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# CALCULATION OF NUCLEAR LEVEL DENSITY RELEVANT FOR THORIUM-BASED REACTORS

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*Abstract*. In this paper the problem of nuclear level density is investigated. The notion is intuitively introduced and then rigurously defined. Several procedures for its calculation, among the most performant, are described. We start with one of the first proposed approach, the equidistant model, continue with empirical methods like Back Shifted Fermi Gas and Gilbert-Cameron and arrive at some modern approaches, as Ignatyuk method and modified Ignatyuk method. Revealing for each method its advantages and limits, we concentrate on Ignatyuk-type methods. Practical recipes for the determination of the needed parameters are given. These are referring to the shape description and to the calculation of deformation energy, shell correction and collective enhancement factors (rotational and vibrational). The presented formalism is applied to study some protactinium isotopes, nuclei of practical interest which appear in the thorium fuelled nuclear reactors.

*Key words:* nuclear reaction, level density, statistical model, nuclear shape parametrization, pairing interaction, shell correction, collective enhancement, neutron induced cross sections, thorium-based reactors.

## 1. INTRODUCTION

The evaluation of the cross sections is one of the main tasks in the field of low-energy nuclear reactions. These reactions are described by different models which depend on the energy of the projectiles. The most investigated range of energies is [0, 200] MeV. In this range one can distinguish three classes of reactions upon the time required for production. The fastest are called direct reactions and the slowest are the reactions giving rise to a compound nucleus. Between these extreme processes there are the pre-equilibrium reactions. To calculate the cross sections in the model of compound nucleus and in pre-equilibrium models, one of the most important ingredients is the level density. This notion is connected to the fact that the typical spacings of the first excited nuclear levels in medium and heavy nuclei are of the order of a tenth or some

tenths of MeV for low excitation energies, but become very densly spaced when these energies increase, so that quickly an individual description of them is no longer possible. Before WWII it was realized that a statistical description is needed [1].

The simplest model resides in considering that an excited level of the nucleus results from the excitation of a certain number of its constituents, the others constituents remaining unperturbed. Then one speaks of intrinsic or incoherent excitations. The level densities involving a fix number of constituents are called partial densities, unlike the total densities, when no restriction on the number of excited fermions is imposed.

One can also consider excited levels of a more complicated nature, namely by treating the fermion ensemble in a coherent manner. For example the nucleus can vibrate around its form of equilibrium: one then speaks of vibration levels. The excited levels resulting from coherent excitations are qualified as collective levels, if all the fermions are involved. In this case, the partial or total densities are called "effective", in contrast to the "intrinsic" densities where the notion of collective levels does not appear.

Many works have been elaborated for the evaluation of these densities. In fact, the calculation of level densities has followed the evolution of the knowledge about the properties of the nuclei. The first studies for the determination of level densities have been achieved at the end of 30'ies, by representing the nucleus as a gas of fermions without interaction confined in a given volume (the Fermi gas model) and, more precisely, by using the zero'th order approximation of this model: the equidistant model. An analytical formula of cumulated densities (based on a mathematical approximation named the approximation of the *saddle point*) has been obtained by Bethe in 1937 [1]. Later on, Ericson (1960) has proposed the first analytical expression for partial densities [2]. This has been modified and improved several times. However, the equidistant model contains too few physical informations to lead at realistic expressions of level densities. Phenomenological adjustments have been considered in order to reproduce some properties revealed by the experimental data. To explain these adjustments, one must go beyond the approximation of equidistant model and calculate the level densities in a shell model. The most common methods of calculation are: (i) a general numerical method, based on the approximation of saddle point, which can lead in certain conditions to analytical results (*partition function method*), and (ii) the combinatorial method, an approach which amounts to finding the number of ways in which the nucleons can be distributed among the available single-particle levels for a fixed energy of the nucleus. These methods of calculation are employing various nuclear models: (i) The model of independent fermions, which allows an easy evaluation of the grand partition function, (ii) the equidistant model, (iii) the shell model, which compared to the previous two models, employs a more realistic single-particle basis in the calculation of the level density, (iv) the model of interacting fermions, where residual interactions are included in the shell-model

Hamiltonian. This is done by means of the pairing interaction. By introducing the notion of pairing of the nuclei, the theoretical description of level densities is more improved, mainly to lower energies. An improvement of these nuclear models was achieved by including the effect of the collective degrees of freedom which are statistically coupled to the intrinsic degrees of freedom. An important issue in this case is the computation of the deformation distribution function with excitation energy.

On the other hand, as numerous shell models exist, the numerical results are difficult to be exploited from a quantitative point of view. The only way to choose a shell model instead of another whould be the comparison of predictions given by each of them with the experimental data. But the data relative to level densities cover only limited energetic domains and are affected by important systematic errors. Therefore, the numerical results are used from a qualitative point of view to modify the pre-established analytical formula. One can infer for example that a parameter considered as constant in the equidistant model is in fact dependent on the excitation energy and one can find a functional form to describe this dependence. The parameters of the functional form are then adjusted on the basis of the existing experimental data. One can easily understand that, in such conditions, the predictive character of the used analytical expressions is very questionable outside the range on which the adjustments have been performed.

Thus, one can see that for a good prediction of densities we have, on the one hand, to dispose of an accurate, general and rapid numerical method to calculate the partial or total level densities on large energetic domains, and, on the other hand, the calculation must rely on a model able to reproduce the experimental data and possessing sufficiently solid physical bases in order to have a real predictive character.

In this paper we shall review some of the fundamental relations, calculation methods and nulear models used in the determination of the level density function with the aim to apply this formalism to nuclei relevant for the Thorium-$^{233}$U cycle.

## 2. THE LEVEL DENSITY PROBLEM

In this section we show why it is necessary to introduce a level density function to describe the excited nuclear levels. We shall then describe the experimental data which permit to obtain informations both qualitative and quantitative on these densities. At the end, some fundamental relations will be presented, required for the calculation of the excited level densities.

### 2.1. THE NOTION OF LEVEL DENSITY

Since the dawn of nuclear physics, the accumulation of experimental data has put in evidence the discrete structure of the excited levels spectra for excitation

energies not exceeding a few MeV. Some characteristics of these discrete levels (the energy, the spin and the parity, for example) are often well explained by the most modern theories of nuclear structure. Beyond a few MeV, an individual description of the discrete levels becomes impossible. Indeed, not only the levels are more and more closed to each other, but acquire larger widths. For these reasons, they become undistinguishable. Therefore, the only possibility to describe them is the statistical frame. For this one introduces a level density function, denoted with $\rho$, which can be defined by the relation

$$\rho(U) = \frac{\mathrm{d}}{\mathrm{d}U} N(U) \tag{2.1}$$

where $N(U)$ is the number of levels with energy lower or equal to the excitation energy $U$.

One can also refine the preceding definition by considering the excited level density $\rho(U, J, \pi)$ for a given excitation energy $U$, spin $J$ and parity $\pi$. When the nucleus possesses a symmetry axis in its intrinsic system of reference, one can also express the excited level density in terms of the diverse projections $M$ of spins $J$ on this axis. This density $\rho(U, M, \pi)$ is called in general density of excited states. The relation between $\rho(U, M, \pi)$ and $\rho(U, J, \pi)$ is

$$\rho(U, M, \pi) = \sum_{J \geq M} \rho(U, J, \pi). \tag{2.2}$$

Of course, one can obtain experimental informations only on the level densities and not on the state densities.

Let us see now in what consist the experimental data at our disposal.

## 2.2. THE EXPERIMENTAL DATA

The level density function, as seen, comes directly from our incapacity to treat individually the excited levels of the nucleus beyond excitation energies of a few MeV. From this reason, one distinguishes naturally two regions of interest: the domain of low energies where the discrete structure is observed and the domain, named continuous, where the notion of level density acquires its whole sense, since one cannot observe anymore the discrete structure of excited nuclear levels.

At low energy it is possible, for certain nuclei, to determine experimentally some characteristics of the first discrete excited levels. More concrete, their energy can be known, which allows to draw the histogram representing the function $N$ from eq. (2.1) in terms of $U$. We will call it in the following *cumulated histogram*. By choosing a logarithmic repesentation, one systematically observes a linear behaviour at low energy (see Fig. 2.2 for $U \leq 7$ MeV), irrespective of the studied

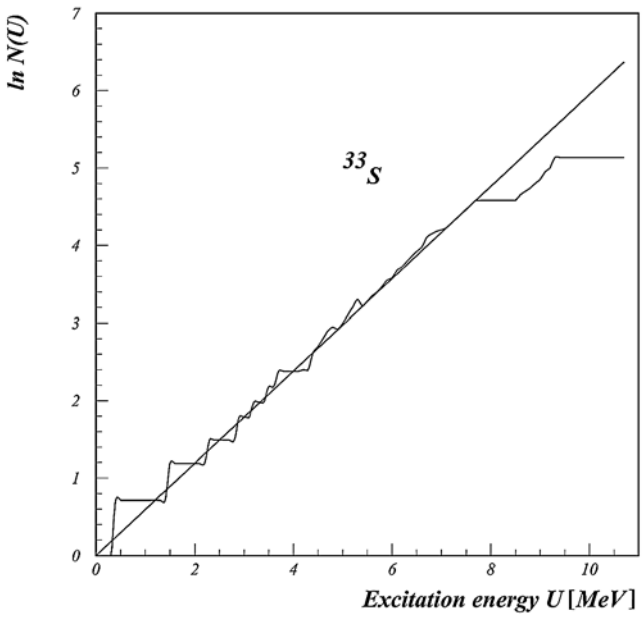


Fig. 1 – The cumulated histogram of discrete levels for $^{33}$S in terms of the excitation energy $U$. The straight line represents the linear function from eq. (2.3) with $U_0 = 0$ and $T = 1.68$ MeV.

nucleus. It is thus possible to describe empirically the function $N(U)$ by adopting the analytic form

$$\ln N(U) = \frac{U - U_0}{T}, \tag{2.3}$$

named *temperature law*, where $U_0$ and $T$ are adjustable parameters.

The level densities seem to increase exponentially with the energy, at least at low energy. In Fig. 2.2 one can also observe, beyond 7.5 MeV, a deviation of the cumulated histogram indicating a smaller number of observed levels than the extrapolation of law (2.3). This remark is valid for any nucleus. In fact, beyond of a certain excitation energy, which depends on the nucleus, some discrete levels cannot be distinguished any longer.

Except this exponential increase with the energy, the analysis of several cumulated histograms, for different nuclei, put into evidence the dependence of level densities on the mass number $A$. One ascertains, in average, a decreasing of the parameter $T$ as a function of the nuclear mass. Given the form of the eq. (2.3), $N(U)$ is thus, in average, an increasing function of $A$ for a fixed energy $U$. Certain mass regions make exception from this rule, namely the regions $A \approx 60$, $A \approx 90$, $A \approx 140$ and $A \approx 120$, where one can clearly distinguish peaks, indicating a decrease of the number of discrete excited levels observed. These peaks, usually

named with the general term of *shell effects*, are due to the presence, in these mass regions, of some nuclei with *magic* properties.

A last remark concerning these histograms can be made. It proceeds from the comparison of the cumulated histograms between nuclei with very close masses, but with a number of neutrons (respectively protons) even or odd. If one defines the parity index $\chi$ of the nucleus ${}^{A}_{Z}X_{N}$ by

$$\chi = \delta_{N,par} + \delta_{Z,par} \tag{2.4}$$

where $\delta_{K\ par}$ is equal with 1 if $K$ is even and 0 if $K$ is odd, one finds that $N(U)$ is larger as much as $\chi$ is smaller. This effect is called *odd-even effect*.

