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STATISTICAL DESCRIPTION OF DEFORMATION IN EXCITED NUCLEI AND DISAPPEARANCE
OF SHELL EFFECTS WITH EXCITATION ENERGY*

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August 1971

Abstract

The deformation of excited nuclei is studied on the basis of the methods of statistical mechanics. The statistical coupling between a system with many internal degrees of freedom and a one-dimensional or multidimensional harmonic oscillator is considered. The relevance of the phase-space volume is discussed in the semiclassical limit. The conclusions are employed to develop a general theory of nuclear deformation for actual nuclei. Calculations for five nuclei are performed on the basis of the Nilsson diagram and of the BCS Hamiltonian. The potential energies of nuclei as a function of deformation are calculated by means of the Strutinski procedure. The level densities are also calculated directly from single particle levels and include pairing and its energy dependence. The deformation probability as a function of excitation energy are derived. The nuclear fluctuations in shape are considered and in particular the disappearance of the ground state deformations with increasing excitation energy is described. The calculations account in a natural way for the washing out of shell effects with excitation energy. Applications of the theory are discussed.

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1. Introduction

The shell model has been successful in explaining the main features of ground state nuclei and of nuclei at low excitation energies: in particular the ground state deformation of a nucleus can now be calculated with a reasonable degree of accuracy. In fact the leading quadrupole term can be predicted as well as higher multipole moments¹). The simplest procedure makes use of the so-called Strutinski normalization²); on the basis of this method the potential energy of a nucleus as a function of deformation is obtained as a sum of a smooth liquid drop term and of the "wiggles" derived from the shell model. The minimum in the potential energy determines the ground state deformation. While such a simple approach yields reliable values for the deformation parameters in nuclei very near closed shells or well between two major shells, the study of the potential energy alone may be inadequate for transition nuclei which are characterized by shallow minima in potential energy and which are not quite spherical nor deformed. The reason for this fact lies in the quantum-mechanical fluctuations in deformation associated with the zero-point motion. Nonetheless we can state that, aside from quantum mechanical fluctuations, a nucleus in its ground state has a well defined deformation. A similar statement holds for a nucleus at a low excitation energy level and its deformation can be obtained, in principle, in the same way as for a ground state nucleus. A new problem arises when we consider a nucleus excited in the statistical region where the energy dispersion is large compared with the level spacing and where the level widths are comparable or larger than the level spacing. For such a nucleus the definition of deformation is more complicated. On one hand we should not expect

unique values for the deformation parameters, because of the large numbers of levels considered at the same time; on the other hand we may expect a coupling between collective and intrinsic degrees of freedom because of the overlapping levels. These circumstances seem to justify the assumption of statistical equilibrium between all the degrees of freedom; therefore the nucleus is expected to explore all the deformations accessible to it on the basis of its excitation energy. Thus, as the statement of the problem suggests, we should expect a distribution in the deformation parameters for an excited nucleus instead of a unique set. Such a distribution can be obtained on the basis of statistical mechanics considerations. For an ordinary macroscopical system, the standard procedure consists in determining the average or the most probable values for the relevant variables. In the present case, the system we are dealing with is composed of a small number of particles: consequently a rather large probability of relative fluctuations is expected in the various dynamical variables, among which the deformation coordinates are included. The possibility of very large fluctuations in shape is proved without question by the fission process where, at low excitation energies, a large fraction of the excitation energy is concentrated in one single degree of freedom. From such considerations the necessity arises of determining the whole probability distribution in the deformation coordinate(s).

The nuclear deformation is a feature which depends upon the details of the shell structure and not upon the smooth nuclear properties. Therefore it is of the utmost importance for the solution of the present problem to develop a statistical procedure which incorporates all the relevant features of the shell model. In this regard, the problem of the level densities assumes two

aspects. On one hand we must be able to evaluate the level density for an arbitrary, fixed deformation. On the other hand, the outcome of the statistical calculation should allow one to define the actual overall level density, accounting also for the deformation degrees of freedom. Preliminary results have been presented in a previous paper³). In the present paper we shall deal first with the case of a many-particle system coupled with one or more harmonic oscillators. Then we shall consider the case of an actual excited nucleus coupled with its collective degrees of freedom (which do not need to be harmonic oscillators). In all these cases the statistical problem is solved in the microcanonical ensemble and the canonical ensemble expansion will be considered. The models involved in the actual calculations are presented and the results for six nuclei ranging from Yb to Pb are discussed. In the appendices we present an analytical formulation of the Strutinski-like potential energy normalization and a general formalism for the level density calculation on the basis of an arbitrary set of single-particle levels including pairing.

2. General Theory

We are interested here in determining the properties of a system with a large number of internal degrees of freedom, statistically coupled to one or more collective modes of motion. The simplest case is perhaps that in which the collective modes of motion are represented by harmonic oscillators.

2.1. COUPLING BETWEEN A MANY-PARTICLE SYSTEM AND ONE OR MORE HARMONIC OSCILLATORS

Let us consider a system with many internal degrees of freedom, whose density of states at an excitation energy x is $\rho(x)$. A harmonic oscillator whose energy quantum is $h\nu$ is statistically coupled to such system. We further assume that the total energy is E and we plan to work within the microcanonical ensemble. The probability of finding the oscillator at the elongation q is:

$$P(E, q) dq = \sum_n \rho(E - nh\nu) \psi_n^2(q) dq \quad (1)$$

where the quantities $\psi_n(q)$ represent the normalized harmonic oscillator wave functions. Such an expression holds for all the excitation energies; however, if the excitation energy is sufficiently high, on the average we shall be dealing with sufficiently high oscillator quantum numbers. For a high quantum number n , we obtain the classical expression for ψ_n^2 :

$$\psi^2(q) \approx \frac{\nu}{v(q)} \quad (2)$$

where $v(q)$ is the velocity at the elongation q . Now, we can substitute eq. (2) in eq. (1) and transform the summation into an integral:

$$P(E, q) dq = dq \int g \rho(E - \xi) \frac{v}{v(q)} d\xi ; \quad (3)$$

where $g = \frac{1}{h\nu}$ is the oscillator level density and ξ is the energy of the oscillator. By changing the integration variable from the energy ξ to the oscillator momentum p we obtain:

$$P(E, q) dq = dq \int \frac{1}{h\nu} \rho\left(E - V(q) - \frac{p^2}{2m}\right) h\nu \frac{m}{p} \frac{p}{m} \frac{dp}{h} \quad (4)$$

or

$$P(E, q) dq = \int \rho\left(E - V(q) - \frac{p^2}{2m}\right) \frac{dp dq}{h} \quad (5)$$

where $V(q)$ is the oscillator potential and m is the inertial parameter of the oscillator.

