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Statistical properties of excited fissioning nuclei

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Abstract. The phenomenon of the disappearance of the shell effects on the thermodynamic properties of nuclei with increasing excitation energy has been examined quantitatively on the basis of numerical calculations based on realistic shell model single particle level schemes. It is shown that shell effects disappear at moderate excitation energies and above these excitation energies, the thermodynamic behaviour of the nucleus is identical to that of the equivalent liquid drop model nucleus. Implications of the above feature in the interpretation of some aspects of fission of excited nuclei such as mass-asymmetry and angular anisotropy are examined. The relationship of the phenomenon of washing out of shell effects at high excitation energies with the temperature smearing method of determining ground state shell correction energies is also outlined.

Keywords. Nuclear shell effects; nuclear fission; thermodynamic properties; shell correction energies.

1. Introduction

From the time the classic paper of Bohr and Wheeler (1939) to explain the nuclear fission process appeared, the concept of nuclear deformation potential energy has been basic to our understanding of the fission phenomenon. Until recently, the interpretation of many fission features such as fission probabilities and fission fragment angular distributions were based on a single-humped fission barrier in the deformation potential energy surface, which results from the surface and Coulomb energy changes of the nucleus on the basis of Liquid Drop Model (LDM). The last few years have seen many intensive theoretical studies of the nuclear potential energy taking into account the nuclear shell and pairing effects. These studies based on the now well-known macroscopic-microscopic method (Strutinsky 1966, 1967) have revealed new structures in the nuclear deformation potential energy surface and for nuclei in the actinide region, the fission barriers have been shown to be double-humped. Much of our current thinking about spontaneous and near threshold fission features such as fission isomers and intermediate structure in fission cross-sections, has resulted from this double-humped fission barrier concept. It should, however, be pointed out here that the static potential energy surface and therefore fission barrier height are of relevance only as far as the interpretation of spontaneous and near threshold fission features is concerned. In the case of fission of an excited nucleus, the nucleons populate a number of single particle states around the Fermi level and consequently the influence of nuclear shell effects on the fission process is expected to decrease and finally disappear with increasing excitation energy since the shell effects have their origin in the non-uniform distribution of single particle states near the Fermi level (Ramamurthy *et al* 1970, Huizenga and Moretto 1972, Adeev and Cherdantsev 1973). In other words, at sufficiently high excitation energies, the nucleus is expected to behave like a liquid drop nucleus and will not exhibit features which are specifically characteristic of a double-humped fission barrier.

In this paper, the phenomenon of the washing out of the shell effects with excitation energy and its implications on some of the observed fission features are examined on the basis of a numerical study of the thermodynamic properties of excited nuclei. It is also shown that from a study of the thermodynamic properties of excited nuclei, the ground state shell correction energies of nuclei can be determined.

2. Thermodynamics of excited nuclei

An important quantity describing the statistical thermodynamic properties of an excited nucleus is its level density, expressed as a function of the various constants of motion like number of particles, excitation energy, angular momentum, parity, etc. In recent years, it has been possible to calculate numerically nuclear level densities starting from shell model single particle states (Ramamurthy *et al* 1970, Huizenga and Moretto 1972), and thereby include the nuclear shell effects on the level densities. This method of calculation of the entropy S versus excitation energy of a specified nuclear system with known single particle states is as follows:

For a system of non-interacting fermions, with total number of particles N and total energy E, one can write the following relations.

$$N = \Sigma\, n_k \tag{1}$$

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$$S = -\Sigma\, \{n_k \ln n_k + (1 - n_k) \ln (1 - n_k)\} \tag{3}$$

Here ϵ_k are the energies of the single particle states and n_k is the Fermi-Dirac distribution function given by

$$n_k = \frac{1}{1 + \exp\, (\epsilon_k - \mu)/T} \tag{4}$$

where T is the thermodynamic temperature and μ is the chemical potential. If the magnetic quantum numbers m_k of the single particle states are known, one can also obtain the spin cut-off parameter σ^2, which determines the width of the distribution of the angular momentum projection M, from the relation

$$\sigma^2 = \Sigma\, n_k (1 - n_k)\, m_k^2 \tag{5}$$

For a specified temperature T the calculation of various thermodynamic quantities, S, E and σ^2 can be carried out numerically on the basis of eqs 1–5, starting from a given set of single particle energies ϵ_k. The corresponding excitation energy E_x is given by $E_x = E - \sum_{i=1}^{N} \epsilon_k$. In applying the above relations for the case of real nuclei, the contributions from both protons and neutrons are added.

It may be pointed out here that the level density ρ is related to the entropy S by the relation $\rho = ce^S$ where c is a weakly energy dependent pre-exponential factor. On the assumption that the density of single particle energy levels near the Fermi-level is nearly constant, the above formalism leads to the well known Bethe expression for the nuclear level densities given by $\rho = c \exp 2\,(aE_x)^{\frac{1}{2}}$, where E_x is the excitation energy of the nucleus. The level density parameter a being proportional to the density of single particle states near the Fermi level increases nearly linearly with the mass number A of the nucleus. It is now known that in a nucleus the density of single particle states near the Fermi level is not constant but exhibits appreciable non-uniformities which can be correlated to the well known shell effects on the nuclear masses and deformation potential energies (Strutinsky 1966, 1967). It is therefore expected that for a nuclear system with non-uniform distribution of single particle states, the actual entropy will deviate from that given by the Bethe expression. The excitation energy dependence of entropy for such a system with ground state shell effects can be studied through eqs 1–4 in the above formalism.

Let us first consider the shell correction to the ground state energy of a nucleus. Since protons and neutrons are considered to be independent in the present formalism, we treat here only one kind of nucleons, say protons, the results and conclusions of the analysis being equally valid for the other kind of nucleons. Let $G(\epsilon) = \Sigma\, \delta(\epsilon - \epsilon_k)$ be the density of single particle states of protons in a nucleus where ϵ_k are a set of single particle states given by the shell model. On the basis of the Strutinsky-Swiatecki concept (Myers and Swiatecki 1965, Strutinsky 1966) $G(\epsilon)$ can be written as the sum of a smoothly varying part $g(\epsilon)$ and a local flucturation $\delta g(\epsilon)$. The shell correction $\triangle_s$ to the total energy is, by definition, equal to the difference between the ground state energies of the actual system and that of a hypothetical smooth system having a density $g(\epsilon)$ of the single particle states, *i.e.*,

$$\triangle_s = E_g - \bar{E}_g = \sum_{k=1}^{Z} \epsilon_k - \int_{-\infty}^{\mu} \epsilon\, g(\epsilon)\, d\epsilon \tag{6}$$

where E_g and $\bar{E}_g$ are the ground state energies for the actual and the corresponding smooth systems, and μ is the Fermi energy for the smooth system. The smooth single particle level density $g(\epsilon)$ corresponding to any level scheme can be obtained by a suitable smearing of the energy states ϵ_k as has been proposed by Strutinsky (1966). A number of calculations of the ground state shell correction energies of nuclei have been carried out in recent years using the Strutinsky method (*see* reviews by Nix *et al* 1973, Brack *et al* 1972).