In the range of low energies, it is thus possible to observe some properties of the level densities. But, for higher excitation energies, nothing guarantees that these properties persist. From here results the necessity of having experimental informations on level densities at high energies. But, as soon as we are placed in the energy range above a few MeV (usually over 6–8 MeV), the data relative to level densities are difficult to be directly obtained, because the levels are no more distinguishable. However some indications are accessible, which are evidently so much the less precise as the higher is the excitation energy.

The first source of experimental information, in continuum, is related to the average spacing of neutronic resonances and, sometimes, protonic. When nuclear reactions are studied by using, as projectiles, the neutrons of very weak incident energy $(U_i \ll 1\,\mathrm{MeV})$, one observes peaks in the curves of total cross sections, for certain energies of incident neutrons. These peaks, or resonances, correspond to some excited levels of the compound nucleus (neutron + target system) with energies slightly superior to the binding energy $B_n$ of the neutron in this compound nucleus. The analysis of their average spacing $D$ supplies an indication on the density of these particular excited levels. More precisely, among the observed resonances, one can especially detect those which are due to the $s$ waves, corresponding to the incident neutrons of null angular momentum ($l = 0$). The average spacing of these particular resonances are denoted by $D_0$.

If one considers a target of spin $J_c$ and a parity $\pi_c$, the usual conservation laws implies that the compound nucleus, created with a neutron of angular momentum $l$ and of spin $s$, has a spin $J_{NC}$ and a parity $\pi_{NC}$ so that

$$\boldsymbol{J}_{NC} = \boldsymbol{J}_c + \boldsymbol{l} + \boldsymbol{s}$$

and

$$\pi_{NC} = \pi_c (-1)^l .$$

Based on these aspects, the values $D_0$ can be related to the level densities of the compound nucleus by the relations:

$$D_0 \approx \frac{1}{\rho(B_n, J_c + 1/2, \pi_c) + \rho(B_n, J_c - 1/2, \pi_c)} \tag{2.5}$$

for a target nucleus of spin $J_c \neq 0$ and

$$D_0 \approx \frac{1}{\rho(B_n, 1/2, \pi_c)} \tag{2.6}$$

for a target nucleus even-even (of spin $J_c = 0$).

The determination of $D_0$ values has been the subject of numerous works and these mean values can be represented in terms of the mass $A$ of the compound nucleus. This representation causes the appearence of two major phenomena, namely: the decrease of $D_0$ when $A$ increases and the rise of peaks, more or less pronounced, at mass regions $A \approx 60$, $A \approx 90$, $A \approx 140$ and $A \approx 210$. This shows that the shell effects, already observed in the case of the cumulated histograms at low energies, persist at higher excitation energies. In the same time, the values of $D_0$ are difficult to obtain and are often affected by errors. In addition, the nuclei for which these values are known are in limited number and near to the stability valley. However, they constitute the most trustful data about level densities, outside the region in which the discrete structure is visible. For this reason they are abundantly used for the adjustment of analytic expression and constitute also a good test for the validation of the microsopic calculations.

The evaluation of level densities for energies over $B_n$ cannot be done directly, as in the previous cases. In fact, in this domain, one can only compare the experimental cross sections with the values computed on the basis of a model of nuclear reactions. If the level density is the single unknown, its value can be then estimated. In this case, the obtained densities are clearly dependent on the approximations made in the model adopted for the calculus of the cross sections. What can be obtained are indications on the orders of magnitude of these densities.

Thus, it is clear that the experimental informations on the excited nuclear level densities are limited. In the best cases, the densities are known until excitation energies of a few MeV. Values for higher energies are often affected by errors. In these conditions, only a theoretical approach to level densities, founded on a microscopic model, could provide us a tool to reproduce the known experimental data at low energy and at $B_n$.

For such calculations, it is necessary a formal definition of the level densities. This will be given in what follows.

## 2.3. DEFINITIONS AND BASIC RELATIONS

We have seen (eq. 2.1) that the level density could be defined as the derivative, with respect to the excitation energy $U$, of the number $N(U)$ of

cumulated levels until the energy $U$. Since the function $N(U)$ is a step function, its derivative is discontinuous, but can be defined with the help of the distributions. In a very general manner, the density of excited levels of a system containing $A$ particles, in terms of the excitation energy $E$, is written as:

$$\rho(A, E) = \sum_{n,i} \delta(A - n)\delta(E - E_i(n)), \tag{2.7}$$

where $E_i(n)$ represents the energy of the quantum level $i$ of the system containing $n$ particles and $\delta$ is the Dirac distribution function.

The Laplace transform of the level density, noted $\mathcal{Z}$, is

$$\mathcal{Z}(\alpha, \beta) = \int_0^\infty \int_0^\infty \rho(A, E) \exp(\alpha A - \beta E) \mathrm{d}A \mathrm{d}E \tag{2.8}$$

and becomes, by using eq. (2.7),

$$\mathcal{Z}(\alpha, \beta) = \sum_{i,n} \exp[\alpha n - \beta E_i(n)]. \tag{2.9}$$

This is the partition function of a system of $n$ particles with corresponding eigenvalues $E_i(n)$ ($i$ = 1, 2, …). The level density is then the inverse Laplace transform of the partition function. Hence it can be written in the form

$$\rho(A, E) = \left(\frac{1}{2\pi i}\right)^2 \int_{-i\infty}^{+i\infty} \mathrm{d}\alpha \int_{-i\infty}^{+i\infty} \mathrm{d}\beta \; \mathcal{Z}(\alpha, \beta) \exp(-\alpha A + \beta E). \tag{2.10}$$

One can also take into account other variables in the expression of the level density, as the spin $J$ of excited nuclei or their parity $\pi$. For this, it is sufficient to add terms of the form $\delta(J - J_i(n))$ or $\delta(\pi - \pi_i(n))$ in eq. (2.9), with the implied consequences for the expression of the partition function.

Thus, the problem resorts to the evaluation of the inverse transform of the Laplace integral (2.10). This can be approximated in the frame of some models, as will be seen in the next section.

## 3. CALCULATION PROCEDURES OF THE LEVEL DENSITIES

For the calculation of the level densities, several models have been elaborated (see, *e.g.* [3]). We shall firstly present one of the simplest case – the equidistant model. It is, on the one hand, instructive, and, on the other hand, it constitutes the basis of the most modern expressions of level densities.

## 3.1. THE LEVEL DENSITIES IN THE EQUIDISTANT MODEL

In this model, the nucleus is represented as a system of fermions susceptible to occupy levels whose energies $\epsilon_i$ are fixed and regularly spaced. We also suppose that the energy scale is such that $\epsilon_i \geq 0$ for any *i*.

For simplicity, we shall limit ourselves for the moment to the case when the protons and the neutrons are not distinguished. The nucleus is thus an ensemble of *A* nucleons. When the system is in its ground state, the first *A* levels are occupied and the rest are empty. When the system has an excitation energy, some fermions are moving towards the levels initially unoccupied. In this case, the nucleus is in an excited state and particle levels appear in the empty places of the ground state, while some levels initially occupied become empty.

In these conditions, the intrinsic density of excited levels, for a certain excitation energy *U* can be calculated with the help of the saddle point approximation [4, 5]. This is based on the fact that the integrand in eq. (2.10) is a function which varies rapidly with respect to $\alpha$ and $\beta$. Thus, the main contribution in integral comes from a little region around the point $(\alpha_0, \beta_0)$ in which the integrand is stationary. The conditions which determine this stationary point are

$$A - \left| \frac{\partial}{\partial \alpha} \ln \mathcal{Z}(\alpha, \beta) \right|_{\alpha_0, \beta_0} = 0 \tag{3.1}$$

and

$$E + \left| \frac{\partial}{\partial \beta} \ln \mathcal{Z}(\alpha, \beta) \right|_{\alpha_0, \beta_0} = 0. \tag{3.2}$$

Expanding the exponent in the integrand up to the second order around the point determined by the conditions (3.1) and (3.2), one gets a Gaussian integral which can be evaluated, resulting for $\rho$ the expression

$$\rho(A, E) = \frac{\mathcal{Z}(\alpha_0, \beta_0) \exp[\beta_0 E - \alpha_0 A]}{2\pi\sqrt{D}} = \frac{\exp[\ln \mathcal{Z}(\alpha_0, \beta_0) + \beta_0 E - \alpha_0 A]}{2\pi\sqrt{D}} \tag{3.3}$$

In eq. (3.3), the argument of the exponential is the entropy *S* of the fermion gas, while $\alpha_0$ and $\beta_0$ are the coordinates of the saddle point which is the point where the entropy of the system is minimum. *D* is the determinant of the matrix whose elements are the second partial derivatives of $\ln \mathcal{Z}(\alpha, \beta)$ with respect to the variables $\alpha$ and $\beta$ evaluated at the saddle point, *i.e.*

$$D = \left| \begin{matrix} \frac{\partial^2 \ln \mathcal{Z}}{\partial \alpha^2} & \frac{\partial^2 \ln \mathcal{Z}}{\partial \alpha \partial \beta} \\ \frac{\partial^2 \ln \mathcal{Z}}{\partial \beta \partial \alpha} & \frac{\partial^2 \ln \mathcal{Z}}{\partial \beta^2} \end{matrix} \right|_{\alpha=\alpha_0, \beta=\beta_0}$$

To evaluate the function $\mathcal{Z}(\alpha,\beta)$ it is supposed that the particles are independent. In this approximation (see [6]) we can write

$$n=\sum_{\nu}(n_\nu)_i \tag{3.4}$$

and

$$E_i=\sum_{\nu}(n_\nu)_i\epsilon_\nu. \tag{3.5}$$

$(n_\nu)_i$ is the occupation number for the single-particle state $\nu$ in the quantum state $i$ of the system of $n$ particles; it has the value 0 or 1 according to the exclusion principle. By using these relations in the expression (2.9) we get

$$\mathcal{Z}(\alpha,\beta)=\prod_{\nu}[1+\exp(\alpha-\beta\epsilon_\nu)]. \tag{3.6}$$

In each factor, the term 1 corresponds to $n_\nu=0,$ while the exponential term corresponds to $n_\nu=1.$ The equidistant model is a particular case of independent particle system, so that the relation (3.6) is valid in the frame of the initial hypothesis.

By taking the logarithm we have

$$\ln\mathcal{Z}(\alpha,\beta)=\sum_{\nu}\ln[1+\exp(\alpha-\beta\epsilon_\nu)]. \tag{3.7}$$

If we define the density $g$ of the individual levels by

$$g(\epsilon)=\sum_i\delta(\epsilon-\epsilon_i) \tag{3.8}$$

we can write

$$\ln\mathcal{Z}(\alpha,\beta)=\int_0^\infty g(\epsilon)\ln[1+\exp\{\alpha-\beta\epsilon)\}]\mathrm{d}\epsilon=\int_0^\infty g(\epsilon)\ln[1+\exp\{\beta(\mu-\epsilon)\}]\mathrm{d}\epsilon, \tag{3.9}$$

by using the notation $\mu=\alpha/\beta.$

Then we separate this integral in two parts by writing

$$\ln\mathcal{Z}(\alpha,\beta)=\int_\mu^\infty g(\epsilon)\ln[1+\exp\{\beta(\mu-\epsilon)\}]\mathrm{d}\epsilon+\int_0^\mu g(\epsilon)\ln[1+\exp\{\beta(\mu-\epsilon)\}]\mathrm{d}\epsilon. \tag{3.10}$$

Let us note with $I_1$, respectively with $I_2$ the two terms.

