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(DENCOM)**

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Abstract

A computer code based on the semimicroscopical combined method of deformed nuclei level density calculation is described. It includes the use of combinatorial and statistical approaches for low and high energies correspondingly, both calculations are fulfilled in the frames of superfluid model. The employed models, the proceeding of the code, the required input data and the output are discussed.

I-Introduction

Actually for level densities calculation both phenomenological and semi-microscopical models are being used. The most of phenomenological models have foundation in Fermi-gas model which has been proposed by Bethe [1]. The phenomenological approach has been developed in several works (see for example [2-4]) taking into consideration the shell, pairing and collective effects. To take into account these effects, a great amount of experimental information about level densities in a broad energy interval is needed. Therefore, the applications of phenomenological formulae for the deformed states in fission or for nuclei far from nuclear stability line are under questions.

The disadvantages of phenomenological models led to the development of semi-microscopical models for level density calculation. The quantum-statistical model for nuclear level density calculations has been investigated by many authors [5-9] taking into account shell and pairing effects in the framework of the nuclei superfluid model (BSC model). But the quantum statistical superfluid approach does not give

the appropriate description of level density at low energy where, the discrete structure of spectrum has to be considered. At low excitation energy the combinatorial method in the frame of quasiparticle-phonon model [10] is more preferable. But for practical calculations this model can not be used because it needs a large computer time. In works [11,12] a combined model of the deformed nuclei level density calculations is proposed. It includes the use of combinatorial and statistical approaches for the low and high energy respectively. Both consideration are fulfilled in the framework of superfluid model, using realistic single-particle spectrum and phenomenological rotation enhancement of deformed nuclei level densities. In this work we propose a computer code for the deformed nuclei level density calculations in the frames of combined model [11,12]. This computer code is useful for nuclear reaction cross section calculations and fission characteristic calculations.

II. Calculation model

The energy range in which the level densities are being considered is divided in two intervals: one is from zero to some value of nucleus excitation energy U_d and the second is the interval from U_d to the final value U_f . In the first interval, level density is calculated in the frame of combinatorial method and in the second energy interval calculations are made in the frame of quantum-statistical method. In both cases the same parameters (single-particle spectra and pairing strength constants) are used.

II.1 Combinatorial model

We use superfluid BSC model taking into account blocking single-particle levels occupied by quasiparticles. The fact that single-particle states must occupy the numbers $n=0,1,2$ is proposed. For deformed nucleus each single-particle level is described by energy ϵ_i , projection of single-particle angular momentum to the nuclear symmetry axis Ω_i and parity π_i . In the case of violation of reflection symmetry of the nucleus shape the single-particle

states have not definite parity. The following consideration is also applied for spherical nuclei, then the single-particle states are characterized by quantum numbers $j \equiv \pi$.

BSC equations for single-component system of N particles with the fixed number of quasiparticles in the definite single-particle states are the following:

$$E_{\Omega}^{\nu} = \sum_1^{\nu} \epsilon_{\Omega_1} + 2 \sum_1^{\nu} \epsilon_{\Omega_1} v_1^2 - \frac{\Delta_{\nu}^2}{G} \quad (1)$$

$$N - N_{\nu} - \nu = 2 \sum_1^{\nu} v_1^2 \quad (2)$$

$$\Delta_{\nu} = G \sum_1^{\nu} u_1 v_1 \quad (3)$$

$$u_1^2 = \frac{1}{2} \left(1 + \frac{\epsilon_{\Omega_1} - \lambda_{\nu}}{E_{\Omega_1}} \right) \quad (4)$$

$$v_1^2 = \frac{1}{2} \left(1 - \frac{\epsilon_{\Omega_1} - \lambda_{\nu}}{E_{\Omega_1}} \right) \quad (5)$$

$$E_{\Omega_1} = \left((\epsilon_{\Omega_1} - \lambda_{\nu})^2 + \Delta_{\nu}^2 \right)^{1/2} \quad (6)$$

Here ϵ_{Ω_1} is the single-particle energy, ν is the number of quasiparticles, λ_{ν} is the chemical potential for a given set of quasiparticles, Δ_{ν} is the correlation function, G is the pairing constant, N_{ν} is the number of particles below the level, from which the summation in the equations (1-3) is fulfilled. ν definite states must be excluded from the sum if the corresponding sign has upper index. E_{Ω}^{ν} is the energy of nucleus with ν quasiparticles in definite states. The total value of momentum projection to the nuclear symmetry axis Ω is the algebraic sum of the quantum number Ω_1 of blocked states. The excitation energy of nucleus with ν quasiparticles is

$$U_{\Omega}^{\nu} = E_{\Omega}^{\nu} - E_0 \quad (7)$$

where E_0 is the ground state BSC energy, which is calculated with the help of the same equations (1-6) with conditions $\nu=0$ for even N , and $\nu=1$ for odd N . The parity of this state is defined

$$\pi_N = \prod_{i=1}^{\nu_N} \pi_i \quad (8)$$

The equations (1-6) are solved separately for protons and neutrons for some values of quasiparticles ν_z and ν_N . Then all the combinations with the following excitation energies and quantum numbers are accounted

$$U_{k\pi} = U_{\Omega_N \pi_N} + U_{\Omega_z \pi_z} \quad (9)$$

$$k = \Omega_z \pm \Omega_N \quad (10)$$

$$\pi = \pi_z \pi_N \quad (11)$$

On each quasiparticle state rotational bands are built with the moment of inertia $F_{\perp}$ corresponding to the given deformation

$$U_{IK\pi} = U_{k\pi} + A_r \left(I(I+1) - K^2 \right) + B_r (I+1/2) (-1)^{I+1/2} \delta_{k,1/2} \quad (12)$$

where A_r and B_r are the rotational constants. Constant A_r can be approximately calculated

$$A_r = \frac{\hbar^2}{2 F_{\perp}} \quad (13)$$

The spin cutoff parameters $\sigma_{\perp}^2$ and $\sigma_{\parallel}^2 = K_0^2$ corresponding to the distribution of the total angular momenta I and the projection K on the symmetry axis can be estimated from calculated quasiparticle spectra

$$2 \sigma_{\perp}^2 = \frac{1}{n} \sum_{I=1}^n I(I+1) \quad (14)$$

$$\sigma_{\parallel}^2 = \frac{1}{n} \sum_{I=1}^n K_I^2 \quad (15)$$

Here n is the state number in the excitation energy interval ΔU .

