = -2.44$ MeV for $^{40}\text{Ca} + ^{40}\text{Ca}$ for a set $\kappa_f = 0.0560$ and $\mu_f = 0.774$ and $E_{shell} = -2.0$ MeV for a pair $^{56}\text{Ni} + ^{56}\text{Ni}$ at $\kappa_f = 0.0597$ and $\mu_f = 0.803$. In the heavier region, proton shell correction $E_{shell}^p = -4.06$ MeV for $\kappa_f = 0.0560$ and

$\mu_f=0.509$ and a neutron shell correction $E_{shell}^n=-4.18$ MeV for $\kappa_f=0.0650$ and $\mu_f=0.890$, for a system $^{132}\text{Sn}+^{132}\text{Sn}$. This arbitrary fit of strength parameters is common practice for phenomenological potentials. It insures however a good agreement with shell correction energies for spherical nuclei (magic numbers) [42]. Also, imposing negative minima for double-magicity of the fragments, one makes sure that fusion valleys due to spherical reaction partners are reproduced. The values of shell corrections are higher than the ones expected for two completely separated fragments. For example at $Z=50$ yields $E_{shell}=-4.12$ MeV for protons, whereas the value calculated here for a pair of Sn fragments is -4.06 MeV, two times higher than expected. In order to obtain the shell corrections for the fragments, calculations have been performed at the touching point configuration. Shell structure within the two center shell model reproduces the final fragment structure starting with the lower levels. Higher levels of the final fragments are reproduced as the distance between centers increase but there will be always an overlapping region at the high energy region of the spectra [31]. Therefore, as the Strutinsky method calculates the shell correction as a difference between the sum of the levels and the energy of a uniform distribution of levels, the region of high energy in the spectrum will not give a significant effect within the two-center shell configuration. This effect induce a lower absolute value of the shell correction energy. Various fitting methods have been used to find κ and μ in order to reproduce the ground state energies for spherical (magic numbers) and deformed nuclei. Bengtsson and Ragnarsson [43] propose a variation of κ and μ within every shell for neutrons and protons as well. Other authors take different sets of strength parameters as function of the mass region. Here we extrapolated the values for magic numbers in order to obtain the ground state deformations for the four nuclei we have worked on. Only the quadrupolar deformation values [42] have been taken into account. After performing a numerical fit, the following law of variation of the strength parameters yielded the best results:

$$\kappa_p = 5.5808 \cdot 10^{-6} \cdot Z^3 - 1.05 \cdot 10^{-3} \cdot Z^2 + 0.0645 \cdot Z - 1.2087 \quad (42)$$

$$\mu_p = 1.1132 \cdot 10^{-5} \cdot Z^3 - 2.861 \cdot 10^{-3} \cdot Z^2 + 0.2223 \cdot Z - 4.6731 \quad (43)$$

$$\kappa_n = 4.1141 \cdot 10^{-7} \cdot N^3 - 1.21 \cdot 10^{-4} \cdot N^2 + 0.0114 \cdot N - 0.26384 \quad (44)$$

$$\mu_n = 7.1868 \cdot 10^{-6} \cdot N^3 - 2.001 \cdot 10^{-3} \cdot N^2 + 0.1772 \cdot N - 4.1773 \quad (45)$$

As can be seen, we used a proton and neutron number dependence for proton and respectively neutron strength parameters, unlikely the usual mass number dependence. The mass number influences the spin-orbit and $\mathbf{I}^2$ terms through the $\hbar\omega$ factor.

Another important feature of the deformation process is the variation law of κ and μ with the distance between centers. For $A > 50$ we used the variation law given by [38]:

$$\kappa = \kappa_i + \Omega \cdot (\kappa_f - \kappa_i) \quad (46)$$

$$\mu = \mu_i + \Omega \cdot (\mu_f - \mu_i) \quad (47)$$

while for $A < 50$ we find a closer value of R corresponding to the ground state deformation for:

$$\kappa = \kappa_i + \sqrt{\Omega} \cdot (\kappa_f - \kappa_i) \quad (48)$$

$$\mu = \mu_i + \sqrt{\Omega} \cdot (\mu_f - \mu_i) \quad (49)$$

where:

$$\Omega = \frac{\omega - \omega_i}{\omega_f - \omega_i}. \quad (50)$$

Here ω_i and ω_f are the frequencies of the initial and final oscillators. These laws of variation can be changed in order to obtain a good agreement with known fission barriers.