By adding and subtracting the term $\beta(\mu-\epsilon)$ in the second intergal, we have

$$I_2=\int_0^\mu g(\epsilon)\beta(\mu-\epsilon)\mathrm{d}\varepsilon+\int_0^\mu g(\epsilon)[\ln(1+\exp\{\beta(\mu-\epsilon)\})-\beta(\mu-\epsilon)]\mathrm{d}\epsilon. \tag{3.11}$$

Noting that

$$\ln(1+\exp\{\beta(\mu-\epsilon)\})-\beta(\mu-\epsilon)=\ln(1+\exp\{\beta(\mu-\epsilon)\})-\ln(\exp\{\beta(\mu-\epsilon)\})=$$
$$=\ln\frac{1+\exp\{\beta(\mu-\epsilon)\}}{\exp\{\beta(\mu-\epsilon)\}}=\ln(1+\exp\{-\beta(\mu-\epsilon)\})$$

we can write

$$I_2=\int_0^{\mu}g(\epsilon)\beta(\mu-\epsilon)\mathrm{d}\varepsilon+\int_0^{\mu}g(\epsilon)\ln(1+\exp\{-\beta(\mu-\epsilon)\})\mathrm{d}\varepsilon. \tag{3.12}$$

In the second integral of $I_2$ we perform the change of variable $\mu-\epsilon=\epsilon'$ and we have

$$\int_0^{\mu}g(\epsilon)\ln(1+\exp\{-\beta(\mu-\epsilon)\})\mathrm{d}\epsilon=-\int_{\mu}^{0}g(\mu-\epsilon')\ln[1+\exp(-\beta\epsilon')]\mathrm{d}\epsilon'=$$
$$=\int_0^{\mu}g(\mu-\epsilon')\ln[1+\exp(-\beta\epsilon')]\mathrm{d}\epsilon'=\int_0^{\infty}g(\mu-\epsilon')\ln[1+\exp(-\beta\epsilon')]\mathrm{d}\epsilon'$$

For the last relation we have taken into account that $g(\epsilon)=0$ if $\epsilon<0$ according to the definition (3.8).

Next we perform in $I_1$ the change of variable $-\mu+\epsilon=\epsilon'$ and we have

$$I_1=\int_0^{\infty}g(\mu+\epsilon')\ln[1+\exp(-\beta\epsilon')]\mathrm{d}\epsilon'$$

Thus, we can now write

$$\ln\mathcal{Z}(\alpha,\beta)=\beta\int_0^{\mu}g(\epsilon)(\mu-\varepsilon)\mathrm{d}\epsilon+\int_0^{\infty}[g(\mu+\epsilon)+g(\mu-\epsilon)]\ln[1+\exp(-\beta\epsilon)]\mathrm{d}\epsilon \tag{3.13}$$

where we returned everywhere to the integration variable $\epsilon$.

Defining the energy $\epsilon_F$ by the equation

$$\int_0^{\epsilon_F}g(\epsilon)\mathrm{d}\varepsilon=A$$

and putting

$$\int_0^{\epsilon_F}\epsilon g(\epsilon)\mathrm{d}\epsilon=E_0$$

the equation (3.13) is transformed in

$$\ln\mathcal{Z}(\alpha,\beta)=\alpha A-\beta E_0+\beta\int_{\epsilon_F}^{\mu}g(\epsilon)(\mu-\epsilon)\mathrm{d}\varepsilon+$$
$$+\int_0^{\infty}[g(\mu+\epsilon)+g(\mu-\epsilon)]\ln[1+\exp(-\beta\epsilon)]\mathrm{d}\epsilon. \tag{3.14}$$

According to the relation (3.5), $E_0$ is the energy of the nucleus in its ground state. The energy $\epsilon_F$ is the energy of the last occupied level and is called the *Fermi energy*.

To analytically calculate the integrals previously obtained, we make use now of the equidistant model hypothesis by supposing that $g(\epsilon)$ is constant and has the value $g_0$. One can then evaluate the integrals of eq. (3.14) and one arrives to

$$\ln \mathcal{Z}(\alpha, \beta) = \alpha A - \beta E_0 + \frac{\pi^2}{6} g_0 \beta^{-1} + \beta g_0 \frac{(\mu - \epsilon_F)^2}{2}. \tag{3.15}$$

The equations (3.1) and (3.2), which define the coordinates of the saddle point, can be now solved. One finds the relations

$$E - E_0 - \frac{\pi^2}{6} g_0 \beta_0^{-2} + g_0 \frac{(\mu_0 - \epsilon_F)^2}{2} = 0 \tag{3.16}$$

and

$$\mu_0 = \alpha_0 / \beta_0 = \epsilon_F .$$

By introducing the excitation energy $U = E - E_0$, as well as the thermodynamic temperature $t = \beta_0^{-1}$, from the relation (3.16) one obtains the state equation of the fermion system

$$U = \frac{\pi^2}{6} g_0 \beta_0^{-2} = at^2 \tag{3.17}$$

in which appears the quantity $a$, named the *the level-density parameter*. We have

$$a = \frac{\pi^2}{6} g_0 .$$

With the help of equation (3.15) one can also calculate the determinant of the second partial derivatives of $\ln \mathcal{Z}(\alpha, \beta)$ with respect to $\alpha$ and $\beta$ at the saddle point:

$$D = \frac{\pi^2}{3} g_0^2 \beta_0^{-4} .$$

Finally,

$$\rho(A, U) = \frac{\exp(2\sqrt{aU})}{4\sqrt{3}U} \tag{3.18}$$

In many cases, this formula, initially derived by Bethe [1], represents a remarkable approximation of the exact value of the level density.

If one makes distinction between the protons and the neutrons, one can show [2, 5]) that

$$\rho(N, Z, U) = \frac{\sqrt{\pi}}{12} \frac{\exp(2\sqrt{aU})}{a^{1/4} U^{5/4}} \tag{3.19}$$

The parameter $a$ is defined by the relation

$$a = \frac{\pi^2}{6}(g_\pi + g_\nu). \tag{3.20}$$

where $g_\pi$ and $g_\nu$ represents the mean density of individual levels of protons, respectively of protons around the last occupied level in the ground state of the considered nucleus.

In the model of the Fermi gas, it is shown [1] that

$$g_\pi = \frac{3Z}{2\epsilon_F}, \quad g_\nu = \frac{3N}{2\epsilon_F}$$

where $Z$ is the number of protons, $N$ is the number of neutrons and the Fermi energy is given by the relation

$$\epsilon_F = \left(\frac{9\pi}{8}\right)^{2/3} \frac{\hbar^2}{2mr_0^2}.$$

In this last expression, $\hbar$ is the reduced Planck constant, $m$ is the mass of the nucleon and $r_0$ is its radius. On the basis of eq. (3.20), one deduces that

$$a = \frac{\pi^2}{4}\frac{A}{\epsilon_F}.$$

With the help of the experimental values for $r_0$, $m$ and $\hbar$ one can then evaluate the value of the parameter $a$ in the frame of Fermi gas model. Thus,

$$a_F \approx \frac{A}{13.5}.$$

For the calculation of total density, one should take into account different factors which can influence its value, as: shell effects, pairing interaction, the nuclear deformation, the collective excitations, the spin and the finite volume of the nucleus.

In what concerns the spin dependence, for a nucleus having a symmetry axis which allows the defining of the projections $M$ of the spin $J$, one considers a gaussian state distribution and we have

$$\rho(N, Z, U, M) = \rho(N, Z, U)\frac{1}{\sqrt{2\pi\sigma}}\exp\left(-\frac{M^2}{2\sigma^2}\right). \tag{3.21}$$

where $\sigma$ is called *spin cut-off* parameter.

For the expression of $\rho(N, Z, U, J)$ one uses the fact that, for a given value of $J$ there are $2J + 1$ values of the projection $M$ of $J$, namely $M = -J, -J + 1, \ldots, J - 1, J$. Also,

$$\rho(N, Z, U, J) = \rho(N, Z, U, M = J) - \rho(N, Z, U, M = J + 1).$$

Assimilating this difference with the derivative

$$-\frac{\rho(N,Z,U,M)}{\mathrm{d}M}|_{M=J+1/2},$$

one gets the relation

$$\rho(N,Z,U,J)\approx\rho(N,Z,U)\frac{2J+1}{2\sqrt{2\pi}\sigma^3}\exp\left[-\frac{(J+1/2)^2}{2\sigma^2}\right]. \tag{3.22}$$

In the following additional specifications will be given on the used parameters and on the introduction of different effects, in the frame of described procedures.

Now, we also mention that using the experimental values of $D_0$ (eqs. (2.5), (2.6)), one can study the evolution of the parameter $a$ of the level density, by comparing the theoretical data with the experimental ones. One finds a linear dependence of it on the mass $A$ of nuclei, with notable deviations in the mass regions 60, 90, 140, 210, where the shell effects are more pronounced. Moreover, there are differences between the even-even, odd and odd-odd nuclei. The equidistant model does not take into account the shell effects and the even-odd effects. These are simulated by adjusting the eq. (3.19). The adjustment is done with the help of experimental data, thus obtaining the so called **empirical level densities**.

## 3.2. EMPIRICAL LEVEL DENSITIES

### 3.2.1. The "Back-Shifted-Fermi-Gas" model

Newton ([7]) has shown that the even-odd effects can be reduced by subtracting from the excitation energy $U$ a quantity $\Delta$ depending on the parity number $\chi$ (see eq. 2.4). To understand the introduction of such a value, one considers that the fermions have the tendency to form pairs (the "pairing" notion) and a certain energy should be supplied to break these pairs, in addition to the energy needed to excite the fermions. The meaning of the quantity $\Delta$ is that of the energy to be spend for breaking the nucleon pairs, so that the nucleus arrives in a state in which can be considered as a gas of independent particles.

If, in a first approximation, one supposes that the energy to be provided is a constant equal to $\delta_n$ for neutrons and to $\delta_p$ for protons, one takes as effective excitation energy the value

$$U^*=U-\Delta, \tag{3.23}$$

which leads to the following formula for the level density:

$$\rho(N,Z,U)=\frac{\sqrt{\pi}}{12}\frac{\exp\left(2\sqrt{a(U-\Delta)}\right)}{a^{1/4}(U-\Delta)^{5/4}}. \tag{3.24}$$

The energy $\Delta$ in the eq. (3.23), called "pairing energy", is defined by the relations:

$\Delta = \delta_n + \delta_p$ for an even-even nucleus,

$\Delta = \delta_p$ for an odd number of neutrons,

$\Delta = \delta_n$ for an odd number of protons and

$\Delta = 0$ for an odd-odd nucleus.

A systematic analysis of mass differences between nuclei allows the estimate of $\delta_n$ and $\delta_p$ values. Thus, one finds that

$$\delta_n = \delta_p = \frac{12}{\sqrt{A}}. \tag{3.25}$$

If such an estimate is adopted, we have

$$\Delta = \chi \frac{12}{\sqrt{A}}, \tag{3.26}$$

where $\chi$ is defined by the eq. (2.4).

The comparison with experimental data shows that the introduction of the effective energy $U^*$ enables the obtaining of a level-density parameter $a$ less sensible to even-odd effects.

One can also consider $\Delta$ as an adjustable parameter, like $a$. One speaks in this case about the "Back-Shifted-Fermi-Gas" formula (*BSFG*) and many tables have been produced with the values of these parameters.