II.2 Quantum-statistical superfluid model

The energy and spin statistical distribution of the deformed nuclei can be written in the form

$$\begin{aligned}\rho(U, I) &= \frac{1}{2} \sum_{K=-I}^I \rho(U - \varepsilon_{\text{rot}}, K) = \frac{1}{2} \sum_{K=-I}^I \rho\left(U - \frac{\hbar^2}{2F_{\perp}} (I(I+1) - K^2), K\right) \\ &= \frac{W(U)}{\sqrt{2\pi} \sigma_{\parallel}} \sum_{K=-I}^I \exp\left[-\frac{I(I+1)}{2\sigma_{\perp}^2} - \frac{K^2}{2\sigma_{\text{eff}}^2}\right]\end{aligned}\quad (16)$$

where $\frac{1}{\sigma_{\text{eff}}^2} = \frac{1}{\sigma_{\parallel}^2} - \frac{1}{\sigma_{\perp}^2}$, $W(U)$ is the total state density in the intrinsic coordinate frame system of deformed nuclei. For the ground and transition states of actinide nuclei we have $\frac{K^2}{2\sigma_{\text{eff}}^2} \ll 1$ therefore we get the following expression

$$\rho(U, I) = (2I+1) \frac{W(U)}{\sqrt{8\pi} \sigma_{\parallel}} \exp\left[-\frac{I(I+1)}{2\sigma_{\perp}^2}\right] \quad (17)$$

In these formulae the contribution of the rotational states is taken into account. The rotation enhancement of the level density for the axial symmetric deformed nuclei can be estimate in the following way [5-7]

$$K_{\text{rot}} = \frac{\rho_{\text{tot}}(U)}{W(U)} = \frac{1}{\sqrt{8\pi} \sigma_{\parallel}} \sum_{I=0}^{\infty} (2I+1) \exp\left[-\frac{I(I+1)}{2\sigma_{\perp}^2}\right] \approx \frac{\sigma_{\perp}^2}{\sqrt{2\pi} \sigma_{\parallel}} \quad (18)$$

In the frame of quantum-statistical superfluid model the intrinsic level density of the fermi system is expressed in the form

$$W(U) = (2\pi)^{-3/2} (\det S'')^{-1/2} e^{S(U)} \quad (19)$$

Here $S(U)$ is entropy, $\det S''$ is the determinant of a matrix, it is built with the second derivations even $\beta=1/T$, $\alpha_z = \mu_z/T$ and $\alpha_n = \mu_n/T$, where μ_n and μ_z are chemical neutron and proton potentials, T is temperature. The entropy of a superfluid fermion particle system is

defined by relation

$$S = 2 \sum_{\tau=N,z} \left[\ln (1 + \exp(-\beta E_{\tau 1})) + \frac{\beta E_{\tau 1}}{1 + \exp(\beta E_{\tau 1})} \right] \quad (20)$$

where τ , $\epsilon_{\tau 1}$ are the single-particle energies in a average nuclear potential for neutrons $\tau=N$ and protons $\tau=z$, $E_{\tau 1}$ are the quasiparticle energies (6). Correlation functions Δ_{τ} together with β , μ_n and μ_z at an excitation energy below the energy of transition from superfluid to normal states U_{cr} are determined by an equation system

$$U + E_0 = \sum_{\tau,1} \left\{ \epsilon_{\tau 1} \left[1 - \frac{\epsilon_{\tau 1} - \mu_{\tau}}{E_{\tau 1}} \operatorname{th} \left(\frac{\beta E_{\tau 1}}{2} \right) \right] - \frac{\Delta_{\tau}^2}{G_{\tau}} \right\} \quad (21)$$

$$N_{\tau} = \sum_1 \left[1 - \frac{\epsilon_{\tau 1} - \mu_{\tau}}{E_{\tau 1}} \operatorname{th} \left(\frac{\beta E_{\tau 1}}{2} \right) \right] \quad (22)$$

$$\frac{2}{G_{\tau}} = \sum_1 \frac{1}{E_{\tau 1}} \operatorname{th} \left(\frac{\beta E_{\tau 1}}{2} \right) \quad (23)$$

where E_0 is the ground state BCS energy, G_{τ} are the pairing constants.

The energy of transition from superfluid to normal state is calculated with the help of the relation (21) at $\Delta_{\tau}=0$ and $T=T_{cr}$ which is defined by equations (15) and (16) at $\Delta_{\tau}=0$ and $E_{\tau 1}=(\epsilon_{\tau 1} - \mu_{\tau})$. At temperatures higher than the critical temperature T_{cr} the entropy is also calculated from system (20-22) at $E_{\tau 1} = |\epsilon_{\tau 1} - \mu_{\tau}|$.