With the above definition of the ground state shell correction energy one can also study quantitatively the influence of shell effects on the thermodynamic properties of an excited nucleus. For example, a comparison of the calculated entropy S of the actual system with the corresponding quantity $\bar{S}$ of the hypothetical smooth system evaluated at the same temperature will bring out the temperature dependence of shell effects on entropy. In the following, we present the results of calculations for the cases of two typical schemes of single particle energy states. The first one was a model scheme with equidistant levels where each level was ten-fold degenerate. The second one was a modified harmonic oscillator level scheme (Seeger and Perisho 1967). For each of these systems, the corresponding smooth density of states was obtained by the Strutinsky smearing procedure (Strutinsky 1965). The thermodynamic quantities S and E were calculated from the set of eqs 1 to 4, while the corresponding quantities $\bar{S}$ and $\bar{E}$ for the smooth reference system were obtained from equations analogue to eqs 1 to 4, where summations are replaced by integrations. Figure 1 shows plots of the calculated $(S - \bar{S})$ and $(E - \bar{E})$ versus the temperature T for the equidistant level scheme for the cases of a closed shell and mid-shell systems having 10 and 5 particles respectively in

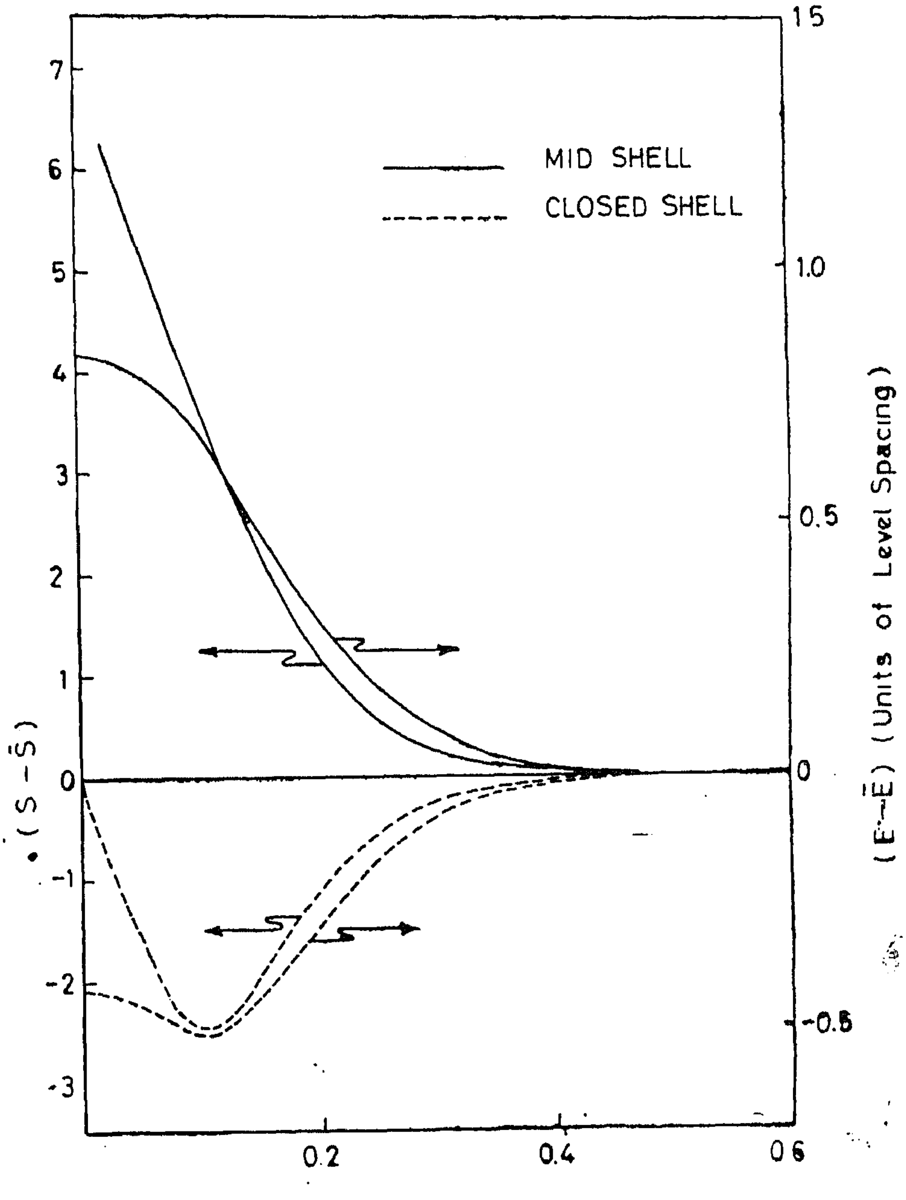

Figure 1. Calculated temperature dependence of the difference in entropy and excitation energy of a system of Fermions in a bunched level scheme and in the corresponding smooth level scheme. The levels in the bunched scheme were equi-spaced and had a degeneracy of 10. The two cases studied refer to the closed shell system with 10 particles in the last occupied level and the mid-shell system with 5 particles in the last occupied level.

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(i) At low temperatures, the actual system and the smooth system behave differently, as a result of the shell effects.

(ii) With increasing temperature, the differences in the calculated values of the total energy and the entropy between the actual system and the reference smooth system decrease and vanish completely at high temperatures. Even for the case of the doubly closed shell nucleus ^{208}Pb a temperature of about 2 MeV ($E_x \sim 100$ MeV) is sufficient to nearly wipe out the shell effects.