The BSFG formula is interesting because contains only two adjustable parameters and allows a convenient reproduction of the experimental data for energies of the order of neutron binding energy. But, in the same time, it exhibits a major inconvenience: it diverges for excitation energies close to $\Delta$. Other expressions permit to remedy this problem, as the Gilbert-Cameron formula, presented in the next paragraph.

### 3.2.2. The Gilbert-Cameron formula

This formula (see [5]) is inspired from the experimental behaviour of discrete level region and from the learnings of BSFG formula. The Gilbert-Cameron procedure consists in the coupling of the description by the BSFG model with the law valid in the domain of discrete levels, *i.e.* the Boltzman law

$$\rho_T = \frac{1}{T} \exp\left( \frac{U - U_0}{T} \right). \tag{3.27}$$

This expression is used for weak energies, while, for higher excitation energies, one adopts the expression of observable level densities $\rho_{obs}$ given by the sum

$$\rho_{\text{obs}}(N, Z, U) = \sum_{J} \rho(N, Z, U, J). \tag{3.28}$$

By using the hypothesis of a distribution with respect to $J$ similar to that of eq. (3.22) one gets

$$\rho_{obs}(N, Z, U) = \frac{1}{\sqrt{2\pi}\sigma} \rho(N, Z, U), \tag{3.29}$$

where for $\rho(N, Z, U)$ one uses the expression (3.24) from BSFG model.

Next, one imposes the continuity of functions $\rho_T$ and $\rho_{obs}$ and their first derivatives at the boundary which separates the regions where each of them are applied.

This formula has a larger domain of applicability then BSFG, but introduces two additional parameters: $U_0$ and $T$.

The presented formulae cover a rather limited energetic range. When disposable, reliable data on level densities seldom go until about 10 MeV excitation energy. The densities obtained by the adjustment of the parameters on such data are difficult to be applied for higher energies (beyond the binding energy $B_n$). Moreover, these expressions are based on the equidistant model, which cannot provide an accurate description. Nothing guarantees for example that a structure effect persists on a large range of excitation energy. In other words, the parameters $a$ and $\Delta$, fitted at $B_n$ to account for the structure effects (of shells for $a$ and of pairing for $\Delta$) change when the energy increases. The only way to improve the results is the use of more realistic nuclear structure models.

## 3.3. REALISTIC LEVEL DENSITIES

### 3.3.1. The levels of a realistic shell model

Qualitatively, the shell effects can be explained in the frame of a model which ignores the pairing (that is an independent particle model), but supposes non-equidistant individual levels. In this model the energy levels of the nucleons are distributed so that they appear grouped in shells. In addition, on a given level of energy at least two fermions can be found, which differ only by the fact that the projections of their angular momenta are of opposite signs. In these conditions, by filling up the levels starting from the deepest ones, one observes shells formed by 2, 8, 20, 28, 50, 82 and 126 occupied levels. These are the *magic numbers*. For this reason, the shell effects are observed to nuclei having a magic number of protons or neutrons and the correspondence with the regions $A \approx 60$, 90, 140, 210 is evident. The mass region $A \approx 210$ contains for example a double magic nucleus, namely $^{208}$Pb with 82 protons and 126 neutrons. One of the consequences of this model for level densities is that, for a magic nucleus, the necessary energy for the

observation of excited levels is more important than for a non-magic nucleus. From here results a weaker level density, at least to low energy, and therefore the parameter $a$ decreases for these levels.

### 3.3.2. Realistic methods for the calculation of level densities

From this category we mention the combinatorial methods (see [8, 9]) and those based on the numerical solution of the saddle point equations (see [10, 11]). These methods allow not only to reproduce the shell effects, but also predict their disappearance when the excitation energy increases.

However, in the independent particle model, the pairing, whose introduction is necessary for the explanation of even-odd effects, is not taken into account. For this, the model is refined, leading to the model called *superfluid*. This is based on the hypothesis that two fermions of the same energy, but whose angular momenta have projections of opposite signs, are not rigorously independent. In order to take into account such a property, one adds to the Hamiltonian which describes the system, a residual interaction which couples the fermions to each other. Making some hypotheses on the form of this interaction, the level densities can be calculated by approximative combinatorial methods or by methods referring to the saddle point. But the calculations become too complicated to allow a systematic study on a large number of nuclei. This model is thus less practical, but enables the theoretical description of the shell effects and of the even-odd effects (without phenomenological approximations of the type $U^* = U - \Delta$). We mention that the superfluid model has predicted the existence of two energetic regions with entirely different characteristics. In the first region, for excitation energies below a certain critical energy $U_c$ (about 5–6 MeV), the nucleons are paired and, for this reason, the ground state energy is diminished by a value $E_{cond}$, named condensation energy, with respect to the energy which the same nucleus would have in an independent particle model. Beyond the critical energy, the pairing disappears and the system behaves like an independent particle one, so that an effective excitation energy defined by $U^* = U - E_{cond}$ must be used.

This energy $E_{cond}$ is, in addition, different, as the nucleus is even-even, odd or odd-odd.

Thus, the superfluid model theoretically justifies the empirical methods in what concerns the pairing, explaining the introduction of the effective energy $U - \Delta$ in the equation (3.24), but restricting its use to energies $U$ above the critical energy $U_c$ (domain to which belongs the energy $B_n$). Moreover, it allows the reproduction of shell effects and predicts their disappearance to high energies. But it is difficult to be used in practice because the complexity of the equations which must be solved. In some simplifying hypotheses, it can give useful quantitative informations, mainly concerning the values of $E_{cond}$ and $U_c$. Also, the realistic

schemes predict the variation of the parameter $a$ with the excitation energy. This variation shows that the shell effects (the decrease of $a$ for the magic nuclei), extremely marked to $B_n$, diminish when the excitation energy increases.

In order to take into account these observations in a simple manner (reasonable computing time) procedures have been developed which we shall call semi-empirical. In the following section two such procedures are presented.

## 3.4. SEMI-EMPIRICAL LEVEL DENSITIES

### 3.4.1. Ignatyuk's method

In this method (see [12]) the intrinsic level density reads

$$\rho_{int} = \frac{\exp S}{\sqrt{D}} \tag{3.30}$$

where the entropy $S$ is defined by

$$S = \begin{cases} 2\sqrt{a(U - E_{cond})} = 2at, & U \geq U_c \\ S_c b, & U \leq U_c. \end{cases} \tag{3.31}$$

The parameter $a$ is taken as follows:

$$a(U, A) = \begin{cases} \tilde{a}(A)[1 + \delta W(Z, N) f(U^*)], & U \geq U_c \\ a(U_c) = a_c, & U \leq U_c \end{cases} \tag{3.32}$$

where $U^* = U - E_{cond}$, and $\delta W$ represents the correction due to the shell effects. The attenuation and dissapearence of the shell effects with increasing excitation energy are modelled by the function

$$f(U) = (1 - \exp(-\gamma U))/U, \quad \gamma = 0.064.$$

The condensation energy, on the basis of the superfluid model, has the expression

$$E_{cond} = \frac{3a_c}{2\pi^2}\Delta_0^2 - \chi\Delta_0, \tag{3.33}$$

where

$$\Delta_0 = \frac{12}{\sqrt{A}} \tag{3.34}$$

is the systematic value of the pairing energy (according to the equation (3.25)) and $\chi$ is the parity index of the nuclei (eq. (2.4)).

The equation (3.32) contains a damping factor $f(u)$ which makes the shell effects to disappear at high energies, so that $a(U, A)$ tends to its asymptotic value $\tilde{a}(A)$, which depends only on the mass $A$. For $\tilde{a}$ one uses the formula

$$\tilde{a}(A) = \alpha A + \beta A^{2/3} \tag{3.35}$$

where α and β are parameters characterizing contribution of the volume and surface regions of nuclei to the level density.

For the determination of $a_c$, one supposes that the individual level density is constant, in order to simplify the equations of the superfluid model. In the range $U \geq U_c$, we can then write the relation

$$U = at^2 + E_{cond}. \tag{3.36}$$

The critical energy is the energy at which the nuclear pairing disappears. From the superfluid model equations one can determine the corresponding critical temperature $t_c$ which has the value

$$t_c = 0.567\Delta_0. \tag{3.37}$$

On the basis of eq. (3.36) we have: $U_c = a_c t_c^2 + E_{cond}$. By introducing this value of $U$ in eq. (3.32), $a_c$ is obtained as a solution of the implicit equation

$$a_c = \tilde{a}\left[1 + \delta W \frac{1 - \exp(-\gamma a_c t_c^2)}{a_c t_c^2}\right]. \tag{3.38}$$

Then one can calculate the values of $E_{cond}$ and $U_c$, thus enabling the calculation of the entropy $S$ on the range $U \geq U_c$.

In the range $U \leq U_c$ one uses the relation

$$\phi = \tanh\left(\frac{t_c}{t}\phi\right) \tag{3.39}$$

where the parameter ϕ is defined by the equation

$$U = U_c(1 - \phi^2). \tag{3.40}$$

From here one gets

$$\phi = \sqrt{1 - \frac{U}{U_c}}. \tag{3.41}$$

The nuclear temperature is then given by the relations

$$t = \begin{cases} \sqrt{\dfrac{U - U_{cond}}{a}}, & U \geq U_c \\ 2\phi t_c / \log\dfrac{1+\phi}{1-\phi}, & U \leq U_c \end{cases} \tag{3.42}$$

The values defining the entropy at energies below $U_c$ are

$$S_c = 2a_c t_c \tag{3.43}$$

and

$$b = \frac{t_c}{t}(1-\phi^2). \tag{3.44}$$

For the calculation of the intrinsic density according to eq. (3.30) we need also the quantity *D*, which is obtained as follows:

$$D = \begin{cases} 144a^3t^5/\pi, & U \geq U_{cr} \\ D_c(1-\phi^2)(1+\phi^2)^3, & U \leq U_c \end{cases} \tag{3.45}$$

where $D_c = 144a_c^3t_c^5/\pi$.

The calculation of the shell correction $\delta W$ along with the macroscopic energy is given in the Appendix.

To resume, the Ignatyuk formalism is quite involved at low energy, because it requires the resolution of the implicit equations (3.38) and (3.39). Its main point is to propose at high energy a relative simple parametrization of the level density parameter which takes into account the the damping of the shell effects with increasing excitation energy. However studies that employed this approach demonstrated the existence of incertitudes in the parameter γ, appearing in the expression of the function $f(U)$ which simulates the damping of the shell effects, and in the shell corrections [13]. Another essential point is the account of collective effects that we discuss below.

The expressions presented so far are referring to the intrinsic excitations, corresponding to the situation when the excitation energy is distributed on a limited number of fermions. But, there are also other types of excited levels: the collective levels. These levels are comming into play by the distribution of the totality or of a part of the excitation energy on the whole set of fermions. Two types of collective levels are usually taken into account. The first ones, the vibrational levels, concern all nuclei and are due to the fact that a nucleus can vibrate around its equilibrium form. The second type is related to the nuclei having a spatial orientation, *i.e.*, the non-spherical nuclei. The excited level spectra of these deformed nuclei display characteristics which can be interpreted as coming from the geometric rotations. One then speaks of rotation levels.

As a rule, to take into account the collective effects, one resorts to the hypothesis called *adiabatic*. This hypothesis consists in the supposition that the intrinsic and collective excitations are independent. One can then define the effective level density $\rho_{eff}$ in the form of a product

$$\rho_{eff} = K_{rot}K_{vib}\rho_{int}, \tag{3.46}$$

where $\rho_{int}$ is the level density without collective effects and $K_{rot}$, $K_{vib}$ are factors representing the enhancement of the level densities because of rotations, respectively of vibrations.