Such an elementary calculation shows that the contribution of the oscillator to the state density is $\frac{dp dq}{h}$ or, as we could have expected, proportional to the classical phase-space volume.

The generalization to an r -dimensional oscillator is immediate:

$$P(E, q_1, q_2, \dots, q_r) = \sum_{\underline{n}} \rho(E - \sum_i n_i h\nu_i) \psi_{\underline{n}}(q_1, q_2, \dots, q_r) dq_1, dq_2, \dots, dq_r \quad (6)$$

where $\underline{n}$ is a vector with components n_i . Again for high quantum numbers we obtain:

$$P(E, p_1, p_2, \dots, p_r) = \int \frac{1}{h^r \prod v_i} \rho\left(E - V(q_1, q_2, \dots, q_r) - \sum \frac{p_i^2}{2m_i}\right) \frac{\prod v_i}{\prod v_i(q_i)} \prod v_i(q_i) dp_1, dp_2, \dots, dp_r, dq_1, dq_2, \dots, dq_r$$

$$= \int \rho \left(E - V(q_1, q_2, \dots, q_r) - \sum \frac{p_i^2}{2m_i} \right) \frac{dp_1, dp_2, \dots, dp_r, dq_1, dq_2, \dots, dq_r}{h^r} \quad (7)$$

where again we can observe the relevance of the phase-space volume in the density of states of the system.

All three results reported above have been obtained in the microcanonical ensemble framework. The calculations for the same system, performed within the canonical ensemble are reported, for instance, by Landau and Lifchitz⁴).

2.2. STATISTICAL PROPERTIES OF A NUCLEUS WITH ONE OR MORE COLLECTIVE DEGREES OF FREEDOM

The present case is more complicated than those considered above; in fact the excitation energy disrupts the nucleon configurations which are responsible for the actual form of the potential energy. However, it is still possible to solve the problem approximately.

We consider a nucleus with total energy E , free to move along the collective coordinate ϵ . Let $V(\epsilon)$ be the potential energy and $E_T = E - V(\epsilon)$ be the local excitation energy (fig. 1).

At fixed deformation ϵ , the available excitation energy E_T can distribute itself between the internal and the collective degrees of freedom. The contribution of the collective degree of freedom to the statistical probability can be taken to be proportional to the collective phase-space volume, as we have seen for the harmonic oscillator case. Therefore the probability that the available excitation energy will distribute itself in any arbitrary way among the internal and the collective degrees of freedom can be written as follows:

$$P(x, \epsilon) d\epsilon dp = \rho(x) \frac{d\epsilon dp}{h}, \quad (8)$$

where x is the energy taken-up by the internal degrees of freedom, $\frac{p^2}{2m}$ is the energy taken-up by the collective degree of freedom, $\rho(x)$ is the state density deriving from the internal degrees of freedom, p is the conjugate momentum of ϵ and m is the inertial mass associated with the collective motion.

In order to obtain the total probability of finding the nucleus at the deformation ϵ , one must integrate over all the possible energy partitions:

$$P_T(E_T, \epsilon) d\epsilon = d\epsilon \int \rho(E_T - \frac{p^2}{2m}) dp \quad (9)$$

In such an integral the integration limits are $\pm \sqrt{2mE_T}$. The evaluation of the integral in eq. (9) can be simplified on the basis of the following considerations.

- a) The integrand presents a sharp maximum for $p = 0$ and decreases rapidly with increasing $|p|$: therefore the main contribution to the integral comes from low $|p|$ values. As a consequence, we can substitute the integration limits with $\pm \infty$.
- b) For the same reasons mentioned above, we can attempt to perform a suitable expansion of the integrand about $p = 0$. It turns out that a more rapid convergence is obtained by expanding the logarithm of the integrand:

$$\ln \rho = A(E_T) - A'(E_T) \frac{p^2}{2m} + A''(E_T) \frac{1}{2} \left(\frac{p^2}{2m} \right)^2 + \dots \quad (10)$$

or

$$\rho(E_T - \frac{p^2}{2m}) = \rho(E_T) e^{-A'(E_T) \frac{p^2}{2m}} e^{A''(E_T) \frac{1}{2} \left(\frac{p^2}{2m} \right)^2} \quad (11)$$

where

$$A'(E_T) = \left(\frac{d \ln \rho(x)}{dx} \right)_{x=E_T} ; \quad A''(E_T) = \left(\frac{d^2 \ln \rho(x)}{dx^2} \right)_{x=E_T} \quad (12)$$

If we employ the approximate expression $\rho(E) \propto \exp 2\sqrt{aE}$, then $A' \approx \sqrt{a} / \sqrt{E}$ and $A'' = -\frac{\sqrt{a}}{2 E^{3/2}}$. For an ordinary nucleus the third term in the expansion given by eq. (10) is clearly small and can be dropped. By means of the two approximations which we have made, the integral of eq. (9) becomes the integral of a gaussian and can be given explicitly:

$$P_T(E_T, \epsilon) d\epsilon = \frac{\sqrt{2\pi m}}{h} A'^{-1/2} \rho(E_T) d\epsilon \quad (13)$$

Since the integrand decreases approximately by a factor of e for $\frac{dA}{dE} \Delta E = 1$, about 85% of the integral comes from the energy interval $E_T \pm \frac{\sqrt{E_T}}{\sqrt{a}}$. The quantity $\frac{\sqrt{E_T}}{\sqrt{a}}$ for an ordinary excited nucleus is very small compared to E_T , and therefore the approximation given by eq. (13) is good.