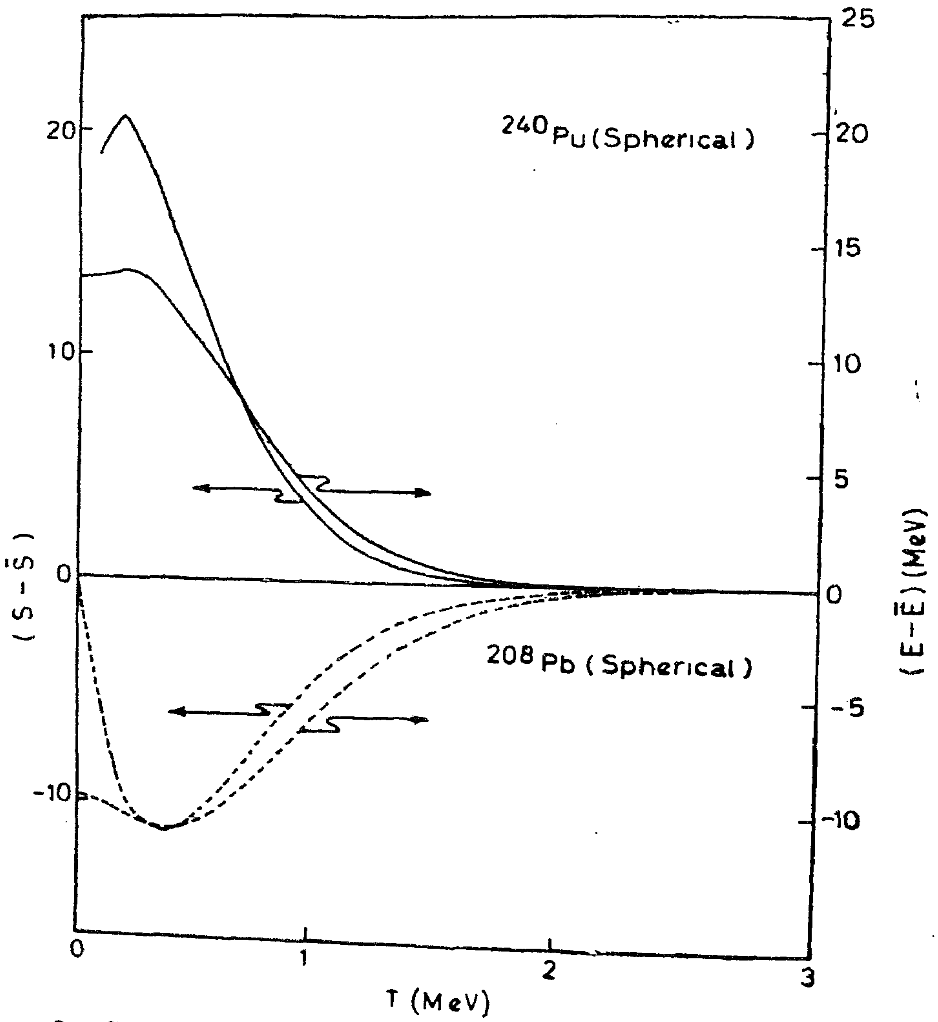

Figure 2. Calculated temperature dependence of the difference in entropy and excitation energy of two typical nuclei, ^{208}Pb and ^{240}Pu, with a shell model single particle level scheme (generated for the modified Harmonic oscillator potential of Seeger and Perisho (1967) and with the corresponding smooth single particle level density generated by the Strutinsky smearing procedure. The parameters used for the Strutinsky smearing are $\gamma = 1{\cdot}2\,\hbar w$ units and $p = 6$.

The same conclusions have also been drawn by Jensen and Damgaard (1973) on the basis of calculations carried out for various nucleon numbers and deformations.

An interesting consequence of the above temperature behaviour of the thermodynamic properties of nuclei is as follows: For a sufficiently high temperature T where the shell effects have disappeared we have $S(T) = \bar{S}(T)$ or $S(E_x) = \bar{S}(\bar{E}_x)$, where E_x and $\bar{E}_x$ are the excitation energies of the actual and smooth systems at temperature T. Considering that at these temperatures we also have $E = \bar{E}$ or $E_x + E_g = \bar{E}_x + \bar{E}_g$, it follows that at sufficiently high temperatures, $S(E_x) = \bar{S}(E_x + \Delta_s)$. Consequently, at temperatures where shell effects have disappeared, the entropy of a nucleus can be obtained simply from LDM calculations of the entropy corresponding to an effective excitation energy obtained by measuring the energy excess with respect to the LDM ground state. If one writes the usual Bethe expression for the smooth system, it follows that in the asymptotic limit of high temperatures, one has $S^2(E_x) = \bar{S}^2(E_x + \Delta_s) = 4a(E_x + \Delta_s)$, where a is related to the average density $\bar{g}$ of the smooth system at the Fermi energy by the expression $a = (\pi^2/6)\,\bar{g}$, on the assumption that the temperature of disappearance of shell effects is not so large as to require inclusion of higher derivatives of $\bar{g}$ in the expression for a. Hence if one plots either dS^2/dE_x or $S^2/(E_x + \Delta_s)$ versus E_x, one finds that these quantities asymptotically reach the same constant value equal to $4a$ after the shell effects have disappeared. On the other hand, a plot of S^2/E_x versus E_x never reaches a constant value which, however, should not be interpreted to imply that shell effects persist at all excitation energies. Plots of $S^2/(E_x + \Delta_s)$, dS^2/dE_x and S^2/E_x versus E_x are shown in figure 3 for a typical case of single particle level scheme of Nix (1972) for the outer barrier deformation of ^{242}Pu, which demonstrate the validity of the preceding remarks. From the preceding discussion it is also apparent that in the phenomenological model, the excitation energy dependence of shell effects on level density can be taken into account by a simple expression of the form $S^2 = 4a(E_x + \delta)$, where $\delta \rightarrow \Delta_s$ at high excitation energies, and a is a constant related to the single particle level density of the smooth system, as defined earlier.

It is seen from the above discussion that as far as its thermodynamic properties are concerned, the nucleus behaves like a liquid drop model nucleus at high temperatures. As is shown in the subsequent sections, the above conclusion has important implications in the interpretation of some of the aspects of fission of excited nuclei.

3. Shell effects on fission transition state

The fission transition state, by definition, corresponds to that shape of the excited fissioning nucleus along the fission path where minimum number of open channels are encountered. In the absence of shell effects, the fission transition state coincides with the LDM saddle shape, since in this case, the level density of the fissioning nucleus at any deformation can be calculated on the basis of the usual Bethe expression $S = 2(aE_x)^{\frac{1}{2}}$ for the entropy S, where E_x is the excitation energy and a is the level density parameter. Since for a given total energy, the excitation energy consequently the influence of nuclear shell effects on the fission process is expected to decrease and finally disappear with increasing excitation energy since the shell effects have their origin in the non-uniform distribution of single particle states near the Fermi level (Ramamurthy *et al* 1970, Huizenga and Moretto 1972, Adeev and Cherdantsev 1973). In other words, at sufficiently high excitation energies, the nucleus is expected to behave like a liquid drop nucleus and will not exhibit features which are specifically characteristic of a double-humped fission barrier.