Instead of giving a rigurous derivation of $K_{rot}$ we show how to evaluate this quantity in some particular cases.

In the case of an axial-symmetric nucleus, one considers that an excited level of energy $U$ and spin $J$ results from a nuclear state whose spin projection onto the symmetry axis is $K$ and the energy is given by $U - E_{rot}(J, K)$, where $E_{rot}(J, K)$ is the rotation energy of the state labeled by $K$. If the nuclear shape is invariant with respect to a plane perpendicular to its intrinsic symmetry axis (left-right symmetry), it can be shown [14] that

$$K_{rot} = \sigma_{\perp}^2 .$$

If we break the left-right symmetry, we obtain an increase two times larger.

For the calculation of $K_{rot}$ in [15] the following formula was proposed [17]:

$$K_{rot} = \begin{cases} 1, \quad \epsilon_2 = \epsilon_3 = \epsilon_4 = 0, \ \gamma = 0, \ \text{(spherical nuclei)} \\ \sigma_{\perp}^2, \quad \epsilon_2 \neq 0, \ \epsilon_3 = 0, \ \gamma = 0, \ \text{(axial – and mirror – symmetric nuclei)} \\ 2\sigma_{\perp}^2, \quad \epsilon_3 \neq 0, \ \gamma = 0, \ \text{(mirror – asymmetric but axially symmetric nuclei)} \\ \sqrt{\frac{\pi}{2}}\sigma_{\perp}^2\sigma_{\parallel}, \ \epsilon_3 = 0, \ \gamma \neq 0, \ \text{(nuclei symmetric to } 180^{\circ} \text{ rotationaround } x, y, z \text{ axes.)} \\ \sqrt{8\pi}\sigma_{\perp}^2\sigma_{\parallel}, \ \text{(nuclei with no symmetry with respect to rotation)} \end{cases} \tag{3.47}$$

The quantities $\epsilon_i$ and $\gamma$ are deformation parameters as explained in Appendix. The four cases correspond respectively to: spherical nuclei, axial and mirror-symmetric nuclei, mirror asymmetric but axially symmetric nuclei and nuclei symmetric with respect to rotation with 180° around all three axes.

The parameters $\sigma_{\perp}$ and $\sigma_{\parallel}$ are the "spin cut-off" parameters and are defined as

$$\sigma_{\perp}^2 = \frac{J_{\perp} t}{\hbar^2}, \quad \sigma_{\parallel}^2 = \frac{J_{\parallel} t}{\hbar^2}. \tag{3.48}$$

The quantities $J_{\perp}$ and $J_{\parallel}$ are the perpendicular and the parallel momenta of inertia and can be obtained from the formulae (see [16]):

$$J_{\perp} = \frac{15}{32 R_0^5} J_0 \int \rho^2 (4z^2 + \rho^2) \, dz \tag{3.49}$$

$$J_{\parallel} = \frac{15}{16 R_0^5} J_0 \int \rho^4 dz \tag{3.50}$$

$J_0$ is the momentum of inertia of an uniform spherical distribution of radius $R_0$ relative to an axis passing through its center of mass:

$$J_0 = \frac{2}{5} M R_0^2, \quad R_0 = 1.16 A^{1/3}, \quad M = m_0 A, \tag{3.51}$$

where $m_0$ is the mass unit.

The adiabatic estimation of $K_{rot}$ increases the nuclear level densities by a factor of 50–100 compared with the calculations taking into account intrinsic excitations alone.

Within the liquid drop model the vibrational enhancement factor reads [18]:

$$K_{vib} = \exp[C A^{2/3} (U^*/a)^{4/3}] \tag{3.52}$$

where $C = 0.0555$ or $C = 0.0480763$.

Note that the subsequent studies shown the disappearance of collective effects at high energies. Therefore, the above factors have been modified to damp them and to make them to converge to $1$ for high energies.

Finally, the spin dependence is introduced by a factor of the form (3.22) as follows:

$$\rho(U, J) = \rho(U) \frac{2J+1}{2\sqrt{2\pi}\sigma_{eff}^3} \exp\left[ -\frac{(J+1/2)^2}{2\sigma_{eff}^2} \right]. \tag{3.53}$$

where

$\sigma_{eff}^2 = \sigma_\perp^{2/3} \sigma_\parallel^{1/3} t$ for deformed nuclei;

$\sigma_{eff}^2 = \sigma_\parallel t$ for spherical nuclei.

### 3.4.2. The modified Ignatyuk method

More recently, A. R. Junghans, A. V. Ignatyuk *et al.* (see [19]) have proposed a new method in order to achieve a better concordance with the accumulated experimental data.

Thus, the intrinsic level density is given by:

$$\rho_{int} = \frac{\sqrt{\pi} \exp(S)}{12 \tilde{a}^{1/4} U^{5/4}} \tag{3.54}$$

where the entropy $S$ depends on the shell corrections $\delta V$ and on the pairing corrections $\delta P$, in the following way

$$S = 2\sqrt{\tilde{a}(U + \delta V\, k(U) + \delta P\, h(U))} \tag{3.55}$$

The level density parameter reads

$$\tilde{a} = 0.073\, A + 0.095\, B_s\, A^{2/3} \quad (\mathrm{MeV}^{-1}), \tag{3.56}$$

where $B_s$ is the surface area of a deformed nucleus, whose formula is given in the Appendix.

The effective pairing energy shift is obtained from:

$$\delta P = -\frac{1}{4}\Delta^2 g + 2\Delta \tag{3.57}$$

where the average pairing gap $\Delta = 12/\sqrt{A}$ MeV (according to equation (3.25)) and $g = 6\tilde{a}/\pi^2$ is the single particle level density at the Fermi energy.

The function

$$h(E) = \begin{cases} 1 - \left(1 - \dfrac{U}{U_c}\right)^2, & U < U_c \\ 1, & U \geq U_c \end{cases} \tag{3.58}$$

describes the damping of the pairing correlations with the critical energy , whereby $U_c$ = 10 MeV.

The effective energy $U$ is shifted with respect to the true excitation energy $U^*$ to accomodate for the different condensation energies of even-even, odd mass and odd-odd nuclei. One takes:

$U = U^*$, for odd-odd

$U = U^* - \Delta$, for odd mass

$U = U^* - 2\Delta$, for even-even.

The total shell correction energy, mentioned in the previous section, is the sum of shell and pairing corrections

$$\delta W = \delta V + \delta P. \tag{3.59}$$

As $\delta P$ is given by eq. (3.57), $\delta V$ results from the above definition.

The factor $k(U) = 1 - \exp(-\gamma U)$ with $\gamma = \tilde{a}/0.4A^{4/3}$ or 1/18 MeV describes the damping of the shell effects with excitation energy (the introduction of shell and pairing effects is in accordance with [13]).

In what concerns the collective enhancement factors, the originary recipe of Ignatyuk has been modified in order to ensure an adequate behaviour of these factors. Thus, the rotational enhancement is expected to be damped, because a separation between intrinsic and collective rotational motion can only be made at temperatures which are low enough to ensure a well defined deformation of the nucleus. Then, for nuclei with a quadrupole deformation $|\beta_2| > 0.15$, the rotational enhancement factor is calculated by the formula

$$K_{rot}(U) = \begin{cases} (\sigma_\perp^2 - 1) f(U) + 1, & \sigma_\perp^2 > 1 \\ 1, & \sigma_\perp^2 \leq 1 \end{cases} \tag{3.60}$$

with $\sigma_{\perp}^2$ previously defined and

$$f(U)=\left[1+\exp\left(\frac{U-E_c}{d_c}\right)\right]^{-1} \tag{3.61}$$

where $E_c=40$ MeV, $d_c=10$ MeV.

Eq. (3.60) was derived in the adiabatic approximation. Hansen and Jensen showed [20], within the algebraic semi-microscopic model SU(3) (oscillator mean-field plus quadrupole-quadrupole interaction of particles), that an empirical formula for the non-adiabatic case can be derived

$$K_{rot}(U)=\frac{K_{rot}^{adiab}(U)}{1+\exp[(U-U_r)/d_r]} \tag{3.62}$$

The parameters of this formula were estimated as

$$U_r=120\,A^{1/3}\beta^2, \qquad d_r=1400\,A^{-2/3}\beta^2$$

where the quadrupole deformation parameter can be easily converted in the $\epsilon$-parametrization.

Ground state deformation, *i.e.*, $|\beta_2|<0.15$ the vibrational enhancement factor reads

$$K_{vib}=25\beta_{eff}^2 K_{rot}(U) \tag{3.63}$$

In this formula the damping of the vibrational enhancement with excitation energy is supposed to be the same as the damping of the rotational enhancement. In addition $K_{vib}$ is required to be greater than 1. In the above formula the rotational enhancement factor $K_{rot}$ is multiplied with the square of a dynamical deformation parameter

$$\beta_{\text{eff}}=0.022+0.003\Delta N+0.005\Delta Z, \tag{3.64}$$

$\Delta N$ and $\Delta Z$ being the absolute values of the number of neutrons and protons above or below the nearest shell closure. In this way the rigid-body moment of inertia $J_{\perp}$ used in (3.60) is substituted by the irotational-flow value of a liquid-drop ($J_{irr}=\beta_{\text{eff}}^2 J_{\perp}$). The factor 25 was chosen in [19] to fit experimental data for the production cross sections.

## 4. APPLICATIONS

We apply the nuclear level density formalism, described in the previous section to the study of some nuclei from the actinide region, namely the protactinium

isotopes $^{232}$Pa, $^{233}$Pa and $^{234}$Pa. These nuclei are less known, but reached a major interest, because of their practical applications. Indeed, they appear in the thorium fuelled nuclear reactors(thorium-$^{233}$U cycle). One considers that nuclear reactors using this fuel might provide safer and cleaner nuclear energy as highly radiotoxic actinide waste (Pu, Am and Cm isotopes) will be produced in much lower quantities compared to the present uranium fuelled reactors. In addition, better material properties and fuel behaviour increase the attractiveness of thorium-based fuel cycles. The primary reaction of importance in the thorium cycle is the one producing the fissile nucleus $^{233}$U after neutron capture on $^{232}$Th. The net production of $^{233}$U is controlled by the long half-life of $^{233}$Pa ($T_{1/2} = 27$ days) according to the following reaction chain:

$$^{232}\mathrm{Th} + n \rightarrow ^{233}\mathrm{Th} \rightarrow ^{233}\mathrm{Pa} + e^- + \overline{\nu}_e \rightarrow ^{233}\mathrm{U} + e^- + \overline{\nu}_e$$

Thus, the ballance of $^{233}$U will be affected by the neutron absorption properties of $^{233}$Pa because every neutron captured by $^{233}$Pa will affect the neutron economy and will cause $^{233}$U to be lost. Such an effect is not encountered in the traditional $^{238}$U-$^{239}$Pu fuel cycle as the equivalent intermediate isotope $^{239}$Np has a relatively shorter half-life ($T_{1/2} = 2.35$ days).

Very recently the fission probability of $^{234}$Pa has been measured using the transfer reaction $^{233}$Pa($^3$He, $p$)$^{234}$Pa [21]. From these measurements it was possible to deduce the equivalent fast neutron induced fission of $^{233}$Pa up to an incident neutron energy of 10 MeV. It is therefore necessary, for comparison purposes, to have a theoretical determination of this quantity.