7 Shell corrections

Shell corrections are obtained by means of Strutinsky procedure [44]. The method extracts a smoothed energy part of the total spectrum from the sum of the energy levels:

$$\delta U = \sum_{\nu} 2E_{\nu} - \tilde{U}. \quad (51)$$

The smoothed part $\tilde{U}$ is obtained with help of a smoothed level density function $\tilde{g}(\epsilon)$, which is calculated by averaging the real distribution $g(\epsilon)$ over the whole energy spectrum. The averaging procedure is applied around every level within a finite energy interval $\Gamma = \hbar\omega$:

$$\begin{aligned} \tilde{g}(\epsilon) &= \frac{1}{\gamma} \int_{-\infty}^{\infty} \zeta\left(\frac{\epsilon - \epsilon'}{\gamma}\right) g(\epsilon') d\epsilon' \\ &= \frac{1}{\gamma} \sum_{i=1}^{\infty} \zeta\left(\frac{\epsilon - \epsilon'}{\gamma}\right) \end{aligned} \quad (52)$$

where $\gamma = \Gamma/\hbar\omega$ and $\zeta(x)$ is the smoothing function. An usual smoothing function is:

$$\zeta(x) = \frac{1}{\sqrt{\pi}} e^{-x^2} \sum_{k=0}^m a_{2k} H_{2k}(x) \quad (53)$$

$H_n(x)$ are the Hermite polynomials. The coefficients a_{2k} are

$$a_{2k} = \frac{H_{2k}(0)}{2^{2k} \cdot (2k)!} \quad (54)$$

The Fermi energy $\tilde{\lambda}$ of the smoothed level distribution is calculated as a solution of the particle number conservation:

$$N_p = 2 \int_{-\infty}^{\tilde{\lambda}} \tilde{g}(\epsilon) d\epsilon \quad (55)$$

Then the total energy of the uniform level distribution, $\tilde{U}$, reproducing the microscopic part which is not submitted to local fluctuations of the spectrum is obtained as:

$$\tilde{U} = 2\hbar\omega \int_{-\infty}^{\tilde{\lambda}} \tilde{g}(\epsilon) \epsilon d\epsilon. \quad (56)$$

After performing the calculations, one obtains the following formula which can be used directly:

$$\delta U = \sum_{\nu} \{ \epsilon_{\nu} [1 - \text{erf}(x_{F_{\nu}})] + \frac{e^{-x_{F_{\nu}}^2}}{\sqrt{\pi}} \cdot [2\epsilon_{\nu} \sum_{k=1}^m a_{2k} H_{2k-1} + \tilde{\gamma} a_{2m} H_{2m}] \} \quad (57)$$

Usually one chose the upper order of Hermite polynomials $m=3$; the variable $x_{F_{\nu}}$ is;

$$x_{F_{\nu}} = \frac{\epsilon_{\nu} - \epsilon_F}{\gamma} \quad (58)$$

and $\text{erf}(x)$ is the error function. Shell corrections are calculated separately for protons and neutrons and the results are added.

8 Macroscopic-microscopic energies for ^{84}Zr , ^{132}Ce , ^{152}Dy and ^{192}Hg

Four nuclei in the 80, 130, 150 and 190 mass regions have been selected and the potential barriers have been computed within the previously defined potential energies aiming to obtain the deformed ground state and the superdeformed isomeric state.

One approximation which has been made is considering the fragments as spheres. This is true in the case of ^{84}Zr , where ^{42}Ca has a proton magic number $Z=20$ and a nearly magic number of neutrons $N=22$. As for the other three cases the fragments are deformed. Deformation in the ground state is always obtained as a result of the shell corrections, since the macroscopic energy is monotonously increasing with R for small elongations. The macroscopic, microscopic and total energies can be seen in Fig.2.a for zero angular momentum and in fig.2.b. for $l=20 \hbar$ in the case of ^{84}Zr deformation. The origin is taken at the macroscopic energy of the sphere. With this respect, for $l=0$ the ground state is at $E=3.2$ MeV. For $l=0$ the second minimum of the shell correction generates only a plateau on the total energy. For $l=20 \hbar$ the second minimum in the total energy appears. Ground state minimum and superdeformed states coexist for an angular momentum within the range $l=20 - 50 \hbar$, as can be seen in fig. 3. Experimentally [45,46] a ND band with maximal spin and excitation energy of around $34 \hbar$ and 25 MeV has been observed as well as a SD band for spins between 21 and $39 \hbar$ corresponding to a deformed minimum with an electric quadrupole moment and a moment of inertia of around $5 eb$ and $28 \hbar^2 \cdot \text{MeV}^{-1}$. The calculations lead to very slightly higher values for the spin and excitation energy of the highest states of the ND band but the second minimum is the lowest for spins higher than $30 \hbar$ which depopulates the ND band. The quadrupole moment and moment of inertia of the superdeformed shape are around $7 eb$ and $31 \hbar^2 \cdot \text{MeV}^{-1}$. For still higher spins, a new plateau appears and the potential energy minimum moves progressively towards the barrier foot due to the action of the centrifugal forces, the shell effects playing no more role. Then, these highest deformed rotating nuclei correspond rather to nascent quasi-molecular systems formed just after the crossing of the fusion barrier and for which the nucleon flow in the neck is hindered by a new potential barrier. This remark is valid for the whole mass range.