Spin cutoff parameters $\sigma_{\parallel}^2 = K_0^2$ and $\sigma_{\perp}^2$ are calculated in the following way

$$\sigma_{\parallel}^2 = \overline{\Omega^2} g T \quad (24)$$

$$\sigma_{\perp}^2 = \frac{F_{\perp} T}{h^2} \quad (25)$$

Here g is a single-particle level density near the Fermi energy, $\overline{\Omega^2}$ is the value of average square single-particle momentum projection on the symmetry axis of the deformed nucleus. The g value is calculated

by averaging over energy interval of a distance between nuclear shells
 $\gamma = 41 A^{-2/3}$

$$g(\lambda) = \frac{1}{\gamma} \sum_i \exp\left(-\frac{(\epsilon_i - \lambda)^2}{\gamma^2}\right) \quad (26)$$

Fermi energy is defined by solving equation

$$N = \int_{-\infty}^{\lambda} f(\epsilon) g(\epsilon) d\epsilon \quad (27)$$

where $f(\epsilon)$ is the correction polynomial

$$\begin{aligned} f(\epsilon) &= \frac{1}{\sqrt{\pi}} \sum_{n=0}^P C_n H_n(u) \\ u &= \frac{(\epsilon - \lambda)}{\gamma} \quad , \quad C_n = \begin{cases} \frac{(-1)^{n/2}}{2^n (n/2)!} & n \text{ even} \\ 0 & n \text{ odd} \end{cases} \\ \gamma &= \hbar \omega_0 = 41 A^{-2/3} \end{aligned} \quad (28)$$

The $\bar{\Omega}^2$ is obtained by averaging over the single-particle energy interval $\Delta\epsilon = (3+4)T$ near the Fermi level. The energetic dependence of the moment of inertia $F_{\perp}$ is approximated in the following way

$$F_{\perp} = \begin{cases} (F_0 - F_{\text{rigid}}) \left(1 - \frac{U}{U_{\text{cr}}}\right) + F_{\text{rigid}} & U < U_{\text{cr}} \\ F_{\text{rigid}} & U \geq U_{\text{cr}} \end{cases} \quad (29)$$

where F_0 is the moment of inertia in ground state, U_{cr} is a maximum value of the transition energy from superfluid to normal states for neutron or protons system, F_{rigid} is the rigid body moment of inertia of the nucleus.

III. ANALYSIS OF THE RESULTS OBTAINED WITH CODE DENCOM.

The necessary base to study the state densities of heavy nuclei, in the region corresponding to high deformations in fission path and which characterizes the extreme points in this process, is the calculation of a single particle spectrum. By using a given model of the nuclei, it will be able to describe variations in nuclear shape, when we have in mind a process where all the internal degrees of freedom the system are involved, as in the case of atomic nuclear fission. In our calculations parameterization of the nuclear shape proposed by V.V Pashkevich and performed in DIANA program [13], is used. Parameterization uses as a base figure the Cassini ovals and operates with a Saxon-Woods type deformed potential, the more suitable procedure for the treatment of the average field of deformed nuclei in actinide region. Potential parameters are selected according with an optimum coincidence with the single-particle excitation spectrum. Single particle spectrum can nonetheless be chosen with another axially-symmetric shape parameterization if it is necessary for work, and, this is not, of course, an obstacle for the operations of DENCOM program.

Combined combinatorial-statistical approach describes the main features of level densities in a wide energy range. This is shown in figure 1 for nuclei of different parity. For the low energy region energy and spin distributions are non-statistical. This is shown in figures 1,2. In fig.3 energy dependence of spin cutoff parameter is presented. The analysis of figures 1-3, shows that ρ^{total} becomes smooth quickly enough. That is not the case for spin distribution, in which shell effects can be seen up to high energies. In fig.1 is illustrated the agreement with experimental data for low energies. The exact account of the superconductivity and shell effects in combined approach guarantees the quality of level density description in a wide energy range.

The analysis of fig.2 convincingly shows the limits from which the quasiparticle excitation spectrum must receive a statistical treatment. This analysis is just the one that allows to fix ECOS

value, which at the same time fixes the limit between combinatorial and statistical calculations. It would be interesting to point out that for energies below ECOS (for each nucleus , in general $2 \text{ MeV} < \text{ECOS} < 3 \text{ MeV}$) distribution behavior for I and K is not statistical. However, with the increase of excitation energy the distribution as a function of I is more rapidly near the statistical behavior than the distribution as a function of K, if we are referring to $\rho^{\text{total}}(u)$; in this case the behavior is typical of statistical dependencies for energies higher than 2.5 MeV .

Calculations can be improved if the parameter set of the average field, as well as the constants of pairing interaction, and the parameters defining rotation bands are separately selected for each nucleus. When working with a given region of interest, of course, mean values of these parameters can be selected, which approximately correspond with the real values and noticeably simplify the calculation volume. To take into account the collective effects is necessary because it leads to a state redistribution according to the energy . The absence of low energy collective states can be substituted by including more recent nuclear models such as the Phonon Quasiparticle Model and the Interacting Boson Model. Statistical- quantum calculation can be improved by including K_{vib} [14].

In fig.4, a comparative analysis is shown for the case of $U^{234}(n, f)$ in which the way to improve the description of σ_f is evident, by including this combined procedure, which even allows to evaluate the unsuccessful moments in a systematic of σ_f .

The calculation carried out using the Combined Method allows to improve the understanding of transition states' role in energetic dependence irregularities of fission cross section. As it is shown in fig.4 example , experimental irregularity present in the energy range from 0.5 to 1.5 MeV could be reproduced. This is very significant to explain irregularities present at these same energies in correlated magnitudes: average kinetic energy and angular distribution of fission fragment. In the frame of the phenomenological method is not possible to reproduce these irregularities due to the fact that nuclear structure is not explicitly considered.