In this regard it is deeply significant to notice that the term A' as given by eq. (12) is equal to the inverse of the local nuclear temperature at the deformation ϵ :

$$A' = \left(\frac{d \ln \rho(x)}{dx} \right)_{x=E_T} = \frac{1}{T} \quad (14)$$

Therefore the expansion given in eq. (10) is just the expansion which allows passage from the energy-preserving microcanonical ensemble to the constant-temperature canonical ensemble. In simpler words, such an approximation physically means that the nucleus at the deformation ϵ acts as an infinite heat reservoir

at constant temperature T with which the collective mode of motion along ϵ is in equilibrium. It is equally important to notice that eq. (13) is the canonical result as far as the energy partition at fixed deformation is concerned and it is the microcanonical result as far as the deformation parameter ϵ is concerned. It is indeed essential to conserve energy as the system moves along ϵ , since the variations in potential energy may be very large and more than one minimum may be present.

In conclusion we may expect that eq. (13) represents a good approximation to the deformation probability of an excited nucleus. Such an expression can be employed if a realistic potential energy $V(\epsilon)$ and state density $\rho(E, \epsilon)$ can be obtained on the basis of the shell model theory. This point will be discussed in the following sections.

The argument that we have developed can be extended to the case of a larger number of collective degrees of freedom. We shall now treat the case of two collective degrees of freedom and then we shall generalize the result for an arbitrary number of them.

Let us assume that the shape of the nucleus is described by two collective coordinates α_1, α_2 . It is always possible to change to a new system of generalized coordinates q_1, q_2 such that the inertia tensor $m_{i,k}$ is diagonal. In this way the kinetic energy of the collective motion can be written as:

$$E_{\text{kin}} = \frac{p_1^2}{2m_1} + \frac{p_2^2}{2m_2} \quad (15)$$

where p_1 and p_2 are the conjugate momenta of the new coordinates and m_1, m_2

are the elements of the diagonalized inertia matrix. The probability of finding the nucleus at the deformations q_1, q_2 will be:

$$P_T(E, q_1, q_2) dq_1 dq_2 = \frac{1}{h^2} \iint \rho(E_T - \frac{p_1^2}{2m_1} - \frac{p_2^2}{2m_2}) dp_1 dp_2 dq_1 dq_2 \quad (16)$$

After the usual approximations the integral can be evaluated:

$$P_T(E, q_1, q_2) dq_1 dq_2 = \frac{2\pi}{h^2} A'^{-1} \sqrt{m_1 m_2} \rho(E_T) dq_1 dq_2 \quad (17)$$

Coming back to the original coordinates α_1, α_2 we obtain the final result:

$$P_T(E, \alpha_1, \alpha_2) d\alpha_1 d\alpha_2 = \frac{2\pi \sqrt{m_1 m_2}}{h^2} A'^{-1} \rho(E_T) J(q_1, q_2/\alpha_1, \alpha_2) d\alpha_1 d\alpha_2 \quad (18)$$

where $J(q_1, q_2/\alpha_1, \alpha_2)$ is the Jacobian determinant.

Such a result can be further generalized for n collective coordinates:

$$P_T(E, \alpha_1, \alpha_2, \alpha_3, \dots, \alpha_n) d\alpha_1 d\alpha_2 d\alpha_3 \dots d\alpha_n = \frac{(2\pi)^{1/2}}{h^n} (m_1 m_2 m_3 \dots m_n)^{1/2} A'^{-n/2} \rho(E_T) J(q_1, q_2, \dots, q_n/\alpha_1, \alpha_2, \dots, \alpha_n) d\alpha_1 d\alpha_2 d\alpha_3 \dots d\alpha_n \quad (19)$$

It is somewhat interesting to notice that the collective kinetic energy contribution to the probability is proportional to $A'^{-n/2}$ or to $T^{n/2}$ where T is the local temperature. This is a small effect when compared with that of the collective potential energy which enters in the argument of the state density, the leading factor in eqs. (13), (18), and (19).

Also the inertial masses do not appear in eq. (19) in a very relevant way. The few microscopical calculations of the collective inertial values which have been carried out^{1,5,6}), show that, at very low excitation energy, there are fluctuations of such quantities about a smooth trend as a function of deformation. Such fluctuations may be of the order of a factor of two at the lowest energies and are quickly smoothed out with increasing energy. Furthermore the inertias appear in eq. (19) as square roots and their fluctuations are smaller than those which appear in the logarithm of the leading term $\rho(E_T)$.

The present formalism also gives an answer concerning how one should account for the nuclear deformation in the evaluation of the overall level density of a nucleus. The answer is straightforward: the overall nuclear state density (or level density) is obtained by integrating eq. (13) or eq. (18) or eq. (19) over the deformation coordinates:

$$\rho(E) = \int P_T(E, \alpha_1, \alpha_2, \dots, \alpha_n) d\alpha_1 d\alpha_2 \dots d\alpha_n \quad (20)$$

Unfortunately this shows again how the task of evaluating a realistic level density on the basis of the shell model theory is indeed rather involved. We shall come back to this problem in the discussion of the calculations. A final point which should be mentioned is the redundancy of the number of degrees of freedom. It is quite clear that the collective degrees of freedom in a nucleus are not independent because the overall number of degrees of freedom is fixed by the number of nucleons. However, the shortcomings of such a redundancy are well balanced by the advantages deriving from the simplicity of the treatment.

3. Calculations

Actual calculations have been performed for some typical nuclei in the region between the heavy rare earths and the doubly magic number 82-126; in this way nuclear deformations from zero up to the maximum value found in the rare earths have been considered. The sequence of the calculations is the following: 1) calculations of the single particle energies and spins; 2) calculation of the potential energy by means of a modified Strutinski procedure; 3) evaluation of the level densities as a function of excitation energy and of deformation; 4) evaluation of the deformation probabilities as a function of excitation energy.