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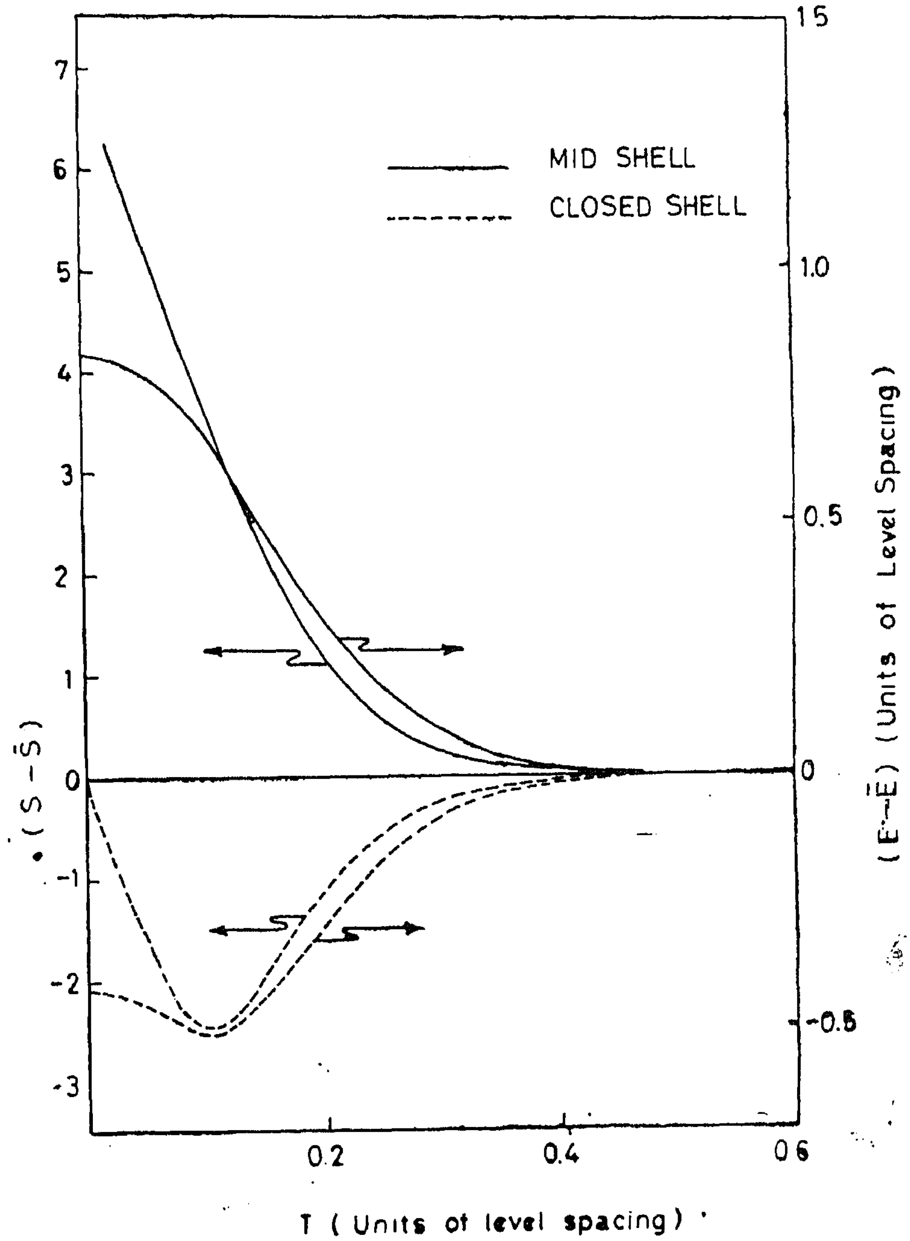

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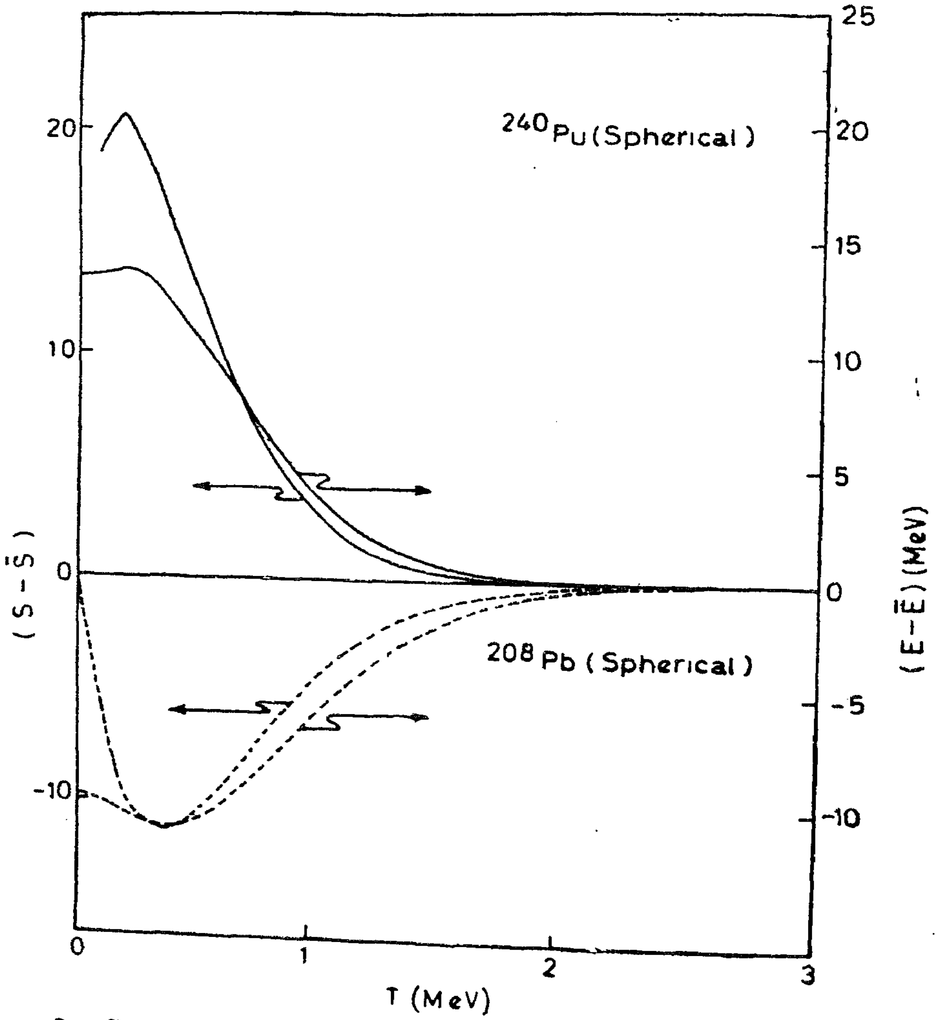