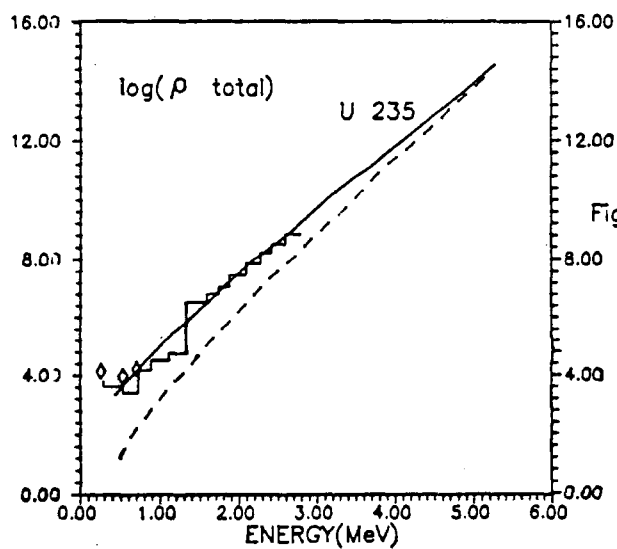
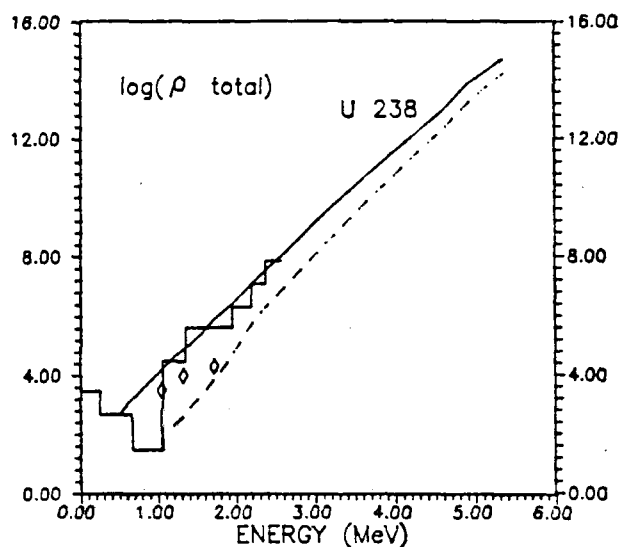
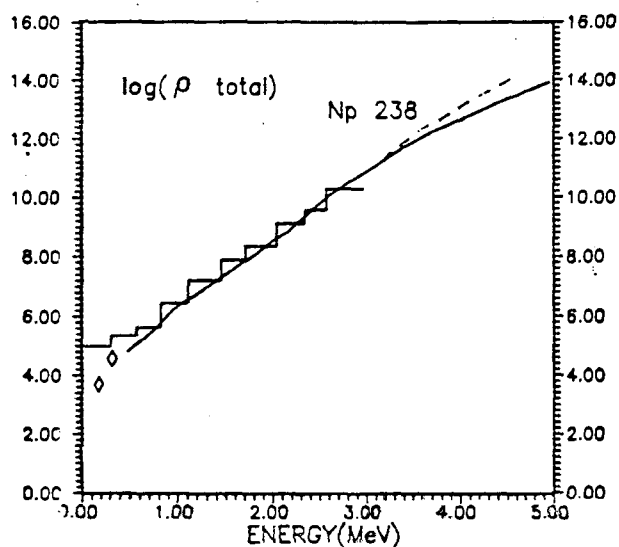


Fig.1 The experimental and calculated level densities. The histogram is the combinatorial, the full line is the quantum statistical model and the dotted curve is the phenomenological superconductivity model /14/ calculation.

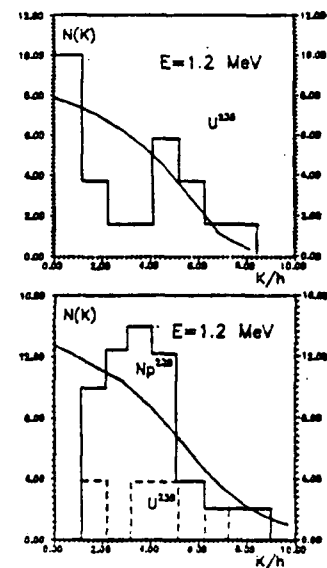
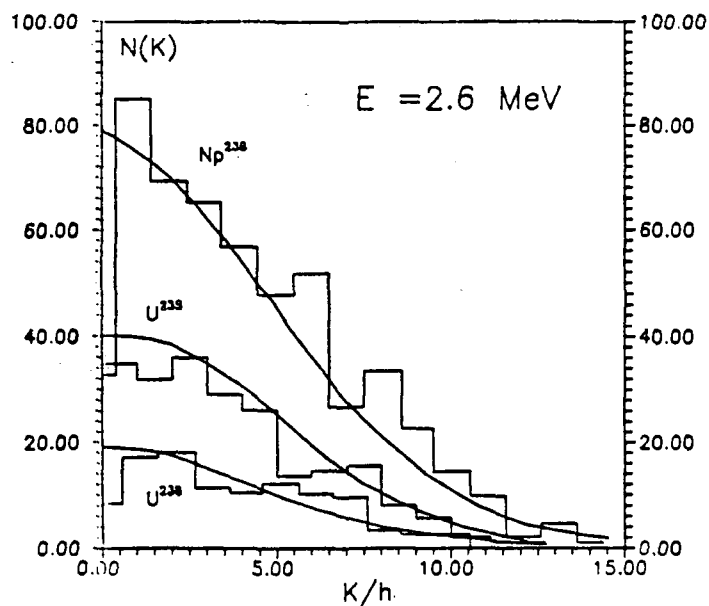


Fig.2a K-distributions of the discrete spectra(histogram) and their statistical approximation at different values of energy.