3.1. THE SHELL MODEL

The calculations have been based on the modified harmonic oscillator potential introduced by Nilsson^{1,7}): such single-particle potential is a function of a set of deformation parameters. A single deformation parameter, ϵ , has been considered in order to simplify the calculations to some extent. The oscillator quantum $\hbar\omega_0$ has been assigned the value $41 A^{-1/3}$ MeV. The quantities k and μ which enter in the Nilsson potential have been considered constant in the range of mass numbers between 170 and 208 and have been assigned the following values:

	k	μ
protons	.0620	.614
neutrons	.0636	.393

3.2. THE POTENTIAL ENERGY

It has been recognized that the potential energy obtained by summation over the single particle levels, even including the coulomb and pairing effects,

is incorrect and unsatisfactory, especially at large deformations⁸⁾. The possibility of a proper use of the shell model calculations avoiding their large errors in the evaluation of the bulk of the potential energy has been shown by Myers and Swiatecki⁹⁾ and by Strutinski²⁾. These authors pointed out that the potential energy as a function of deformation, calculated by means of the shell model, may predict the fluctuations or wiggles about the average value quite well, while the average bulk of the potential energy may be grossly in error. Therefore it is possible to calculate such wiggles by subtracting a smoothed-out potential energy to the potential energy calculated with the shell model. The wiggles can be added to the liquid drop potential energy which is known to be an accurate average of the nuclear potential energy.

Let us first calculate the shell model energy by means of the B.C.S. Hamiltonian¹⁰⁾ to account for pairing:

$$E_{SM} = 2 \sum e_k v_k^2 - \frac{\Delta^2}{G} - G \left[\sum_k v_k^4 - \sum_k' 1 \right] \quad (21)$$

In this expression e_k are the single particle energies, G is the pairing strength, Δ is the gap parameter, v_k is given by the expression:

$$v_k = \frac{1}{\sqrt{2}} \left(1 - \frac{e_k - \lambda}{E_k} \right)^{1/2}, \quad (22)$$

$$E_k = [(e_k - \lambda)^2 + \Delta^2]^{1/2} \quad (23)$$

The symbol Σ' refers to a summation over the single particle levels below the Fermi surface. The quantities λ and Δ are the solution of the system formed by the gap equation and the particle equation:

$$\sum_k \frac{1}{E_k} = \frac{2}{G} \quad (24)$$

$$\sum_k \left(1 - \frac{e_k - \lambda}{E_k}\right) = N \quad (25)$$

In such calculation we have used the following expressions for the pairing strengths¹⁾:

$$G \times A = g_0 \pm g_1 \frac{N - Z}{A}$$

$$g_0 = 19.2 \text{ MeV}; g_1 = 7.4 \text{ MeV}$$

In the summation we have included $\sqrt{15Z}$ or $\sqrt{15N}$ levels above and below the Fermi surfaces. Such a prescription¹⁾ is chosen in order to reproduce approximately the experimental even-odd mass differences. In order to obtain the wiggle or the fluctuation we must subtract a smooth shell energy and a smooth pairing energy:

$$E_W = E_{SM} - \bar{E}_{Str.} - \bar{E}_{pair} \quad (26)$$

The quantity $E_{Str.}$ is the smoothed-out shell model energy, without pairing, obtained with a modified Strutinski procedure. Such a procedure is illustrated in Appendix A. The quantity $\bar{E}_{pair}$ is the average pairing energy, which we take to be independent of A and to which we assign the value 2.3 MeV inclusive of neutrons and protons.

The overall potential energy can now be calculated

$$V(N, Z, \epsilon) = E_{LD} + E_W \quad (27)$$

In the present calculation we have used the parameters of the liquid drop expression proposed by Myers and Swiatecki⁹). Examples of calculations of potential energies as a function of deformation, together with the liquid drop potential energies are shown in fig. 2 through fig. 7.

3.3. THE LEVEL DENSITIES

This represents the crucial point of the whole calculation. A level density suitable for the present calculation should account for the shell effects as a function of the deformation; it should include the pairing in a consistent way and reproduce the washing out of the pairing and the shell effects with increasing excitation energy. Calculations of level densities on the basis of a shell-model set of single particle levels without pairing have been presented elsewhere³). Also a formalism for the level density calculation on the basis of the shell model with inclusion of pairing has been presented by Sano and Yamasaki¹¹) and by Decowski et al.¹²). The derivation of our own formalism, similar, to some extent to that of Decowski is presented in Appendix B. Such formalism predicts that the pairing effects decrease with increasing energy until, at a critical energy, the system reverts back to a normal uncorrelated Fermi gas. In fig. 8 the energy dependence of the neutron and proton gap parameters is shown for the nucleus ¹⁷²Yb at a deformation $\epsilon = 0$. In the same figure the level density denominator is presented: this quantity is a smooth function of the specific heat of the system. The discontinuities

associated with the second-order phase-transition are visible. In fig. 9 and fig. 10 the level density and the spin cutoff parameters are presented as a function of excitation energy for the two deformations $\epsilon = 0$ and $\epsilon = .250$. The latter quantity, which determines the angular momentum distribution, is calculated assuming that the gap parameter Δ does not depend upon the angular momentum. This is not a very satisfactory assumption for large angular momenta. The correct angular momentum dependence of Δ and the level density formalism including angular momentum and pairing have been presented elsewhere¹³).

The shell model used in the level density evaluation is that described in section 3.1. The neutron and proton pairing strengths are calculated following the prescriptions given in section 3.2.