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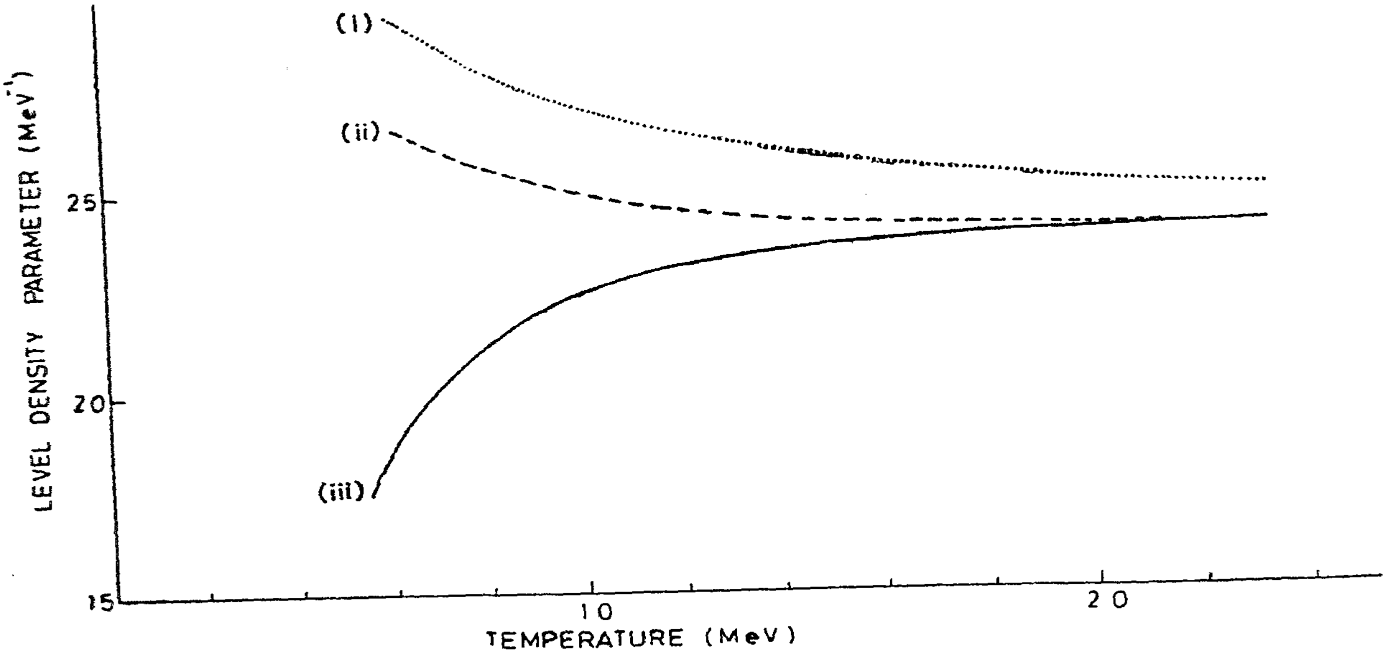

Figure 3. Plots of the calculated level density parameter a versus temperature for the nucleus ^{242}Pu having the symmetric outer barrier deformation. Curves (i), (ii) and (iii) are the results of calculations based on the three definitions of a.

$$a = \frac{S^2}{4\,E_x}\,, \qquad a = \frac{1}{4}\,\frac{dS^2}{dE_x}$$

and

$$a = \frac{S^2}{4\,(E_x + \Delta_s)} \text{ respectively}$$

where Δ_s is the ground state shell correction energy for that deformation.

is minimum at the LDM saddle point, the level density also shows a minimum at the same shape which then becomes the fission transition state. If, however, the shell effects are included, the above considerations are no longer valid and the transition state shape needs to be determined directly from the level density considerations. Just as the LDM saddle point is located by finding out the maximum in the locus of conditional minima in the deformation energy surface, the transition state shapes of excited nuclei should be determined by locating minima in the locus of conditional maxima of level density for different nuclear elongations. Interpretation of super-barrier fission data is, therefore, closely linked to the calculation of level density as a function of nuclear shapes taking into account shell effects. Such calculations have been made possible in recent years with the availability of single particle energy levels for different nuclear shapes and the application of numerical methods of calculation of nuclear level densities, as described in the previous section. In the present work, numerical calculations of the entropy of fissioning nuclei have been carried out for various nuclear shapes starting from appropriate single particle level schemes. The results of these calculations are used to discuss the excitation energy dependence of the fission transition state shape and the relevant thermodynamic properties.

3.1. *Influence of mass-asymmetric co-ordinate on the fission transition state of excited nuclei.*

Calculations (Nix 1973) of nuclear deformation potential energy surfaces have shown that for actinide nuclei, the second fission barrier has a lower deformation potential energy for mass-asymmetric shapes as compared to mass-symmetric shapes. In the present work, we have carried out calculations of the entropy surface near the outer fission barrier starting from the single particle level scheme of Nix (1972), for the folded Yukawa potential whose shape is specified by suitable parameters including mass-asymmetric co-ordinate α_2. Results of these calculations for a typical case of ^{242}Pu fissioning nucleus are shown in figure 4.

In these calculations the deformation potential energy was taken from the microscopic-macroscopic calculations of Nix and co-workers (Bolsterli 1971). Following conclusions can be directly drawn from the figure:

(1) At low excitation energies corresponding to near threshold fission, the entropy is maximum for $\alpha_2 = 0 \cdot 8$ implying that the nucleus predominantly passes through a mass-asymmetric shape at the second barrier.

(2) At excitation energies exceeding 25 MeV, the entropy is maximum for $\alpha_2 = 0$, again implying that at these energies the nucleus predominantly passes through a mass-symmetric shape at the second barrier. This result is a direct consequence of the rapid washing out of shell effects on entropy, as discussed in the earlier section.

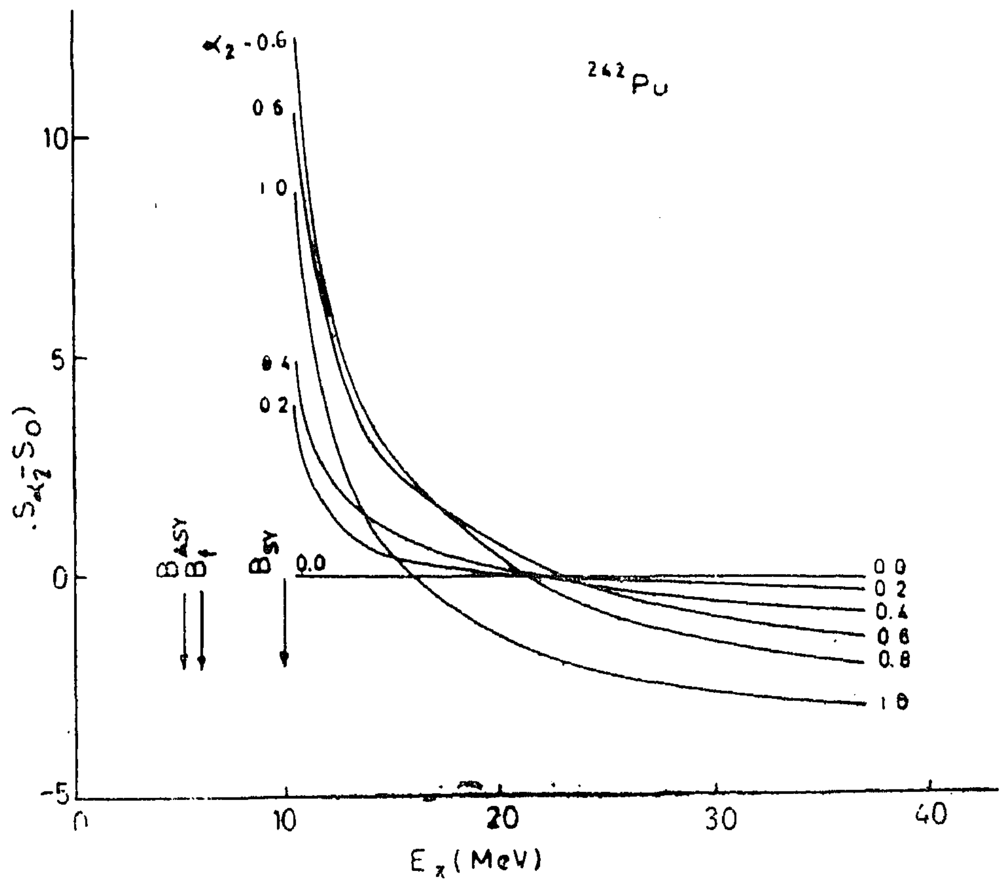

Figure 4. Plots of the calculated entropy difference $(S_{\alpha_2} - S_0)$ of the fissioning nucleus ^{242}Pu as a function of the compound nucleus excitation energy E_x, where S_{α_2} and S_0 are the entropies for the mass-asymmetric shape specified by the parameter α_2 and for the mass-symmetric shape respectively corresponding to the outer barrier deformation.