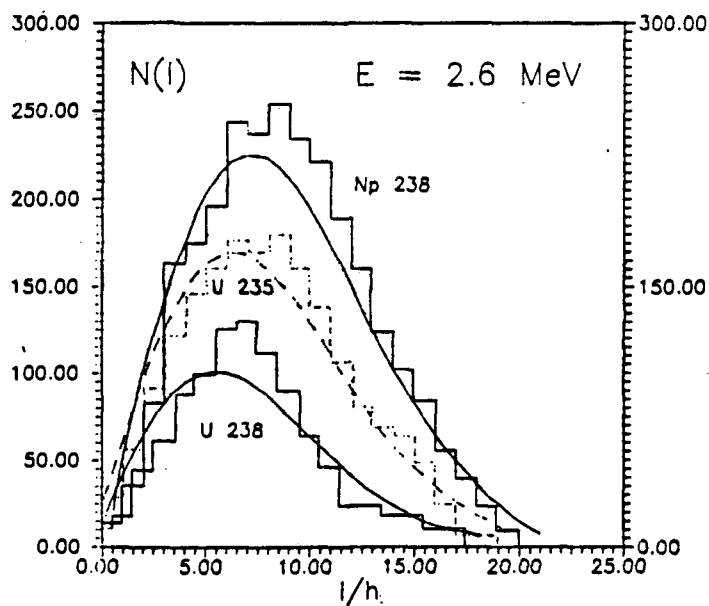


Fig.2b I-distribution of the discrete spectra(histogram) and their statistical approximation

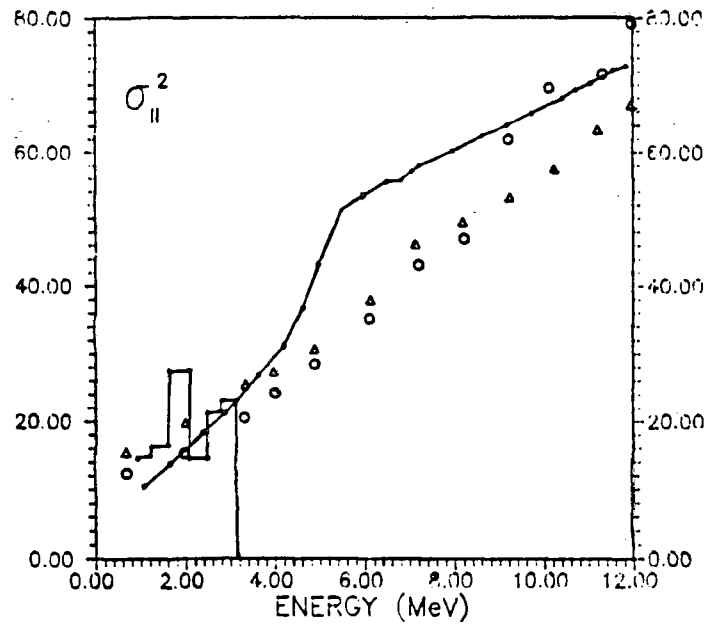


Fig.3 The histogram and the full line are the combinatorial and the superconductivity models calculations. The circles and the triangles show the results of the statistical approximation with averaging in 3 and 4T intervals.

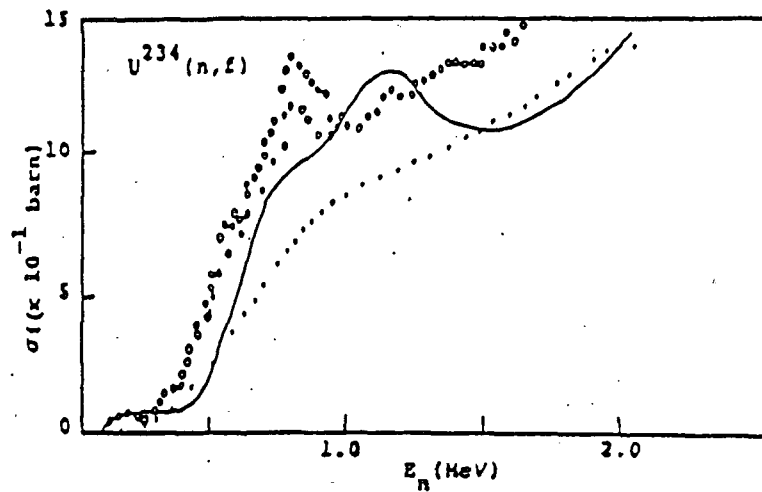


Fig4. Fission Cross Section of U^{235}
 (-----) result of [15] where DENCOM code is used
 (.....) result of [16]
 (o o o o) experimental data [17,18]

III ORGANIZATION OF THE COMPUTER CODE

1. General Structures of the Code

The computer code permits the calculation for the deformed nucleus with axial-symmetry of the next magnitudes :

- a. Quasiparticle spectrum of the nucleus and its rotational bands.
- b. Nuclear level densities using the superfluid model
- c. Spin cutoff parameters and its energetic dependence.

The code's work is divided in two fundamental sections. The first one, done by subroutine COMBIL calculates the quasiparticle discrete spectrum and its rotational bands up to a maximum energy (ECOS), introduced as an input data. The second one, carried out by subroutine DELSTA calculates the nuclear level densities from the same energy ECOS to UMAX (maximum considered excitation energy). UMAX is an input data.

Calculation are performed for fixed values of the nuclear deformation parameters, which are included implicitly in the single particle spectrum given as an input data.

Subroutines COMBIL and DELSTA call a set of subroutines that allow the performance of the calculations. In Fig.1 the general structure of the code and the name of all subroutines are used shown.

The code is a set of 25 subroutines. It needs 90 Kbytes of operating memory using the Microsoft FORTRAN v 5.1 Compiler.