3.4. CALCULATION OF THE DEFORMATION PROBABILITIES

The deformation probabilities are evaluated by means of eq. (13). At any given excitation energy E , the local excitation energy E_T at the deformation ϵ is evaluated. Since the level densities are generated in tabular form, their logarithmic value is interpolated by means of a three point Lagrange's method which gives the derivative of the function with respect to the energy at the same time. In this way also the quantity A' in eq. (13) is obtained. Since, as discussed above, the relevance of the inertial parameters is rather small, we have chosen to drop the factor $\frac{\sqrt{2\pi m}}{h}$ altogether. Therefore the quantity which we have calculated is the following:

$$\ln \frac{P_T(E_T, \epsilon)}{\frac{\sqrt{2\pi m}}{h}} = \ln [A'^{-1/2} \cdot \rho(E_T)]$$

Examples of such calculations are shown in fig. 11 through fig. 16 for the nuclei ^{172}Yb , ^{184}Os , ^{190}Pt , ^{192}Pt , ^{200}Hg , ^{208}Pb . Such calculations range from $-.5$ to $+.5$ in deformation ϵ in steps of $.05$, and from 6 MeV to 60 MeV in excitation energy.

4. Discussion of the Results

The nuclei for which the calculations have been performed were chosen in such a way as to explore the behaviour of shell effects from a mid-shell region to a magic region. In fig. 2 through fig. 7 the nuclear potential energies, calculated by means of the Strutinski procedure, are shown, together with the corresponding liquid drop energies. The ^{172}Yb nucleus presents a sharp minimum in the potential energy at a deformation $\epsilon = +.250$ and a secondary minimum (not necessarily a minimum when more than one collective coordinate is used!) at the oblate deformation $\epsilon = -.200$. Such minima are separated by a very high barrier with its maximum at sphericity. Similar features are observed in the other nuclei of increasing mass number: however the difference in deformation between the two minima decreases as well as does their difference in energy and the height of the intermediate barrier. When the nuclei are close to the doubly magic number $Z = 82$, $N = 126$ the two minima tend to merge into one single minimum centered at sphericity while another small minimum begins to appear at large prolate deformations. Such potential energies show the relevance of the shell effects in cold nuclei in the most pictorial way.

The relevance of the shell effects in excited nuclei can be seen instead in fig. 11 through fig. 16 where the logarithms of the deformation probabilities for different excitation energies are plotted against the deformation parameter ϵ .

At the lowest excitation energies the variations in deformation probability as a function of deformation are quite impressive, being in the most dramatic case of the order of many powers of 10, as for example in the cases of

^{172}Yb , ^{200}Hg , and ^{208}Pb . Such variations tend to follow the potential energy variations quite closely when the excitation energy is very low. Very sharp maxima occur in correspondence of the minima in the potential energy and vice versa. The compound nuclei are characterized by one or two peaks in deformation which account for nearly all the probability. With increasing excitation energy a rather dramatic washing out of such structures takes place. In the case of a ground state deformed nucleus, the two probability peaks, the oblate and the prolate ones, tend to become broader, to equalize their height and to move closer to sphericity, while the minimum in between becomes shallower. At excitation energies close to 60 MeV the two probability peaks have merged together completely, giving rise to a broad peak centered at sphericity and very little residual influence remains of the shell effects visible in the potential energy and in the low energy probability curves. Actually the 60 MeV probability curve reflects the smooth liquid drop potential energy quite well. Similar considerations can be made for the nuclei which are spherical in their ground states, such as ^{200}Hg and ^{208}Pb . In this case a prominent sharp probability peak is present at sphericity and a small peak is visible at large deformations; with increasing excitation energy the peak at sphericity broadens and the small peak at large deformations disappears altogether.

In order to better appreciate the extent of the smearing-out of the shell effects, let us consider the potential energy curve of ^{172}Yb . The energy difference between the deepest minimum of the potential energy and the top of the intermediate maximum at sphericity is larger than 7 MeV. While the effect of such energy difference is quite remarkable at low energies, at 60 MeV it is non existent, since at this energy the deformation probability is essentially

constant in such a range of deformations. This is to be compared with the fact that the ratio of the level densities at 60 MeV and at 53 MeV for $\epsilon = .250$ is $e^{4.1}$. This implies also that the level density at 53 MeV for $\epsilon = 0$ is equal to the level density at 60 MeV for $\epsilon = .250$ (fig. 9).

The smearing of the shell effects is an obvious effect of the excitation energy, although some smearing of the shell effects already exists for a cold nucleus because of pairing. Formally we may consider the shell effects to be at their maximum for a cold nucleus without pairing. The pairing interaction smears-out the Fermi surface in an energy interval of $\sim 2\Delta$ and this implies an averaging of the single particle features which extend over such an energy range. The excitation energy acts as a much more powerful smearing agent by spreading-out nucleons above and below the Fermi surface. The rate at which the washing-out of shell effects takes place depends upon the range of the perturbation of the single particle level density which gives rise to such effects. The largest shell effects have a range of the order of one major oscillator shell and consequently they are the last to be washed out. This can be observed in the case of ^{208}Pb where the shell effects are still quite visible at 60 MeV in comparison with ^{172}Yb where at the same excitation energy a strong smoothing has taken place.

As far as the evaluation of level densities is concerned, there are a few difficulties left. As mentioned in section 2, the overall level density should be obtained by integrating the deformation probability over the collective coordinate space. This presents two kinds of difficulties: the first has to do with the extremely large amount of calculations necessary in order to explore the whole deformation space suitably, the second, of more

basic nature has to do with the necessity of truncating the number of collective coordinates. Because of the arbitrariness of such a truncation, it follows that the level densities will depend somewhat upon the parametrization. An inspection of eq. (19) shows how the introduction of a new collective degree of freedom multiplies the deformation probability by a factor $\frac{\sqrt{2\pi m}}{h} T^{1/2}$. Such an effect is the necessary result of the redundancy of the degrees of freedom employed in describing the system.

Many applications can be found for the present formalism. Perhaps a most interesting one could be a consistent evaluation of the fission probabilities; this involves the calculation of the deformation probability for very large deformations, the identification of the transition state at each excitation energy, and the calculation of both the fission and neutron emission widths. In particular such calculations become relevant for very heavy or superheavy nuclei where the shell effects make a substantial contribution as far as the fission barrier height and the saddle point deformations are concerned. An example of such calculations for superheavy nuclei has been reported by the author¹⁴⁾ and more extensive calculations are in progress.

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Appendix A

The Strutinski smoothing procedure.