The barriers standing against a rotating ^{132}Ce nucleus are shown in figures 4 and 5 and the contribution of the shell effects is underlined. Macroscopic energy curves are monotonously increasing up to a maximum situated beyond the touching point (fig. 4.a). When shell corrections are added a hump appears due to microscopic effects (fig. 4.b). The two minima are visible even at $l=0$. The deformed ground state has a depth of about 1.5 MeV with respect to the sphere and is slightly deeper than the superdeformed state. A second minimum even at $l=0$ appears because of negative shell correction. For ^{132}Ce , at $l=20 \hbar$ the superdeformed state has already a lower energy value than the ground state. Experimentally [45,47,48], ND bands have been observed till $28 \hbar$ and SD bands for an assigned spin range of 20 to $52 \hbar$ corresponding to deexcitation of superdeformed nuclei characterized by Q around $8.8 eb$ and $I \sim 57 \hbar^2 \text{MeV}$. It is important to recall that up to $\beta \sim 0.8$ the differences between the values of I and Q for ellipsoidal and quasi-molecular shapes are very small even though these two configurations are so different [27]. Therefore, the values of I and Q deduced from experimental data lead to a poor understanding

of the nucleus elongation and neck development and do not necessary prove the ellipsoidal nature of the strongly deformed rotating states. The SD bands become yrast around $25 \hbar$ and decay into the yrast sequence at spin $16 - 18 \hbar$. The calculations lead to superdeformed shapes characterized by $I \sim 60 \hbar^2 \text{MeV}^{-1}$ and $Q \sim 10 \text{ eb}$ in correct agreement with experimental data. The theoretical ND states exist at relatively high spins but do no more correspond to the lowest minimum and furthermore the barrier between the two minima is thin and low. The second minimum appearing at $l=0$ does not allow to explain the sudden decay out of the SD bands.

When the rotation energy increases (fig. 5.a) the macroscopic curves become descendent and a minimum is observable. Shell correction are only deepening the second minimum with about 1.5 MeV within the same region of deformation.

One can perform the same analysis for ^{152}Dy , for which the hump in the first stages of elongation is also generated by the shell corrections (fig. 6.a). Negative values of δE_{shell} induces the second minimum in the total energy. As the angular momentum increases, the slope of macroscopic energy curve approaches to zero. For $l=40 \hbar$ (fig. 6.b) one obtains nearly a plateau and the ground state minimum almost disappeared. The only minimum in the total energy now is the superdeformed state. The two minima coexist up to $l=40 \hbar$ (fig. 7.a). Experimentally [7,13,45,49,50], ND bands have been observed with a highest spin of around $40 \hbar$ and an excitation energy of 13 MeV . SD states extend in spin from 22 to $60 \hbar$, in excitation energy from 12 to 30 MeV and become yrast around $55 \hbar$. The associated quadrupole moment and moment of inertia are around 17 eb and $85 \hbar^2 \text{MeV}^{-1}$. Theoretically the first minimum which lodges the ND states disappears effectively around $40 \hbar$ at an excitation energy around 13 MeV . The second minimum seems to be lower than experimentally observed both in spin and excitation range. Nevertheless the theoretical values $Q \sim 15 \text{ eb}$ and $I \sim 80 \hbar^2 \text{MeV}^{-1}$ are in reasonable agreement with the experimental results. Furthermore, the stability against fission of these superdeformed states at $60 \hbar$ is ensured by a barrier of more than 15 MeV in this deformation valley. The fusion-fission barrier survives to spin around $110 \hbar$ (fig. 7b) and macroscopic hyperdeformed states appear in a very high spin range [26]. The possibility to conciliate low fission barrier heights and high maxima angular momenta is really a specificity of this deformation valley through quasi-molecular shapes.