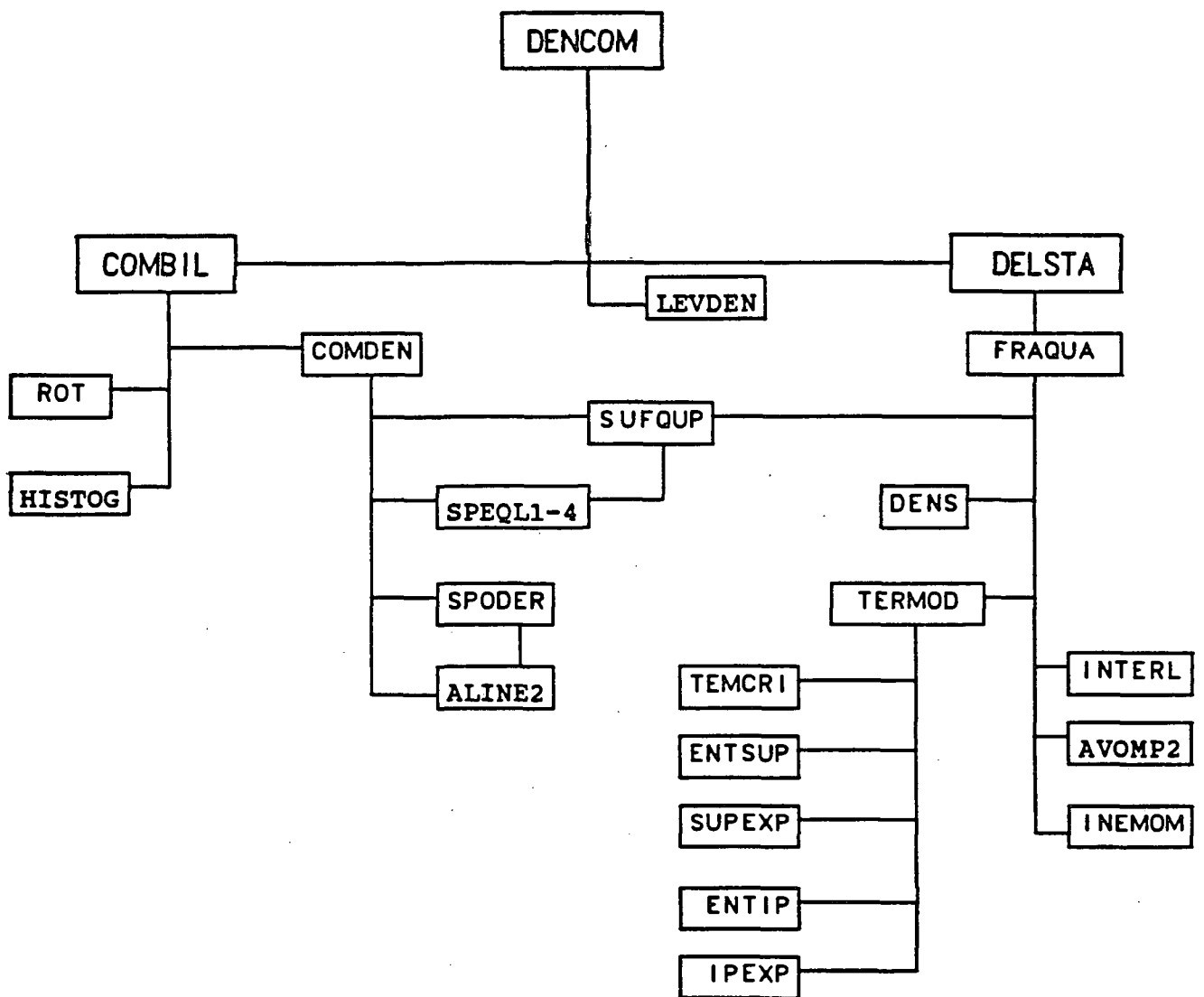


Fig.1 General Structure of the code.

2.- Input data

Single particle spectrum for neutron and proton system are read from file3='NEUTRON.SPE' and file4='PROTON.SPE' respectively.

READ FROM FILE 3.4.9

1.- card 1

AA(1),AC,HA(2),ZC [A4, F5.0, A4, F4.0]

AA(1)- identifiers.

AC - mass number of the base nucleus.

ZC - atomic number of the base nucleus.

2.- card 2

AA(3), EPSI, AA(4), ALPHA3, AA(5), ALPHA4, AA(6), NUM
[A8, F5.2, 2(A9, F5.2), A6, I4]

AA(I) I=3,6 : identifiers.

EPSI - quadrupole deformation parameter.

ALPHA3 - octupole deformation parameter.

ALPHA4 - hexadecapole deformation parameter.

NUM - number of single-particle levels to be read.

3.- card 3

(ENE(I), IQNE(I), I=1,NUM) [5(F8.3, I5)]

ENE(I) - neutron single-particle spectrum array.

IQNE(I) - K in symmetric rotational model. (array).

file4 has the same cards for protons.

The rest of the data and options are read from
file9= 'DENCOM.INP'.

1.- card 1

AA(7) [A3]

AA(7) - Chemical symbol of the nucleus.

2.- card 2

(NA,NZ) [2I4]

NA - Nucleus mass number.

NZ - Charge number.

3.- card_3

(NUQN,NUQZ) [2I2]

NUQN - Neutron quasiparticle number.

NUQP - Proton quasiparticle number.

4.- card_4

ECOS [F4.2]

ECOS - Matching energy.

5.- card_5

(KTEST,KRHO) [2I2]

KTEST - Key to print Δ_n , Δ_z and $\bar{g}_n$, $\bar{g}_z$.

KRHO - Key to compute partial level density.

0 - Compute partial level density by eq.17.

1 - Compute partial level density by eq.16.