Although such procedure has been described elsewhere^{1,2,15}), we report here the entire formalism which we have obtained in a complete analytical form.

The gaussian-smoothed single particle level density can be written as:

$$g(e) = \frac{1}{\gamma \sqrt{\pi}} \sum_k f_k \exp(-u_k^2) \quad (A1)$$

where

$$u_k = \frac{e - e_k}{\gamma} \quad (A2)$$

e_k are the single particle levels, and γ is the width of the smoothing function. The function f_k is chosen in such a way that the averaged function retains the long range variations up to a fixed order. For our purpose we shall retain the terms up to the 6th order. The function f_k has been shown to be¹⁵):

$$f_k = 1 + (1/2 - u_k^2) + (\frac{3}{8} - \frac{3}{2} u_k^2 + 1/2 u_k^4) + (\frac{15}{10} - \frac{15}{8} u_k^2 + \frac{5}{4} u_k^4 - \frac{1}{6} u_k^6) \dots \quad (A3)$$

we notice that such function can be rewritten in a much simpler way:

$$f_k = \sum_{n=0}^3 \frac{(-1)^n}{2^{2n} n!} H_{2n} \quad (A4)$$

where H_{2n} are the Hermite polynomials of even order. The smoothed-out shell model energy is

$$E = \int_{-\infty}^{\lambda} 2 e g(e) de \quad (A5)$$

The Fermi level λ is defined by the equation:

$$N = \int_{-\infty}^{\lambda} 2 g(e) de \quad (A6)$$

For technical reasons the lower limits in the last two integrals is to be chosen equal to $-\infty$ instead of zero: this depends upon the choice of the gaussian smoothing function which spreads-out the strength of a level over an infinite interval.

In order to perform the above integrals analytically, the following relations are needed:

$$\frac{d^n}{dx^n} e^{-x^2} = (-1)^n H_n(x) e^{-x^2} \quad (A7)$$

$$\int x H_n(x) e^{-x^2} dx = -e^{-x^2} (x H_{n-1}(x) + H_{n-2}(x)) \quad (A8)$$

Let us now evaluate the integral in A6:

$$N = \sum_k \left(\operatorname{erf} \left(\frac{\lambda - e_k}{\gamma} \right) + 1 \right) - \sum_v \frac{2}{\sqrt{\pi}} \sum_{n=1}^3 \frac{1}{n! 2^{2n}} H_{2n-1} \left(\frac{\lambda - e_k}{\gamma} \right) \exp - \frac{(\lambda - e_k)^2}{\gamma^2} \\ = F_k \quad (A9)$$

The integral in A5 is

$$E = \sum_k e_k F_k - \frac{\gamma}{\sqrt{\pi}} \sum_k \exp - \frac{(\lambda - e_k)^2}{\gamma^2} - \frac{2\gamma}{\sqrt{\pi}} \sum_k \sum_{n=1}^3 \frac{(-1)^n}{n! 2^{2n}} \exp - \frac{(\lambda - e_k)^2}{\gamma^2} \times$$

$$\times \left[\frac{(\lambda - e_k)^2}{\gamma^2} H_{2n-1} \left(\frac{\lambda - e_k}{\gamma} \right) + H_{2n-2} \left(\frac{\lambda - e_k}{\gamma} \right) \right] \quad (A10)$$

The eq. (A9) is numerically solved for the chemical potential λ , which is then introduced in the expression A10 in order to obtain the smoothed-out shell model energy. Such a procedure allows a rather wide choice for the smoothing parameter γ . Actually the value which has been used here was 1 MeV.

The summations over the single particle levels should be carried out up to a very high energy in such a way that the Fermi energy will result to be independent upon the upper limit of the sum.

Appendix B

Level density formalism for an arbitrary sequence of single particle levels with inclusion of pairing.

Let us assume that the nucleus can be described in terms of the B.C.S. Hamiltonian;

$$H = \sum_k e_k (a_k^+ a_k + a_{-k}^+ a_{-k}) - G \sum_{kk'} a_k^+ a_{-k'}^+ a_k a_{-k} \quad (B1)$$

where e_k is the energy of the k^{th} doubly degenerate energy level, $a_{\pm k}^+$ and $a_{\pm k}$ are the creation and annihilation operators for particles with opposite spin projections. The grand partition function e^Ω of such a system can be defined according to Sano and Yamasaki¹¹⁾ as:

$$\Omega = -\beta \sum_k (e_k - \lambda - E_k) + 2 \sum_k \ln[1 + \exp(-\beta E_k)] - \beta \frac{\Delta^2}{G} \quad (B2)$$

where Δ is the gap parameter

$$E_k = [(e_k - \lambda)^2 + \Delta^2]^{1/2}$$

$\beta = \frac{1}{T}$ (T being the temperature) is the Lagrange multiplier which fixes the amount of excitation energy

$\lambda = \frac{\alpha}{\beta}$ is the chemical potential of the system.

The relation B2 represents the grand partition function provided that the quantities β , λ , Δ be related by the following equation:

$$\frac{2}{G} = \sum_k \frac{\text{tgh} (1/2 \beta E_k)}{E_k} \quad (\text{B3})$$

The level density, which is the inverse Laplace transform of the grand partition function, can be written as:

$$\rho(E, N, Z) = \left(\frac{1}{2\pi i} \right)^3 \oint d\beta \oint d\alpha_N \oint d\alpha_Z e^S \quad (\text{B4})$$

where

$$S = \Omega_N + \Omega_Z - \alpha_N N - \alpha_Z Z + \beta E$$

and N and Z are the neutron and proton numbers and E the total energy. The integral in (B4) can be evaluated by means of the saddle point technique. The quantity S presents a saddle point at:

$$N = \frac{\partial \Omega}{\partial \alpha_N}, \quad Z = \frac{\partial \Omega}{\partial \alpha_Z}, \quad E = -\frac{\partial \Omega}{\partial \beta} \quad (\text{B5})$$