In Fig. 2 are shown the intrinsic level densities (in logarithmic form) for $^{232}$Pa and $^{234}$Pa with both Ignatyuk formulae at the ground state and at the barrier values (for this nucleus the macroscopic-microscopic model provides a double-humped fission barrier (saddle points A and B)). The shell correction has been obtained as described in the Appendix. The barrier values have been extracted from the tables of Howard and Moeller ([23]).

A prerequisite of a theoretical analysis of the $^{233}\mathrm{Pa}(n, f)$ cross section is the level density. The absorbtion of a neutron of incident energy $E_n$ by the nucleus $^{233}$Pa will determine the compound nucleus $^{234}$Pa to decay subsequently by fission, neutron or γ emission. Averaging over many levels of the fissioning system, the neutron induced fission cross section reads [22, 21]

$$\sigma_f(E_n) = \sum_{J\pi} \sigma_{\mathrm{CN}}(E_n, J, \pi) \frac{\left\langle \Gamma_f^{J,\pi} \right\rangle}{\left\langle \Gamma_f^{J,\pi} \right\rangle + \left\langle \Gamma_n^{J,\pi} \right\rangle + \left\langle \Gamma_\gamma^{J,\pi} \right\rangle} F \tag{4.65}$$

where $\sigma_{\mathrm{CN}}(E_n, J, \pi)$ represents the compound nucleus formation cross (CN) in states $(J, \pi)$ in $^{234}$Pa. The quantities under brackets arising in the nominator and

denominator of the second factor under the above sum are the partial widths. In order to determine these widths a specific fission model should be considered. We assume that the fission process is governed by the double humped barrier [24]. In this approach the fission is pictured as the crossing of an inner barrier (A) followed by the crossing of the outer barrier (B) (see Fig. 3). At the corresponding saddle point deformations ($\epsilon_{\mathrm{A}}$ and $\epsilon_{\mathrm{B}}$), the barrier shapes are approximated by inverted parabolas which define the barrier heights and curvatures of the inner barrier $(E_A, \hbar\omega_A \equiv \partial^2 E_{def}/\partial\epsilon^2\big|_A)$ and of the outer barrier $(E_B, \hbar\omega_B$ respectively. Then the partial width corresponding to each barrier $i$ reads

$$\left\langle \Gamma_f^{J,\pi}(U) \right\rangle = \frac{\left\langle D_{gs}^{J,\pi}(U) \right\rangle}{2\pi} \int_{-\infty}^{U-E_i} \frac{\rho_i(U-E_i-\varepsilon)}{1+\exp\left(-\frac{2\pi\varepsilon}{\hbar\omega_i}\right)} \mathrm{d}\varepsilon \tag{4.66}$$

where $\varepsilon$ and $\rho_i(U-E_i-\varepsilon)$ represent, respectively, the kinetic energy in the fission degree of freedom and the level density of compound states $(J\pi)$ at the top of the

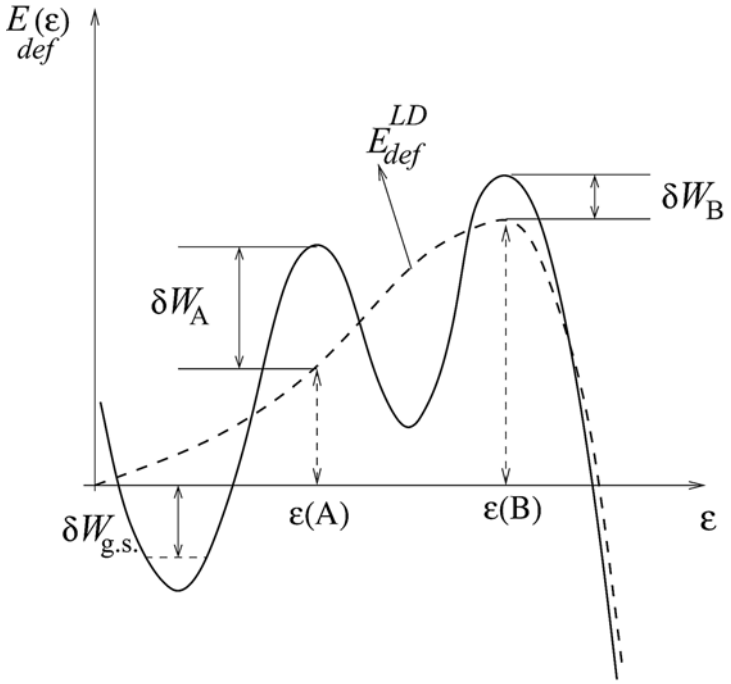


Fig. 3 – Schematic illustration of the deformation energy computed in the liquid drop model $E_{def}^{LD}$ (dashed line) and with shell corrections (full line). The shell corrections $\delta W$ in the ground-state, and the top of the barriers is also indicated.

barrier $E_i$. The quantity $\left\langle D_{gs}^{J,\pi}(U)\right\rangle$ is the mean level spacing of the compound states at an energy $U$ above the g.s. of the $^{234}$Pa nucleus.

As for the γ decay width of states $(J\pi)$, it was computed assuming that only electric dipole transitions (E1) contribute to the γ-decay channel respectively. Then the partial width corresponding to each barrier $i$ reads

$$\left\langle \Gamma_{\gamma}^{J,\pi}(U)\right\rangle = C\frac{\left\langle D_{gs}^{J,\pi}(U)\right\rangle}{2\pi}\sum_{J_f=J-1}^{J+1}\int_0^U \rho_i(E_f,-\pi,J_f)(U-E_f)^3\,\mathrm{d}E_f \qquad (4.67)$$

The summation is done over the continuous final states $(E_f,\pi_f-\pi,J_f)$ of $^{234}$Pa nucleus after emission of a γ ray energy $E_\gamma = U - E_f$. The constant $C$ has been adjusted in order to reproduce the experimentally known average γ width at the neutron binding energy.

The partial width in the neutron channel is computed according to the formula

$$\begin{aligned}\left\langle \Gamma_{n}^{J,\pi}(U)\right\rangle &= \\ &= \frac{\left\langle D_{gs}^{J,\pi}(U)\right\rangle}{2\pi}\int_{E_d}^{U-B_n}\sum_{j=\left|J-J_f\right|}^{\left|J+J_f\right|}\sum_{l=\left|j-\frac{1}{2}\right|}^{\left|j+\frac{1}{2}\right|}\delta(\pi,\pi_f,(-)^l)\rho(E_f,J_f,\pi_f)T_l^j(E_n)\mathrm{d}E_f \qquad (4.68)\\ &+\sum_{E'J',\pi'}\sum_{j=\left|J-J'\right|}^{\left|J+J'\right|}\sum_{l=\left|j-\frac{1}{2}\right|}^{\left|j+\frac{1}{2}\right|}\delta(\pi,\pi_f,(-)^l)T_l^j(E_n)\end{aligned}$$

In the above formula $T_l^j(E_n)$ is the transmission coefficient for emission of a neutron with kinetic energy $E_n = U - S_n - E_f$, an orbital angular momentum $l$ and channel spin $j$. The border between the continuous and discrete levels was set at $E_d = 0.8$ MeV

Formula (4.65) contains also a fluctuation factor $F$ important in case of subthreshold fission of even-even fissioning systems where a few channels contribute to the fission cross section.

In the calculation of the cross section for the neutron induced fission of $^{233}$Pa we take into account only the rotational enhancement factor. The relevant moment of inertia in the ground state of $^{233}$Pa (and $^{234}$Pa) and at the deformations corresponding to the barriers A and B have been computed, for consistency, also with the set of prolate deformations calculated in [23].

At the second barrier (B), the level density $\rho(U,J)$ calculated from eq. (3.53) has been doubled because it is assumed that reflection against a cut perpendicular to the symmetry axis has been lost: thus levels of opposite parity and the same energy are added to the intrinsic levels.

Fig. 4 shows for the nucleus $^{232}$Pa the fitting on experimental data of the cross sections obtained on the basis of the continuous densities given by the mentioned methods and including some discrete densities, experimentally measured at low energies. We see that the calculations are in a good agreement with data up to 6 MeV. Fig. 5 shows similar data for the nucleus $^{234}$Pa.

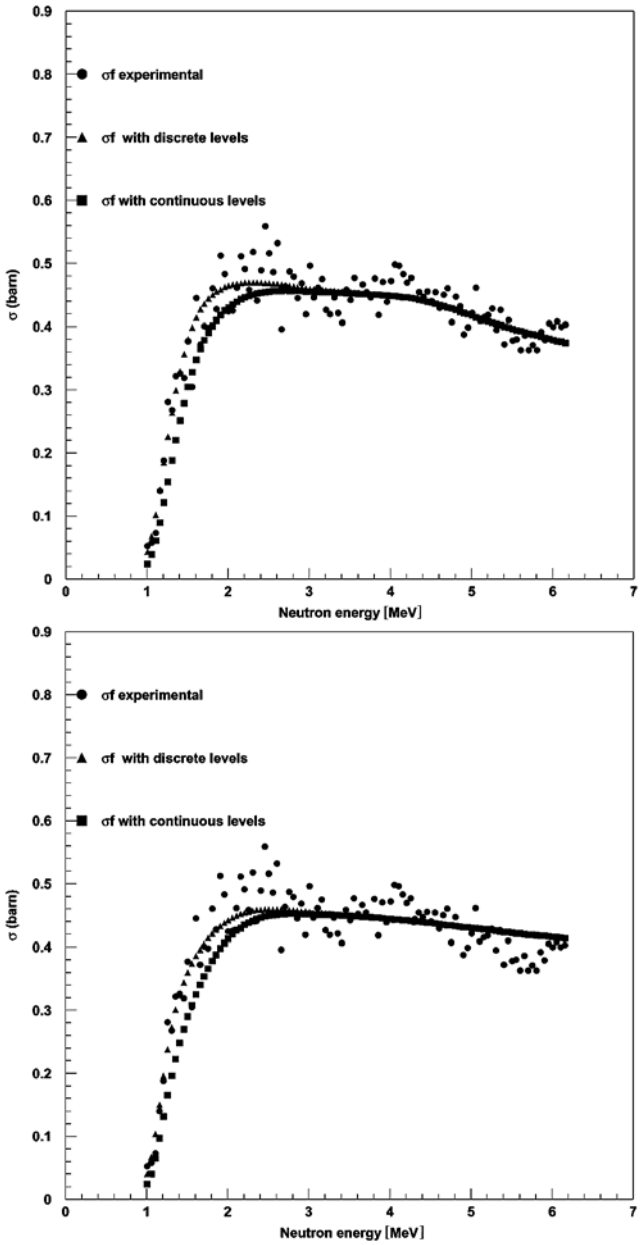


Fig. 4 – The comparison with experimental data of the cross sections for the neutron induced fission of $^{232}$Pa calculated from the continuous densities given by the Ignatyuk method (upper panel) and by the modified Ignatyuk method (lower panel).