6.- card_6

This card is read only if KTEST=1.

(BN,STAR) (2F5.2)

BN - Neutron binding energy.

STAR - Spin of the target nucleus. ${}^{N A-1}_{N Z} X$.

7.- card_7

KLQP [I2]

KLQP - Key to options calculus.

0 - Only compute quasiparticle spectrum.

1 - Only compute statistical level density.

2 - Both.

3- Output data

The results are given in files 5,6,7,21,22.

FILE5='SPEQP.DAT' the total quasiparticle spectrum.

FILE6='SPEQPROT.DAT' the total rotational spectrum and histogram of
 $.dn/du$, K_0^2 , σ_1^2

The histogram is stored in this file if KLQP=0.

FILE7='STATIST.DAT' intrinsic state density and spin cutoff parameters.

FILE8='LEVELD.DAT' partial level density : $\rho(u,i)$
total level density, : $\rho^{\text{total}}(u)$
rotational enhancement : $K^{\text{rot}}(u)$

The histogram is stored in this file if KLQP=2.

FILE21='NEUT.FIN' Correlation function and $\bar{g}$ for neutron.

FILE22='PROT.FIN' Correlation function and $\bar{g}$ for proton.

4. Short description of the subroutines.

SUBROUTINE COMDEN

This subprogram conforms the quasiparticle excitation spectrum of the nucleus by a combinatorial method in the energy interval [UMAXI,UMAX].

The most important variables and arrays are:

ND: half of the interval for the sum by BCS

SPZE (SPNE): It stores energy of quasiparticle spectrum for proton and neutron system.

SPZO(SPNO) : It stores quantum number of quasiparticle spectrum for proton and neutron system.

SPE(SPO) :arrays to store the energy and quantum number of quasiparticle spectrum of the nucleus.

SUBROUTINE SUFOUP.

It constitutes the main routine of every calculations. The energy of quasiparticle spectrum is calculated in it according to the BCS model, with a fixed number of quasiparticles (up to 4) in prefixed states. The blocking effect is considered.

The most important variables and arrays are the following:

N : Number of particles

NL,NU : numbers of the lowest and highest levels for the energy interval in which pairing is considered .

NUQ : number of quasiparticles

L1,L2,L3,L4 : number of levels, beginning from the ground, in

single-particle spectrum, in which the quasiparticles are located

EPS: result accuracy

F: chemical potential

EBCS: Energy value by BCS

/ENERGC/ : array in which level spectrum is stored .

If every L_k and $NUQ=0$,then this is the basic state of the nucleon even system.

States with two or four quasiparticles can be taken into account for nucleons even system. States with one or three quasiparticles can be taken into account for nucleons odd system.

Equation system is solved by the method of "steepest descent".

SUBROUTINE SPODER.

This subprogram conforms quasiparticle excitations spectra corresponding to a given even or odd system of nucleons (neutrons or protons). It organizes the spectrum in an ascending order of excitation energy. It accepts no more than two types of excitations (2 and 4, or 1 and 3).

The most important variables and arrays are :

UMAX: maximum value of the spectrum energy stored in SPE.

SPE: energy of the quasiparticle spectrum of the given nucleon system

SPO: quantum numbers K and Π stored as :

$$2 \cdot (0.5 - \Pi) \cdot (\Omega + 1)$$

$$\Pi = (0 +, 1 -)$$

SP1, SP2: arrays where spectra obtained for a given quasiparticle system in the subroutines SPEQL(1) are stored.

NM: number of particles in the one-component system.

SUBROUTINE SPEQL(i)

This subprogram conforms spectrum with quasiparticle excitations of a given type (with 1, 2, 3 and 4 quasiparticles) according to the BCS model , considering the blocking effect for a deformed potential and for a given system (proton or neutron).

The most important variables and arrays are the following:

NMAX: It is used to define the spectrum interval in which the quasiparticles are located (I1,I2)

I1=NN/2-NMAX.

I2=NN/2+NMAX.

SP:array in which calculation results are kept
(quasiparticle spectrum)

NSP: SP array dimension

SUBROUTINE LEVDEN.

This subprogram carries out the calculation of energy and spin statistical distribution of the deformed nuclei: $\rho(U,I)$ according to the formula (16) or (17) if key KRHO is 1 or 0. Furthermore, the total level density of the nucleus, and the coefficient of rotational enhancement are calculated (K_{rot}).

The most important arrays are :

ALEVDEN: It stores distribution $\rho(U,I)$

TOTALD: Total $\rho^{total}(U)$ density are stored

AROT: K_{rot} values are stored

SUBROUTINE ROT

This subroutine performs the rotational band on the quasiparticle spectrum obtained by COMDEN and writes it in file 6 (='SPEQROT.DAT').

The most important arrays are :

QPS : stores quasiparticle spectrum (energy)

OMQPS : stores quantum number K and parity of quasiparticle spectrum.

QPROTS: stores the total rotational spectrum (energy).

QNIKPI: stores the quantum number (I,K,PI) of the total rotational spectrum.

The order of the total rotational spectrum is carried out by ALINE2.

SUBROUTINE HISTOG

This subroutine performs the histogram calculation of the total discrete spectrum obtained by COMBIL.

The energy histogram (HIRO) is obtained, from K_0^2 (HIK02) and σ_1^2 (HISIP2).

SUBROUTINE ALINE2

This subroutine organizes the tables of the different values of the function in an increasing order of energy.

SUBROUTINE DELSTA

Fixes two sets for performed calculations of values of nuclear temperatures; (initial and final temperature and variation step) afterwards, subroutine FRAQUA is called.

SUBROUTINE FRAQUA

Organizes the calculations of the continuous part of the spectrum and stores the final results in an array (FRAD). It obtains the parameters of the parallel and perpendicular spin cutoff $\sigma_{\parallel}^2$, $\sigma_{\perp}^2$ in the frame of the quantum-statistical model.