The level density is approximately:

$$\rho = \frac{e^S}{(2\pi)^{3/2} D^{1/2}} \quad (\text{B6})$$

where

$$D = \begin{vmatrix} \frac{\partial^2 \Omega}{\partial \alpha_N^2} & \frac{\partial^2 \Omega}{\partial \alpha_N \partial \alpha_Z} & \frac{\partial^2 \Omega}{\partial \alpha_N \partial \beta} \\ \frac{\partial^2 \Omega}{\partial \alpha_N \partial \alpha_Z} & \frac{\partial^2 \Omega}{\partial \alpha_Z^2} & \frac{\partial^2 \Omega}{\partial \alpha_Z \partial \beta} \\ \frac{\partial^2 \Omega}{\partial \alpha_N \partial \beta} & \frac{\partial^2 \Omega}{\partial \alpha_Z \partial \beta} & \frac{\partial^2 \Omega}{\partial \beta^2} \end{vmatrix} \quad (B7)$$

It can be noticed that:

$$E = E_N + E_Z$$

$$S = S_N + S_Z$$

$$D = \frac{\partial^2 \Omega}{\partial \alpha_N^2} D_Z + \frac{\partial^2 \Omega}{\partial \alpha_Z^2} D_N \quad (B8)$$

where

$$D_N = \begin{vmatrix} \frac{\partial^2 \Omega_N}{\partial \alpha_N^2} & \frac{\partial^2 \Omega_N}{\partial \alpha_N \partial \beta} \\ \frac{\partial^2 \Omega_N}{\partial \alpha_N \partial \beta} & \frac{\partial^2 \Omega_N}{\partial \beta^2} \end{vmatrix} \quad (B9)$$

and D_Z is similarly defined. Let us write down explicitly the eq. (B5); with some algebra we obtain:

$$N = \frac{\partial \Omega_N}{\partial \alpha_N} = \frac{\beta \partial \Delta^2}{\partial \alpha_N} \left(\sum_k \frac{1}{2 E_k} \operatorname{tgh} (1/2 \beta E_k) - \frac{1}{G_N} \right) +$$

$$+ \sum_k \left[1 - \frac{e_k - \lambda}{E_k} \operatorname{tgh} (1/2 \beta E_k) \right] ; \quad (B10)$$

because of the gap equation (B3) the quantity within brackets in the first term is equal to zero, therefore,

$$N = \sum_k \left[1 - \frac{e_k - \lambda}{E_k} \operatorname{tgh} (1/2 \beta E_k) \right] . \quad (B11)$$

A similar relation holds for Z. The total energy can be calculated in a similar way:

$$- E_N = \frac{\partial \Omega_N}{\partial \beta} = \beta \Delta \frac{\partial \Delta}{\partial \beta} \left(\sum_k \frac{1}{E_k} \operatorname{tgh} (1/2 \beta E_k) - \frac{2}{G_N} \right) + \Delta^2 \left(\sum_k \frac{1}{E_k} \operatorname{tgh} 1/2 \beta E_k - \frac{2}{G_N} \right)$$

$$- \sum_k e_k \left(1 - \frac{e_k - \lambda}{E_k} \operatorname{tgh} 1/2 \beta E_k \right) + \frac{\Delta^2}{G_N} \quad (B12)$$

Because of the gap equation, the first two terms are equal to zero. We can write then:

$$E_N = \sum_k e_k \left(1 - \frac{e_k - \lambda}{E_k} \operatorname{tgh} (1/2 \beta E_k) \right) - \frac{\Delta^2}{G_N} \quad (B13)$$

A similar relation holds for E_Z . It is quite interesting to notice that, although in the above calculations we have properly differentiated Δ with

respect to α_N and β , the resulting expressions for the number of particles and for the energies are independent of such derivatives.

For the entropy we can write:

$$S_N = 2 \sum_k \ln[1 + \exp(-\beta E_k)] + 2 \beta \sum_k \frac{E_k}{1 + \exp(\beta E_k)}, \quad (B14)$$

and similarly for S_Z . The second derivatives of the grand partition function which appear in the determinants D_N , D_Z can be written down explicitly:

$$\begin{aligned} \frac{\partial^2 \Omega}{\partial \beta^2} = & \sum_k e_k^2 (e_k - \lambda)^2 a_k + \Delta^2 \lambda \sum_k e_k b_k + \Delta^2 \sum_k e_k (e_k - \lambda) a_k \\ & + K \left[\frac{2}{\beta G_N} + \sum_k e_k (e_k - \lambda) (a_k - b_k) \right] \end{aligned} \quad (B15)$$

$$\frac{\partial^2 \Omega}{\partial \alpha_N^2} = \sum_k (e_k - \lambda)^2 a_k + \Delta^2 \sum_k b_k - M \sum_k (e_k - \lambda) (a_k - b_k) \quad (B16)$$

$$\frac{\partial^2 \Omega}{\partial \alpha_N \partial \beta} = - \sum_k e_k (e_k - \lambda)^2 a_k - \Delta^2 \lambda \sum_k b_k - \Delta^2 \sum_k (e_k - \lambda) a_k - K \sum_k (e_k - \lambda) (a_k - b_k) \quad (B17)$$

In these equations we have set:

$$a_k = \frac{1}{2E_k^2} \operatorname{sech}^2(1/2 \beta E_k); \quad b_k = \frac{1}{\beta E_k^3} \operatorname{tgh} 1/2 \beta E_k$$

$$K = \beta \Delta \frac{\partial \Delta}{\partial \beta}, \quad M = \beta \Delta \frac{\partial \Delta}{\partial \alpha_N} \quad \text{for} \quad \Delta > 0$$

$$K = 0, \quad M = 0 \quad \text{for} \quad \Delta = 0$$

The gap parameter Δ is a decreasing function of excitation energy: it goes to zero at a critical temperature T_c that, together with the critical chemical potential λ_c can be obtained by solving eq. (B3) and eq. (B11) after setting $\Delta = 0$.