It is interesting to see how the protons and neutrons are contributing at the shell corrections. Fig. 8 displays the proton - $E_{sh}^{(p)}$ and neutron - $E_{sh}^{(n)}$ shell corrections and their sum E_{sh} for ^{192}Hg . Because $Z=80$ is very close to the magicity of $Z=82$, one has a negative value of $E_{sh}^{(p)} = -2.7 \text{ MeV}$ at the sphere, whereas the neutron contribution starts with a positive value. The result is a slightly positive total shell correction. Unfortunately the model does not

reproduce oblate like shapes, therefore the oblate minimum which normally corresponds to a negative ϵ_2 deformation [42] is not seen. In this case, the sphere is a step further from the deformed ground state. As the distance between centers increase, the neutron shell correction becomes negative. The total shell correction follows this behaviour in the same region.

The macroscopic, microscopic and total energies are displayed in Fig. 9 at $l=0$ and $40 \hbar$, while in fig. 10, the evolution of the total energy with the angular momentum is shown. Experimentally [45,51–53] almost spherical rotational bands have been observed till $34 \hbar$ while SD bands have been detected in the $8 - 40 \hbar$ spin range with a limit of 14 MeV for the excitation energy, their geometrical characteristics being $Q \sim 20 \text{ eb}$ and $I \sim 120 \hbar^2 \cdot \text{MeV}^{-1}$. Theoretically, the shell effects lead also to a first quasi-spherical minimum and a second well corresponding to SD shapes. The calculated geometrical characteristics are $Q \sim 21 \text{ eb}$ and $I \sim 119 \hbar^2 \text{MeV}^{-1}$, in very good agreement with the experimental data. The potential barriers at $l=0$ and $10 \hbar$ are very similar. They cannot explain the sudden decay-out of the SD bands at around $8 \hbar$.

The characteristics of the hyperdeformed nuclei found in this peculiar quasi-molecular deformation valley are not deeply changed by the shell effects. The following formulas fitted from the macroscopic energy give the lower and upper limits for the angular momentum, excitation energy, mass quadrupole moment and moment of inertia of the predicted hyperdeformed β -stable nuclei [27]:

$$\begin{aligned} L_{sup}(A_\beta) = & 43.7 - 3.89A_\beta + 0.18563A_\beta^2 - 3.3903 \times 10^{-3}A_\beta^3 + \\ & 3.311395 \times 10^{-5}A_\beta^4 - 1.776482 \times 10^{-7}A_\beta^5 + \\ & 4.9078 \times 10^{-10}A_\beta^6 - 5.4568 \times 10^{-13}A_\beta^7 \end{aligned} \quad (59)$$

$$\begin{aligned} L_{inf}(A_\beta) = & 9.63 - 0.4076 \times A_\beta + 0.02399A_\beta^2 - 2.7475 \times 10^{-4}A_\beta^3 + \\ & 1.3615 \times 10^{-6}A_\beta^4 - 2.5824 \times 10^{-9}A_\beta^5 \end{aligned} \quad (60)$$

$$E_{exc,sup}(A_\beta) = 26.5 + 1.503A_\beta - 9.02 \times 10^{-3}A_\beta^2 + 1.16 \times 10^{-5}A_\beta^3 \quad (61)$$

$$\begin{aligned} E_{exc,inf}(A_\beta) = & 7.4 + 0.682A_\beta - 4.234 \times 10^{-3}A_\beta^2 - 3.86 \times 10^{-6}A_\beta^3 + \\ & 6.783 \times 10^{-8}A_\beta^4 - 1.3121 \times 10^{-10}A_\beta^5 \end{aligned} \quad (62)$$

$$\begin{aligned} Q_{20,sup}(A_\beta) = & -26.3 + 2.893A_\beta - 0.114374A_\beta^2 + 2.4297 \times 10^{-3}A_\beta^3 - \\ & 2.73872 \times 10^{-5}A_\beta^4 + 1.692903 \times 10^{-7}A_\beta^5 - \\ & 5.37284 \times 10^{-10}A_\beta^6 + 6.8204 \times 10^{-13}A_\beta^7 \end{aligned} \quad (63)$$

$$\begin{aligned} Q_{20,inf}(A_\beta) = & -3.9 + 0.415A_\beta - 0.01029A_\beta^2 + 1.5928 \times 10^{-4}A_\beta^3 - \\ & 1.1136 \times 10^{-6}A_\beta^4 + 3.694 \times 10^{-9}A_\beta^5 - 4.485 \times 10^{-12}A_\beta^6 \end{aligned} \quad (64)$$

$$\begin{aligned} I_{sup}(A_\beta) = & 26.3 - 2.4013A_\beta + 0.08908A_\beta^2 - 1.28912 \times 10^{-3}A_\beta^3 + \\ & 9.78952 \times 10^{-6}A_\beta^4 - 3.59728 \times 10^{-8}A_\beta^5 + \\ & 5.07115 \times 10^{-11}A_\beta^6 \end{aligned} \quad (65)$$

$$I_{inf}(A_\beta) = 0.97 + 0.0525A_\beta + 0.003006A_\beta^2 + 1.19 \times 10^{-5}A_\beta^3 - 1.3589 \times 10^{-7}A_\beta^4 + 3.756 \times 10^{-10}A_\beta^5 \quad (66)$$