If one makes the assumption that the probability $P(\alpha_2)$ of the fissioning nucleus going through a mass-asymmetric shape at the second barrier deformation is proportional to the total number of open channels for that configuration, the following analysis can also be carried out. Restricting oneself to the study of super-barrier fission, where excitation energy of the compound nucleus is above both the symmetric and asymmetric barriers, one can write

$$P(\alpha_2) \propto \int_0^{E_x - E(\alpha_2)} \rho(x)\, dx \tag{7}$$

where $E(\alpha_2)$ is the deformation potential energy of the asymmetric shape relative to ground state and E_x is the compound nucleus excitation energy.

Qualitatively, it follows from eq. (7) that in this case $P(\alpha_2)$ is proportional to $\rho\{E_x - E(\alpha_2)\}$, due to the fact that most of the contribution to the integral comes from the upper limit. Also, since predominant energy dependence of the level density is governed by the entropy, one can write

$$P(\alpha_2) \propto e^{S(\alpha_2)} \tag{8}$$

where $S(\alpha_2)$ is the entropy of the nuclear configuration α_2 for a given compound nucleus excitation energy E_x.

Figure 5 shows the results of calculations of the probabilities for the same

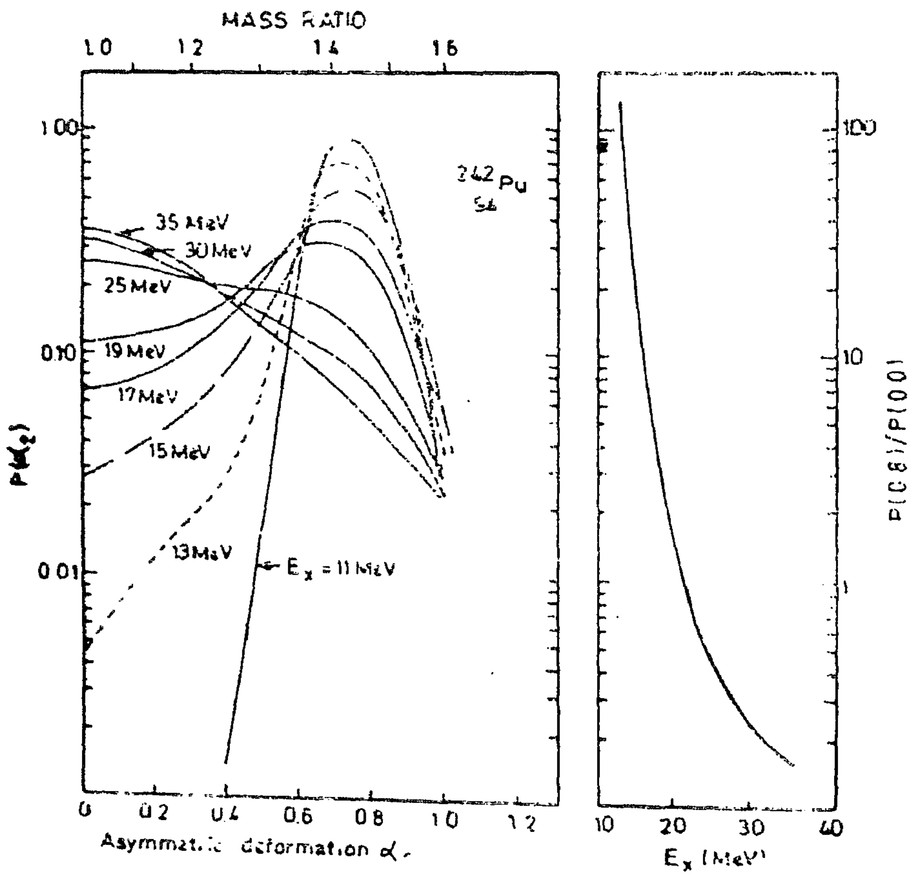

Figure 5. Plots of the probability $P(\alpha_2)$ of the nucleus going through a mass-asymmetric shape α_2 at the outer barrier deformation versus the parameter α_2 for different excitation energies. Also shown in figure is the ratio $P(\alpha_2 = 0.8)/P(\alpha_2 = 0)$ as a function of the excitation energy, showing the variation of the peak to valley ratio with excitation energy.

nucleus ^{242}Pu and it can be seen that the points of the earlier qualitative discussion are also brought out in this figure. Also shown in figure 5 is a plot of the calculated variations of the ratio of the probabilities for the nucleus to go through asymmetric and symmetric shapes as a function of the compound nucleus excitation energy. This plot clearly brings out the rapid filling up of the valley in the mass distribution with excitation energy resulting in a symmetric mass division at excitation energies exceeding about 30 MeV. It may be pointed out here that the present calculations of $\rho\ (\alpha_2)$ versus excitation energy are based on a set of single particle levels corresponding to the second barrier deformation. However, as is pointed out in the next section, the fission transition state itself shifts from the second barrier towards the LDM saddle point with increasing excitation energy. Inclusion of this effect in the present calculations should lead to a more rapid filling up of the valley than indicated in figure 5. For lower values of E_x, the plots in figure 5 are expected to be quantitatively correct since at these values of E_x the transition state coincides with the second barrier. The relation between expected fragment mass ratio and the asymmetry parameter α_2 on the assumption of a " knife cut " at the middle of the nuclear shape at the outer barrier is also indicated in figure 5. It is seen that in the range of excitation energies where the mass distributions are asymmetric, the calculated most probable mass ratio is surprisingly close to the experimental value. However, at the lowest excitation energy of 11 MeV for which the present calculations were carried out, the width of the calculated mass distribution is only about 5 mass units, which is considerably smaller than the experimental value. This comparison therefore shows that considerable broadening of the fragment mass distributions takes place during its descent from the second barrier to scission. Considering that the present calculations do not have any free parameter, it can be concluded that the experimental fragment mass distribution cannot be quantitatively understood on the basis of the properties of the transition state of the fissioning nucleus alone, without including the dynamics during the descent from the transition state to scission.