We need to calculate $\frac{\partial \Delta}{\partial \beta}$ and $\frac{\partial \Delta}{\partial \alpha_N}$; in order to calculate such derivatives we observe that eq. (3), which we rewrite:

$$\frac{2}{G} - \sum_k \frac{\tanh(1/2 \beta E_k)}{E_k} = 0$$

defines Δ as an implicit function of β and α_N . We can write:

$$f(\Delta, \alpha_N, \beta) = 0;$$

the total differential is:

$$\frac{\partial f}{\partial \beta} d\beta + \frac{\partial f}{\partial \alpha_N} d\alpha_N + \frac{\partial f}{\partial \Delta} \left(\frac{\partial \Delta}{\partial \beta} d\beta + \frac{\partial \Delta}{\partial \alpha_N} d\alpha_N \right) = 0$$

or

$$\left(\frac{\partial f}{\partial \beta} + \frac{\partial f}{\partial \Delta} \frac{\partial \Delta}{\partial \beta} \right) d\beta + \left(\frac{\partial f}{\partial \alpha_N} + \frac{\partial f}{\partial \Delta} \frac{\partial \Delta}{\partial \alpha_N} \right) d\alpha_N = 0$$

Such equation is satisfied if and only if:

$$\frac{\partial f}{\partial \beta} + \frac{\partial f}{\partial \Delta} \frac{\partial \Delta}{\partial \beta} = 0 \quad ; \quad \frac{\partial f}{\partial \alpha_n} + \frac{\partial f}{\partial \Delta} \frac{\partial \Delta}{\partial \alpha_n} = 0$$

It follows then:

$$\frac{\partial \Delta}{\partial \beta} = - \frac{\frac{\partial f}{\partial \beta}}{\frac{\partial f}{\partial \Delta}} \quad ; \quad \frac{\partial \Delta}{\partial \alpha_n} = - \frac{\frac{\partial f}{\partial \alpha_n}}{\frac{\partial f}{\partial \Delta}}$$

By using the above formulae we obtain:

$$\frac{\partial \Delta}{\partial \beta} = - \frac{\sum_k a_k e_k (e_k - \lambda) + \Delta^2 \sum_k a_k - \lambda \sum_k (e_k - \lambda) b_k}{\beta \Delta \sum_k (a_k - b_k)} \quad (B18)$$

$$\frac{\partial \Delta}{\partial \alpha_n} = \frac{\sum_k (e_k - \lambda)(a_k - b_k)}{\beta \Delta \sum_k (a_k - b_k)} \quad (B19)$$

The angular momentum dependent level density is given by the expression:

$$\rho(E, J) = \frac{(2J + 1)}{2(2\pi)^{1/2} \sigma^3} \rho(E) \exp - \frac{J(J + 1)}{2\sigma^2} \quad (B20)$$

where

$$\sigma^2 = \sigma_N^2 + \sigma_Z^2 \quad (B21)$$

and

$$\sigma_N^2 = 1/2 \sum \frac{m_k^2}{\cosh^2 1/2 \beta E_k} \quad (B22)$$

In the development of this formalism we agree with Sano and Yamasaki and Decowski et al. in the quantities Ω , E , N , S . The level density denominator derived here differs from that of Sano and Yamasaki because while we searched for the saddle point with respect to β , α_N , and α_Z , they searched for the saddle point with respect to β only. Our level density denominator differs from that derived by Decowski et al. in the values of the quantities K and M . We have no explanation for the disagreement.

The actual calculations are executed in the following way:

- a) the ground state energy is calculated by setting $T = 0$ and by solving eqs. (3) and (11) for Δ_0 and λ_0
- b) the critical quantities T_c and λ_c are evaluated by solving eqs. (3) and (11) after setting $\Delta = 0$.
- c) the nuclear temperature T is taken as the independent variable; the quantities $\Delta(T)$ and $\lambda(T)$ are evaluated by solving again eqs. (3) (11) for a given value of T and used to evaluate E , S , D and finally p .

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Figure Captions

Fig. 1. Schematic representation of the potential energy V of a nucleus as a function of a deformation parameter ϵ . The total energy of the system E , measured from the deepest minimum in the potential energy can be divided, at any deformation in two portions; a potential energy part V and a local excitation energy E_T . The latter is shared by the internal and collective degrees of freedom.

Fig. 2. Potential energy as a function of the deformation parameter ϵ for ^{172}Yb calculated from the Nilsson diagram by means of the Strutinski procedure (black circles). The continuous line represents the liquid drop energy.

Fig. 3. Same as fig. 2 for ^{184}Os .

Fig. 4. Same as fig. 2 for ^{190}Pt .

Fig. 5. Same as fig. 2 for ^{192}Pt .

Fig. 6. Same as fig. 2 for ^{200}Hg .

Fig. 7. Same as fig. 2 for ^{208}Pb .

Fig. 8. Statistical quantities calculated for ^{172}Yb at $\epsilon = 0$ from the Nilsson diagram and the B.C.S. Hamiltonian. Neutron and proton gap parameters as a function of excitation energy (left scale). Level density denominator as a function of excitation energy (right scale) showing the two discontinuities associated with the second-order phase transitions.

Fig. 9. Natural logarithm of level densities as a function of excitation energy for ^{172}Yb at sphericity and at the ground state deformation. It can be noticed how the different rate of growth of the two curves compensates, at ~ 40 MeV for the 7 MeV difference in ground state potential energies.

Fig. 10. Spin cut-off parameters for ^{172}Yb calculated at sphericity and at the ground state deformation.

Fig. 11. Natural logarithm of the deformation probabilities (see text for details) for different excitation energies for ^{172}Yb . The labeling of each curve is in MeV.

Fig. 12. Same as in fig. 12 for ^{184}Os .

Fig. 13. Same as in fig. 12 for ^{190}Pt .

Fig. 14. Same as in fig. 12 for ^{192}Pt .

Fig. 15. Same as in fig. 12 for ^{200}Hg .

Fig. 16. Same as in fig. 12 for ^{208}Pb .

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6

Fig. 7

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Fig. 9

Fig. 10

Fig. 11

Fig. 12

Fig. 13

Fig. 14

Fig. 15

Fig. 16

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