The most important arrays are:

DEST : stores the intrinsic level density.

SIGPE2 : stores the perpendicular spin cutoff.

SIGPA2 : stores the parallel spin cutoff.

The following subroutines are called SUFQUP, DEN, TERMOD.

SUBROUTINE INTERL

Performs the interpolation of the function using Lagrange polynomial. The function and its argument are stored in the array PLUR of NP dimension

EX : argument values for which the functions are calculated .

DENS: function values to interpolate.

PLUR: table of arguments and functions x1, f1, x2, f2.

NP : dimension of PLUR.

SUBROUTINE INEMON

Computes the perpendicular inertial momentum of the nucleus for a given excitation energy according to (29).

SUBROUTINE AVOMP2

Computes the average square single-particle momentum

projection on the symmetry axis of the deformed nucleus.

CTAV : energy interval near the Fermi level for which the average of $\bar{\Omega}^2$ is estimated.

AOMN2 : variables where the values of the $\bar{\Omega}_N^2$, $\bar{\Omega}_Z^2$ are stored.
(AOMZ2)

SUBROUTINE DENS

This subroutine computes the level densities for different values of a scaling factor γ at different energies. Average is estimated taking into consideration energy intervals of a distance between nuclear shells, for neutron and proton system (26).

The single-particles spectra are transmitted by the COMMON ENERG. The results are transferred by the COMMON DENSIC.

The $\bar{g}_{(E)}$ is calculated taking into account (26-28) where the optimum choice for $P=6$ is $\gamma=41 A^{-2/3}$.

The C_α coefficients are expressed by the Gardner scheme.

SUBROUTINE TERMOD

Calculates the thermodynamic functions and their dependence on energy and temperature. Calculated values as a function of temperature are placed into the array TERM in the following sequence:

- K+1. E- energy.
- K+2. S- entropy.
- K+3. GAP- correlation function.
- K+4. DET- determinant of matrix of second derivates for one type of particle.
- K+5. Second derivate on alpha.

In the first five elements of the array there are:

- 1- E₀- total energy of the ground state.
- 2- GAP.
- 3- SP- ground state entropy.
- 4- TEC- critical temperature.
- 5- UCR- critical energy.

Subroutine TERMOD uses external subroutine TEMCRI for calculating of the critical temperature. When temperature $T < T_{crit}$, it is called ENTSUP and SUPEXP by the superfluid model (BCS). When $T \geq T_{crit}$, it is called ENTIP and IPEXP in the frame of independent particle model.

SUBROUTINE TEMCRI

This subroutine computes the critical temperature (TECR), the critical energy (UCR) and the accurate calculation of the chemical potential (HIMPOT).

Computer calculations are made resolving the system (21-23) by taking in account $\Delta=0$ y $T=T_{crit}$. To resolve the system the method of "steepest descent" is used.

SUBROUTINE ENTSUP

This subroutine computes, by the superfluidity model, the energy (E), the entropy (S), the correlation function (GAP) and the chemical potential (HIMPOT). For this purpose, the system (21-23) is solved using the method of "steepest descent".

SUBROUTINE SUPEXP

This subroutine is used to compute the matrix of entropy's second derivatives for the superfluid system. (det S'' of (19)). Exit pairs are:

$$DET = \left[\frac{\partial^2}{\partial p^2} \ln(Z) \right] \frac{1}{\beta^2 \partial \lambda^2} \ln(Z) - \left[\frac{\partial}{\partial \beta} \left(\frac{1}{\beta} \frac{\partial}{\partial \lambda} \ln(Z) \right) \right]^2$$

$$DAT = \frac{1}{\beta^2} \frac{\partial^2}{\partial \lambda^2} \ln(Z)$$

The calculations are carried out for a given temperature of the Fermi system.

The single-particles energies, which in this subroutine are closely related with the partition function Z, are given in the COMMON /ENERGC/.

SUBROUTINE ENTIP

This subroutine has the same purpose as that of the ENTSUP, but for the non interacting particle system.

When temperature $T > T_{crit}$, the system (21-23) is changed in

$$\begin{aligned} N^{IP} &= 2 \sum_i \frac{1}{1 + \exp(\beta(E_i - \lambda))} \\ E^{IP} &= 2 \sum_i \frac{E_i}{1 + \exp(\beta(E_i - \lambda))} \\ S^{IP} &= 2 \sum_i \left\{ \ln[1 + \exp(-\beta(E_i - \lambda))] + \frac{\beta(E_i - \lambda)}{1 + \exp(\beta(E_i - \lambda))} \right\} \end{aligned}$$

This system is solved employing the Newton method.

The total energy(E), the entropy (S) and the chemical potential ($HIMP$) of the system are calculated in this subroutine.

SUBROUTINE IPEXP

This subroutine has the same purpose as that of the SUPEXP, but for the non interacting particle system.

IV. CONCLUSIONS.

For deformed nuclei and especially for extreme points of fission path, the fenomenological methods in level density calculations have many disadvantages. In these cases, the semi-microscopical approach is more adequate. The semi-microscopical Combined Method includes the use of combinatorial and statistical methods for low and high energy correspondingly

The code DENCOM is apt to calculate level densities for axial-symmetric deformed nuclei, using the Combined Method. When applying the results of the code, the adequacy of the models used must be assured. The results obtained using DENCOM code allow to consider in the analysis of the state densities, the particular properties of state spectrum, in a wide energy and deformation range.

Work on the DENCOM code is in progress to improve the accuracy and to consider new effects in a more realistic way. In the next version of code configuration with higher numbers of quasiparticles and vibrational enhancement will be included among others features.

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