3.2. *Statistical interpretation of the fragment angular distributions*

The washing out of shell effects with excitation energy introduces a new feature which need to be taken into account in the statistical interpretation of the fission fragment angular distributions at moderate excitation energies. According to the statistical theory, (Halpern-Strutinsky 1958) the fragment angular distributions are determined by the distribution of K quantum number of the levels of the transition state nucleus, and can be characterized by a parameter $K_0^2 = J_{eff} \cdot T/\hbar^2$ where T is the temperature and J_{eff} is the effective moment of inertia of the transition state nucleus. For nuclei in the actinide region where the shell effects result in a pronounced double-humped barrier, the question arises as to which nuclear shape does the effective moment of inertia J_{eff} derived from the analysis of the fragment anisotropies correspond. In near threshold fission, the anisotropy data show that the angular distributions are characteristic of the states on the top of the second barrier (Strutinsky and Pauli 1969). However, as pointed out earlier, at excitation energies where shell effects have completely disappeared, the nucleus should thermodynamically behave as a LDM nucleus and therefore the transition state should coincide with the LDM saddle shape. Consequently, one would expect a shift of the transition state shape from the second barrier shape to the LDM shape at intermediate excitation energies. This would imply that J_{eff} becomes excitation energy dependent not only because of the shell and pairing effects on the moments of inertia for a given shape but also because the shape itself changes with excitation energy. This feature then need to be included in the interpretation of the parameter K_0^2 ($= J_{eff} \cdot T/\hbar^2$) versus excitation energy, derived from the statistical analysis of the fragment anisotropy data.

A calculation of the effective moment of inertia J_{eff} ($= J_{\perp} J_{\parallel}/J_{\perp} - J_{\parallel}$) at a specified excitation energy consequently involves (i) determination of the transition state shape relevant for fragment angular distributions and (ii) calculation of J_{eff} for that nuclear shape. The transition state shapes of the nucleus at a specified excitation energy can be located from the map of entropy calculated for different mass-asymmetric shapes for each elongation parameter y, from the criterion of minima in the locus of conditional maxima with respect to the coordinate α_2 for different elongation parameter y. Having located the transition state shape, microscopic calculation of J_{eff} can then be carried out starting with the single particle levels for the appropriate nuclear shape. It is shown in the appendix that numerical calculations of the moment of inertia starting from the shell model scheme, should also incorporate a normalisation procedure.

It has been shown in the earlier section that at $E_x \gtrsim 25$ MeV, the fissioning nucleus predominantly goes through mass-symmetric shapes at the second barrier. Therefore at these excitation energies, the transition state can be located from the calculated entropy S versus excitation energy E_x considering only the symmetric deformation parameter y. The results of these calculations for the typical case of the fissioning nucleus ^{242}Pu are shown in figure 6. For these calculations the deformation potential energy as a function of symmetric deformation parameter y was obtained with the use of the LDM parameters of Pauli-Ledergerber (1971) for the smooth part and the shell corrections calculated by Bolsterli *et al* (1971). For this nucleus the fissionability parameter $x = 0 \cdot 805$ and therefore the LDM saddle point is at the deformation $y = 1 - x = 0 \cdot 195$. It can be seen from the figure and the insert that with increasing excitation energy the transition state point (minimum entropy point) gradually shifts from the second barrier to the LDM saddle point and at $E_x \sim 40$ MeV, the transition state point coincides with the LDM saddle point.

It should be pointed out here that the excitation energy at which the transition state shape coincides with the LDM saddle shape depends on the shape of the LDM potential energy surface and thereby on the LDM parameters used. Some recent calculations for the same nucleus by Vandenbosch (1973) show that the LDM saddle point is reached only at $E_x \gtrsim 65$ MeV, but this appears to be due to the use of LDM parameters which are different from the more reliable Pauli-Ledergerber parameters since these latter parameters were extracted from fission barrier systematics. There is, however, one feature of the results shown in figure 6 which is somewhat disturbing. It is seen that as the excitation energy is further increased, the minimum entropy point further shifts at excitation energy of about 90 MeV to a deformation $\sim 0 \cdot 18$ which remains the minimum entropy

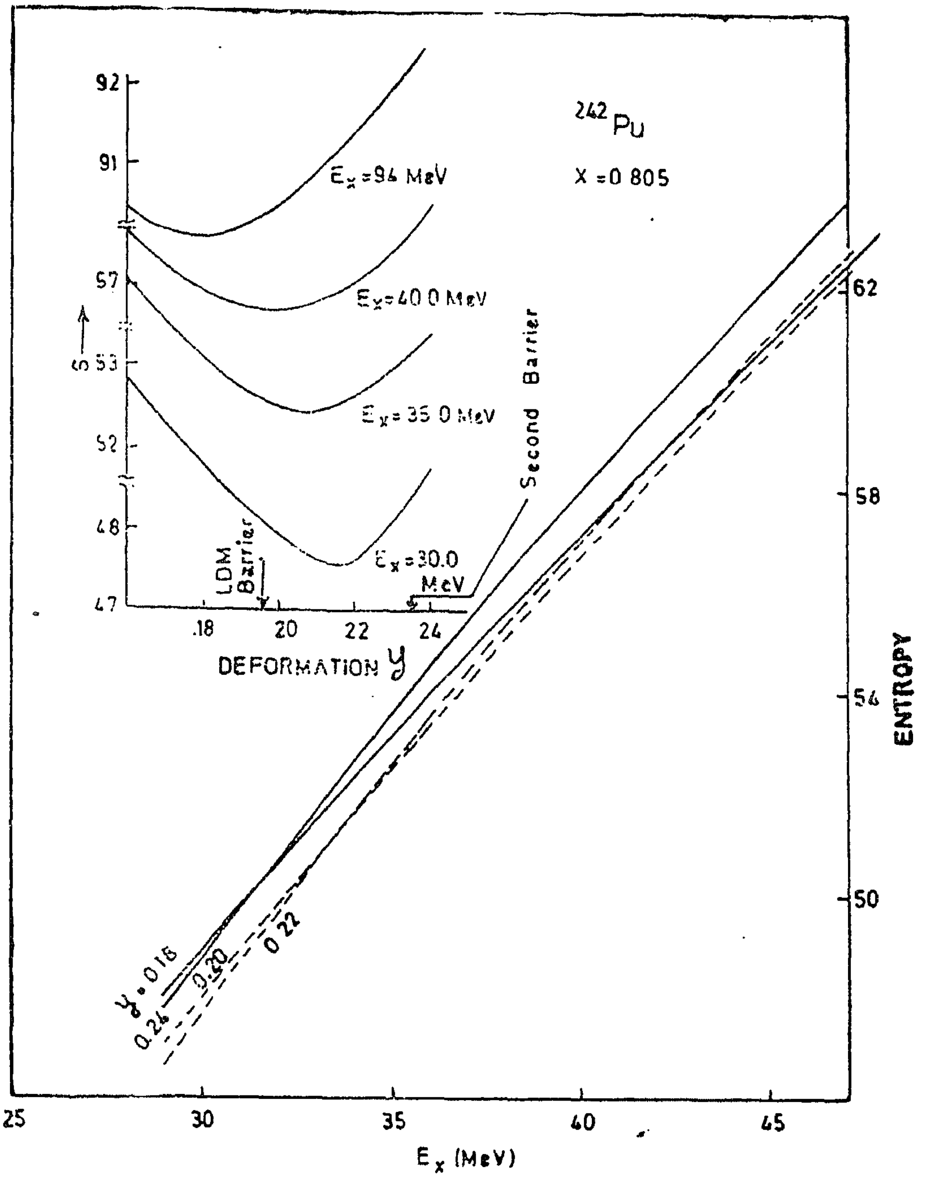

Figure 6. Plots of calculated entropy S for the nucleus ^{242}Pu as a function of the compound nucleus excitation energy E_x for different values of the symmetric deformation parameter y. The insert shows entropy S versus deformation parameter y, for specified values of E_x.