9 Conclusions

The macroscopic-microscopic energy of rotating nuclei in the fusion-like deformation valley has been determined within a generalized liquid drop model, the two-center shell model and Strutinsky shell corrections. The l -dependent potential barriers of the ^{84}Zr , ^{132}Ce , ^{152}Dy and ^{192}Hg nuclei have been particularly calculated. The observed first and second potential wells are reproduced and the calculated moment of inertia and quadrupole moment of the associated normally and superdeformed nuclei are in correct agreement with the experimental results. For the lightest nucleus, the second well does not exist at $l=0$ but a plateau already appears in the deformation barrier allowing the progressive appearance of the second minimum with increasing spins. For the heavier nuclei such picture is absent and the second potential well exists at $l=0$, as in most theoretical studies. Consequently, it is difficult to explain the sudden decay-out of the superdeformed bands at low spins. The shell effects at large deformations are perhaps overestimated. The influence of the relative height of the two potential minima and of the thickness and height of the barrier between the two minima is also poorly understood.

The shell effects explain alone the existence of the first well while the macroscopic and microscopic energies both contribute to the stabilization of the superdeformed states. A third well corresponding to hyperdeformed quasi-molecular shapes appears at very high angular momenta. It is generated by the centrifugal forces and the persistence of a fusion-fission barrier, the maximum of which corresponds to two well-separated spherical nuclei. These highly deformed potential pockets might be directly populated in cold fusion reactions, the asymmetry degree of freedom playing in such a case an important role.

Acknowledgement

We thank G. Legoux who determined several analytic fits. One of us (RAG) is thankful for support of his visit by the french Institut National de Physique Nucleaire et de Physique de Particules and Ecole des Mines de Nantes.

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Figure captions

Fig. 1. Typical compact and necked shape with quasi-spherical ends in the fusion-like deformation valley.

Fig. 2a. Deformation barrier for ^{84}Zr in the fusion-like deformation valley as a function of the deformation parameter R . The microscopic, macroscopic and total energies are respectively given by the thin solid, dashed and thick solid curves.

Fig. 2b. Same as fig. 2.a but for $l=20 \hbar$.

Fig. 3. Sum of the macroscopic-microscopic and rotational energies as functions of the angular momentum ($\hbar$ unit) and the deformation for ^{84}Zr . The vertical dashed line indicates the touching point between the spherical fragments.

Fig. 4a. Sum of the macroscopic and rotational energies as functions of the angular momentum ($\hbar$ unit) and the deformation for ^{132}Ce . The vertical dashed line indicates the touching point between the spherical fragments.

Fig. 4b. Same as fig. 4a with microscopic energy included.

Fig. 5a. Same as fig. 4a but for higher angular momenta.

Fig. 5b. Same as fig. 4b but for higher angular momenta.

Fig. 6a. Deformation barrier for ^{152}Dy in the fusion-like deformation valley as a function of the deformation parameter R . The microscopic, macroscopic and total energies are respectively given by the thin solid, dashed and thick solid curves.

Fig. 6b. Same as fig. 6a but for $l=40 \hbar$.

Fig. 7a. Sum of the macroscopic-microscopic and rotational energies as functions of the angular momentum ($\hbar$ unit) and the deformation for ^{152}Dy .

Fig. 7b. Same as fig. 7a but for higher angular momenta.

Fig. 8. Microscopic energy in the fusion-like deformation valley for ^{192}Hg . The shell corrections for the neutrons and protons are given by the dashed curves while the total shell effects are indicated by the thick solid curve.

Fig. 9a. Deformation barrier for ^{192}Hg in the fusion-like deformation valley as a function of the deformation parameter R . The microscopic, macroscopic and total energies are respectively given by the thin solid, dashed and thick solid curves.

Fig. 9b. Same as fig. 9a but for $l=40 \hbar$.

Fig. 10. Sum of the macroscopic-microscopic and rotational energies as functions of the angular momentum ($\hbar$ unit) and the deformation for ^{192}Hg .

Fig. 1

Fig. 2a

Fig. 2b

Fig. 3

Fig. 4a

Fig. 4b

Fig. 5a

Fig. 5b

Fig. 6a

Fig. 6b

Fig. 7a

Fig. 7b

Fig. 8

Fig. 9a

Fig. 9b

Fig. 10