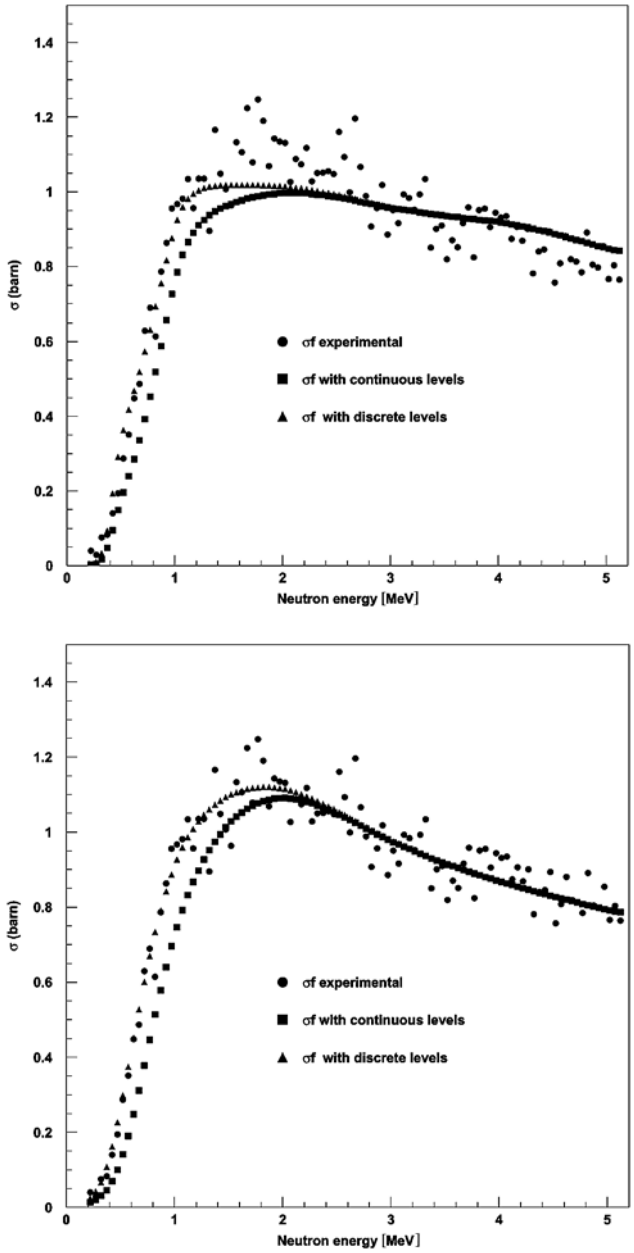


Fig. 5 – The comparison with experimental data of the cross sections for the neutron induced fission of $^{234}$Pa calculated from the continuous densities given by the Ignatyuk method (upper panel) and by the modified Ignatyuk method (lower panel).

We have also deduced the capture, compound nucleus formation and inelastic cross sections for the reactions $^{231}$Pa + $n$ and $^{233}$Pa + $n$. They are shown in Fig. 6 (the continuous densities have been obtained by the modified Ignatyuk method).

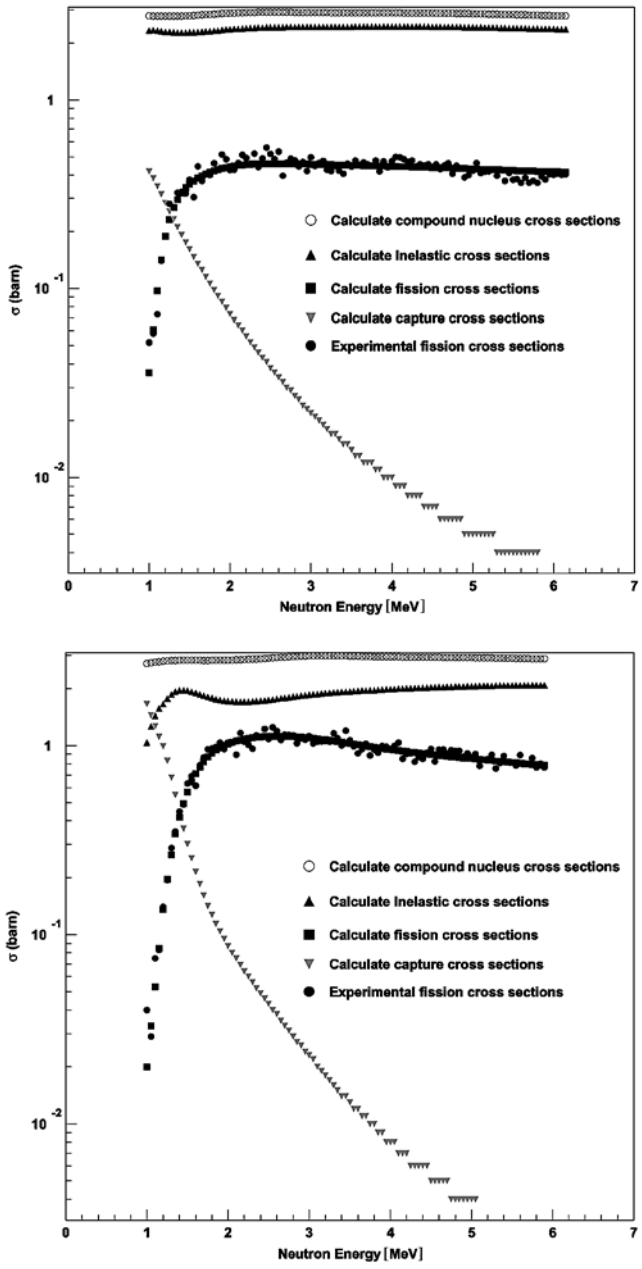


Fig. 6 – The comparison with experimental data of the fission cross sections for the neutron induced fission of $^{232}$Pa together with the calculated capture, compound nucleus and inelastic cross sections (upper panel) and of $^{234}$Pa (lower panel).

## 5. SUMMARY

In the present paper we have discussed the level density calculation, a long-standing problem of nuclear physics. Firstly, the notion of level density is

introduced and several definitions and basic relations are given. The density of levels near the ground state varies markedly due to the odd-even effect, the vicinity of a closed shell and the spherical or deformed nature of the nucleus. The accurate study of the decay products of an excited nucleus requires the ability not only to describe these variations in level density at low excitation but also to extrapolate the level density into regions of excitation energy, angular momentum, and nuclear shape for which there is little direct experimental knowledge.

Then some of the most relevant calculation procedures of the level densities are presented. We started with the formula of level density in the equidistant model. It was very useful at the early moments of nuclear physics and has given a basis for developing new approaches. After that we described methods of two types: empirical and semi-empirical. To the first class belong the "Back-Shifted-Fermi-Gas" model and the Gilbert-Cameron formula. From the second class we discussed rather extensively the Ignatyuk method and the modified Ignatyuk method. We emphasized on the practical evaluation of the involved ingredients, like shell correction.

Finally, some applications to $^{232,233,234}$Pa nucleus are presented. The study of such nucleus became very important, since it appears in a safer type of nuclear reactor, namely the thorium fuelled reactor. Fueling nuclear reactors with thorium instead uranium could produce half as much radioactive waste and reduce the quantity of resulting plutonium. Also, the element thorium is naturally more abundant than uranium.

The numerical techniques for level densities described here supply an useful input to accurate computation of some quantities of highest interest in nuclear reactions, as partial widths and cross sections.

Apart the practical needs, the theoretical study of the nuclear level density provides a fundamental insight into an important property of nuclei and how it is affected by the microscopic, *i.e.*, shell-related aspects of nucleonic motion.

## APPENDIX: SHAPE PARAMETRIZATION, DEFORMATION ENERGY AND PHENOMENOLOGICAL SHELL CORRECTIONS IN FISSION

To study the fission, one needs the level densities at equilibrium state and at the saddle points (of extremum) of the fissionable nucleus. To describe these states, different models are used. One of them is based on the $\epsilon$ parametrization of Nilsson [29], which has been introduced in order to reproduce as well as possible the modifications of nuclear shapes during the fission process (elongation, necking, mass-asymmetry and axially asymmetry). There is also another parametrization introduced by Pashkevich based on the Cassini ovals [28].

The literature provides tables for different nuclei with fission barriers and deformation parameters at extremum points (see [23, 25]). To calculate the total

shell corections, at each point of interest the value $E_{def}$ of the barrier is extracted from tables and with the corresponding $\epsilon$ parameters one determines the deformation energy $E_{def}^{LD}$ in the liquid drop model. Then, $\delta W = E_{def} - E_{def}^{LD}$.

However, since in the ground state there is a computed microscopic correction $E_{mic}$ (see [25]) then the barrier's heights provided by Howard and Möller [23] should be corrected by this quantity . One then computes the total shell corrections at each extremum point according to $\delta W_i = E'_{def}(\epsilon_i) - E_{def}^{LD}(\varepsilon)$, where the prime indicates that the barrier was corrected as follows: $E'_{def} = E_{def} - |E_{micro}|$. This procedure is illustrated in Fig. 3. It should be stressed that for nuclei of interest these shell corrections are negative in the ground state and positive at the barriers. As a consequence the level density parameters could be rather different at the extrema of the fission path.

To show how $E_{def}^{LD}$ is obtained, we shall firstly define the perturbed-spheroid $\varepsilon$ parametrization [25] with quadrupole $\epsilon_2$, octupole $\epsilon_3$, hexadecapole $\epsilon_4$ axial-symmetric deformations and also the axial-asymmetric deformation ($\gamma$).

As the first step a "stretched" representation is introduced. The stretched coordinates $\xi$, $\eta$ and $\zeta$ are defined by

$$\xi = \left\{ \frac{m\omega_0}{\hbar} \left[ 1 - \frac{2}{3}\epsilon_2 \cos\left(\gamma + \frac{2}{3}\pi\right) \right] \right\}^{1/2} x \tag{5.69}$$

$$\eta = \left\{ \frac{m\omega_0}{\hbar} \left[ 1 - \frac{2}{3}\epsilon_2 \cos\left(\gamma - \frac{2}{3}\pi\right) \right] \right\}^{1/2} y \tag{5.70}$$

$$\zeta = \left\{ \frac{m\omega_0}{\hbar} \left[ 1 - \frac{2}{3}\epsilon_2 \cos(\gamma) \right] \right\}^{1/2} x \tag{5.71}$$

where $\hbar\omega_0$ is the oscillator energy, $\epsilon_2$ is the ellipsoidal deformation parameter, and $\gamma$ is the nonaxiality angle. It is then convenient to define a stretched radius vector $\rho_t$ by

$$\rho_t = (\xi^2 + \eta^2 + \zeta^2)^{1/2} \tag{5.72}$$

a stretched polar angle $\theta_t$ by

$$u = \cos\theta_t = \frac{\zeta}{\rho_t} = \left[ \frac{1 - \frac{2}{3}\epsilon_2 \cos\gamma}{1 - \frac{2}{3}\epsilon_2 \cos\gamma P_2(\cos\theta) + \left(\frac{1}{3}\right)^{1/2} \epsilon_2 \sin\gamma \sin^2\theta \cos 2\phi)} \right]^{1/2} \cos\theta \tag{5.73}$$

and a stretched azimuthal angle $\phi_t$ by

$$v=\cos 2\phi_t=\frac{2\eta}{(\xi^2+\eta^2)^{1/2}}=\frac{[1+\frac{1}{3}\epsilon_2\cos\gamma]\cos 2\phi+\left(\frac{1}{3}\right)^{1/2}\epsilon_2\sin\gamma}{1+\frac{1}{3}\epsilon_2\cos\gamma+\left(\frac{1}{3}\right)^{1/2}\epsilon_2\sin\gamma\cos 2\phi}. \tag{5.74}$$

The Nilsson modified-oscillator potential is defined by

$$\begin{aligned}V=&\frac{1}{2}\hbar\omega_0\rho_t^2\left\{1+2\epsilon_1P_1(\cos\theta_t)-\frac{2}{3}\epsilon_2\cos\gamma P_2(\cos\theta_t)+\right.\\&+\frac{1}{3}\epsilon_2\sin\gamma\left(\frac{8\pi}{5}\right)^{1/2}[Y_2^2(\theta_t,\phi_t)+Y_2^{-2}(\theta_t,\phi_t)]+2\epsilon_3P_3(\cos\theta_t)+\\&\left.+2\epsilon_4V_4(\cos\theta_t,\cos 2\phi_t)+2\epsilon_5P_5(\cos\theta_t)+2\epsilon_6P_6(\cos\theta_t)\right\}-\\&-\kappa\hbar\omega_0^0\left[2\boldsymbol{l}_t\times\boldsymbol{s}+\mu\left(\boldsymbol{l}^2-\left\langle\boldsymbol{l}_t^2\right\rangle\right)\right],\end{aligned} \tag{5.75}$$

where $\boldsymbol{l}_t$ is the angular-momentum operator in the stretched coordinate system, $\boldsymbol{s}$ is the spin-operator and

$$V_4(u,v)=a_{40}P_4+\left(\frac{4\pi}{9}\right)^{1/2}[a_{42}(Y_{42}+Y_{4-2})+a_{44}(Y_{44}+Y_{4_4})]. \tag{5.76}$$

The hexadecapole potential $V_4(u,v)$ depends on $\gamma$ in such a way that axial symmetry is preserved when $\gamma=0,60°$, $-120°$ and $-60°$, for axial-symmetric shapes and for $\epsilon_6=0$. This is accomplished by choosing the coefficients $a_{4i}$ so that they have the transformation properties of a hexadecapole tensor. Thus,

$$a_{40}=\frac{1}{6}(5\cos^2\gamma+1),\quad a_{42}=-\frac{1}{12}\sqrt{30}\sin 2\gamma,\quad a_{44}=\frac{1}{12}\sqrt{70}\sin^2\gamma.$$

Assuming that the shape of the nuclear surface is equal to the shape of an equipotential surface given by eq. (5.75) and neglecting the terms $\boldsymbol{l}_t\times\boldsymbol{s}$ and $\boldsymbol{l}_t^2$, solving for $\rho_t$, and then using eqs. (5.69)–(5.74) to derive an expression for the radius vector $R(\theta,\phi)$ in the non-stretched laboratory system, we obtain (eq. (24) from [25]):

$$R(\theta,\phi)=\frac{R_0}{\lambda}\left(\frac{p_1}{p_2q}\right)^{1/2} \tag{5.77}$$

where

$$\begin{aligned}p_1=&1-\frac{1}{3}\epsilon_2\cos\gamma\left(1+\frac{2}{3}\epsilon_2\cos\gamma\right)+\epsilon_2\left(\cos\gamma+\frac{1}{3}\epsilon_2\cos 2\gamma\right)u^2-\\&-\left(\frac{1}{3}\right)^{1/2}\epsilon_2\sin\gamma\left(1-\frac{2}{3}\epsilon_2\cos\gamma\right)(1-u^2)v\end{aligned} \tag{5.78}$$

$$p_2 = 1 - \frac{2}{3}\epsilon_2 \cos\gamma P_2(u) + \left(\frac{1}{3}\right)^{1/2} \epsilon_2 \sin\gamma(1-u^2)v + 2\epsilon_1 P_1(u) + \\ + 2\epsilon_3 P_3(u) + 2\epsilon_4 V_4(u,v) + 2\epsilon_6 P_6(u) \tag{5.79}$$

$$q = \left[1 - \frac{2}{3}\epsilon_2 \cos\left(\gamma + \frac{2}{3}\pi\right)\right]\left[1 - \frac{2}{3}\epsilon_2 \cos\left(\gamma - \frac{2}{3}\pi\right)\right]\left[1 - \frac{2}{3}\epsilon_2 \cos\gamma\right] \tag{5.80}$$

The quantity $\lambda = \omega_0/\overline{\omega}_0$ is determined by requiring that the volume is preserved when deformation is increased

$$\lambda^3 = \frac{1}{4\pi} q^{-1/2} \int_0^{\pi} \mathrm{d}\theta_t \int_0^{2\pi} \mathrm{d}\phi_t \sin\theta_t \times \\ \times \left[1 - \frac{2}{3}\epsilon_2 \cos\gamma P_2(u) + \epsilon_2 \sin\gamma \left(\frac{8\pi}{45}\right)^{1/2} (Y_{22} + Y_{2-2}) + \right. \\ \left. + 2\epsilon_1 P_1(u) + 2\epsilon_3 P_3(u) + 2\epsilon_4 V_4(u,v) + 2\epsilon_5 P_5(u) + 2\epsilon_6 P_6(u)\right]^{-3/2} \tag{5.81}$$

The functions $P_l$ are the Legendre polynomials and $Y_{lm}(\theta, \phi)$ are the spherical harmonics. In the above expressions the following sums appear:

$$SY_{22} = Y_{22}(\theta,\phi) + Y_{2-2}(\theta,\phi), \quad SY_{42} = Y_{42}(\theta,\phi) + Y_{4-2}(\theta,\phi), \\ SY_{44} = Y_{44}(\theta,\phi) + Y_{4-4}(\theta,\phi)$$

When the arguments of the spherical harmonics are the stretched angles $\theta_t$ and $\phi_t$ we obtain

$$SY_{22} = \left(\frac{15}{8\pi}\right)^{1/2} \sin^2\theta_t \cos 2\phi_t = \left(\frac{15}{8\pi}\right)^{1/2} (1-u^2)v$$

$$SY_{42} = \left(\frac{45}{32\pi}\right)^{1/2} \sin^2\theta_t (7\cos^2\theta_t - 1)\cos 2\phi_t = \left(\frac{45}{32\pi}\right)^{1/2} (1-u^2)(7u^2-1)v$$

$$SY_{44} = \left(\frac{315}{128\pi}\right)^{1/2} \sin^4\theta_t \cos 4\phi_t = \left(\frac{315}{128\pi}\right)^{1/2} (1-u^2)^2(2v^2-1)$$

Considering only axial-symmetric shapes (*i.e.* $\gamma = 0$) and retaining only quadrupole and hexadecapole deformations, the expression of the radius vector $R(\theta)$ is

$$R(\theta) = \frac{R_0}{\lambda} \sqrt{\frac{\varpi_1}{\varpi_2}} \frac{1}{(1+\epsilon_2/3)\sqrt{1-2\epsilon_2/3}} \tag{5.82}$$

where

$$\varpi_1 = 1 - \frac{1}{3}\epsilon_2 \left(1 + \frac{2}{3}\epsilon_2\right) + \epsilon_2 \left(1 + \frac{1}{3}\epsilon_2\right) u^2$$

$$\varpi_2 = 1 - \frac{2}{3}\epsilon_2 P_2(u) + 2\epsilon_3 P_3(u) + 2\epsilon_4 P_4(u)$$

with

$$u = \cos\theta \sqrt{\frac{1 - \frac{2}{3}\epsilon_2}{1 - \frac{2}{3}\epsilon_2 P_2(\cos\theta)}}$$

Then, the cylindrical coordinates $\rho$ and $z$ can be derived as follows:

$$\rho = R\sqrt{1 - x^2}, \quad z = Rx, \quad x = \cos\theta. \tag{5.83}$$

The total deformation energy is computed according to the standard liquid drop model, *i.e.* the actual total energy minus the value for a sphere (see [16], p. 14, eq. (1.74))

$$E_{def}^{LD} = E_{surf} - E_s^0 + E_{coul} - E_c^0. \tag{5.84}$$

where $E_s^0$ and $E_c^0$ are the surface and Coulomb energies of a charged liquid drop.

Using the parametrization of Myers and Swiatecki [26] we have that

$$E_s^0 = 17.9439\left[1 - 1.7826\left(\frac{A-2Z}{A}\right)^2\right]A^{2/3} \quad \text{MeV} \tag{5.85}$$

$$E_c^0 = 0.7053\frac{Z^2}{A^{1/3}} \quad \text{MeV}. \tag{5.86}$$

Strutinsky [27] proposed another ansatz

$$E_s^0 = \sigma A^{2/3}, \quad E_c^0 = \frac{2\sigma}{(Z^2/A)_c}\frac{Z^2}{A^{1/3}} \tag{5.87}$$

with $\sigma = 16$, $(Z^2/A)_c = 45$.

The ratio $x = \dfrac{E_c^0}{2E_s^0} \sim Z^2/A$ is called *fissility* and is a characteristic parameter of nuclear fission.

For practical calculations another parametrization is however more convenient, namely the parametrization based on the Cassini ovaloids (see [28]). Therefore, we adopted a numerical procedure to fit a curve which describe the contour of a nucleus in the Nilsson parametrization with a curve given in the Cassini parametrization.

In the Cassini parametrization an axially deformed shape can be described in cylindrical coordinates

$$\rho = \frac{1}{\sqrt{2}}[G(x)^{1/2} - R^2(x)(2x^2 - 1) - \epsilon R_0^2]^{1/2} \tag{5.88}$$

$$z = \frac{\text{sign}(x)}{\sqrt{2}}[G(x)^{1/2} + R^2(x)(2x^2 - 1) + \epsilon R_0^2]^{1/2} \tag{5.89}$$

where

$$G(x) = [(R^4(x) + 2\epsilon R_0^2 R^2(x)(2x^2 - 1) + \epsilon^2 R_0^4)^{1/2}.$$

The curve $R(x)$ is expanded in Legendre polynomials

$$R(x) = R_0\left(1 + \sum_m \alpha_m P_m(x)\right) \tag{5.90}$$

Thus a deformed shape in Cassini parametrization is described by the following deformation parameters: $\epsilon, \alpha_m, m = 1, 2..., M$ .

Next the surface $E_{surf}$ and Coulomb $E_{coul}$ terms entering in the expression of the total deformation energy are computed according to [28]:

$$E_{surf} = E_s^0 B_{surf}, \quad B_{surf} = \frac{1}{2R_0^2}\int_{Z_L}^{Z_R} \rho\sqrt{1 + \left(\frac{d\rho}{dz}\right)^2}\,\mathrm{d}z \tag{5.91}$$

$$E_{coul} = E_c^0 B_{coul}, \quad B_{coul} = \frac{1}{2R_0^2}\int_{Z_L}^{Z_R} \Phi_s(z)\left(\rho^2 - z\rho\frac{\mathrm{d}\rho}{\mathrm{d}z}\right)\mathrm{d}z \tag{5.92}$$

were

$$\Phi_s(z) = \frac{3}{4\pi R_0^2}\int \mathrm{d}\,\overline{z}\,\frac{k}{\sqrt{\rho(z)\overline{\rho}(\overline{z})}}\cdot \\ \cdot\left\{\left[\rho(z)\overline{\rho}(\overline{z}) + \overline{\rho}^2(\overline{z}) + (z - \overline{z})\rho(z)\frac{\mathrm{d}\overline{\rho}(\overline{z})}{\mathrm{d}\,\overline{z}}\right]K(k^2) - 2\rho\overline{\rho}D(k^2)\right\} \tag{5.93}$$

$K(k^2)$ and $D(k^2) = [K(k^2) - E(k^2)]/k^2$ being complete elliptic integrals of the argument

$$k^2 = \frac{4\rho(z)\overline{\rho}(\overline{z})}{(z - \overline{z})^2 + (\rho + \overline{\rho})^2}$$

(see [16], p. 74, eq. 7.10).

For each set of Nilsson deformations $(\epsilon_2, \epsilon_3, \epsilon_4)$ we determined a set of Cassini parameters $(\epsilon, \alpha_1, \alpha_2, ..., \alpha_M)$ by a least square fit procedure for the g.s., saddle points and minimum points. It was proved that a number of eight $\alpha$ parameters are necessary in order to provide a good fit for large deformations.

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