point even at higher excitation energies. This small further shift of the minimum entropy point towards a lower deformation ($y = 0\cdot 18$) at these excitation energies appears to arise due to small errors of about 0·5 MeV in the relative values of the shell corrections for the deformations $y = 0\cdot 18$ and 0·20 and uncertainties of this order are known to be present in the shell correction values given by the Strutinsky smearing procedure. It should also be pointed out here that this feature of figure 6 cannot be understood on the basis of any other known mechanism such as a complicated excitation energy dependence of shell effects since, by definition, in the limit of high excitation energies where shell effects are completely wiped out, the minimum entropy point must coincide with the LDM saddle point shape. It is further shown below that the experimental results of fragment anisotropies for a wide variety of nuclei in the actinide region at excitation energies $E_x \sim 37$ MeV present evidence that for these fissioning nuclei the transition state shape coincides very nearly with the LDM saddle point shape at these energies.

The first chance anisotropy values for a number of actinide nuclei have been obtained by Reising *et al* (1966) for the case of 42·8 MeV alpha induced fission. These anisotropy values were used to determine the parameter K_0^2 on the basis of the statistical theory (Halpern and Strutinsky 1958) neglecting the effect of target spin. From the values of K_0^2 thus obtained for each case, the values of J_{eff} were determined. The values of temperature T used were those corresponding to the excitation energy at the LDM saddle point deformation and were obtained from the numerical thermodynamic calculation with single particle level schemes of Bolsterli *et al* (1971) after normalisation to correspond to $r_0 = 1 \cdot 16 f$. The pairing effect were approximately taken into account by substracting a condensation energy equal to $\frac{1}{4} g \Delta_0^2 - k\Delta_0$ from the excitation energy, where $k = 0$ for even nuclei and 1 for odd mass nuclei, $\Delta_0 = 11/\sqrt{A}$ MeV and the single particle level density g is that corresponding to the level scheme used. The moment of inertia J_0 for the spherical shape was also calculated with $r_0 = 1 \cdot 16 f$. Assuming that the transition state shape corresponds to the LDM saddle point, each value of J_0/J_{eff} was converted to give the fissionability parameter X of the nucleus on the basis of the liquid drop model calculations (Hasse 1972) without curvature correction. Figure 7 shows the values of the parameter $\xi = (Z^2/A)/X$ derived in this manner versus the isospin parameter $I^2 = \{(N-Z)/A\}^2$. It can be seen from figure 7 that the values of ξ derived in this manner from anisotropy data appear to bring out even such details as the isospin dependence of surface energy. It should be pointed out that part of the scatter in the data points can be ascribed to the effect of target spin which was not included in the above analysis. In fact, the points showing maximum deviation from the average trend do correspond to targets with spins of 5/2 and 7/2. The curves based on the Pauli-Ledergerber (1971) and Myer-Swiatecki (1967) LDM parameters are also shown in the figure for the sake of comparison, where it is seen that the anisotropy data is in better agreement with the Pauli-Ledergerber LDM parameters. It should be pointed out that if, in fact, at excitation energies of about 37 MeV encountered in these experiments, the transition state was either at the second barrier or between the second barrier and the LDM saddle point, the above analysis should lead to values of ξ significantly higher than the LDM prediction, whereas it in fact leads to values of ξ which are smaller than those shown in figure 7 if the temperature T is evaluated at the second barrier deformation. Considering that the experimental points are well below the Myer-Swiatecki curve and lie almost on the Pauli-Ledergerber curve, it can be concluded that even at compound nucleus excitation energies of about 37 MeV, the fission transition state relevant for fragment angular distributions indeed coincides almost with the LDM saddle point shape. The same conclusions were reached on the basis of the results of figure 6 where at $E_x \sim 40$ MeV the transition state point (minimum entropy point) is found to coincide with the LDM saddle point.

4. Evaluation of relative shell correction energies of nuclei

It was shown in section 2 that at high temperatures, the influence of nuclear shell effects on the thermodynamic properties of nuclei disappear. In particular it was shown that the calculated entropies and the total energies asymptotically

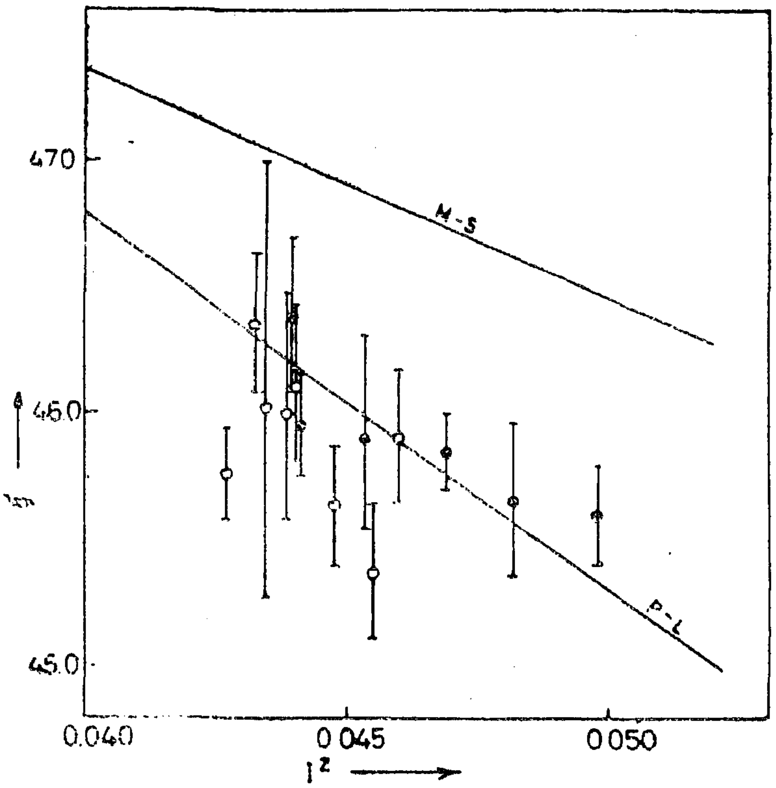

Figure 7. The values of $\zeta = (Z^2/A)/X$ versus the square of $I = (N - Z)/(N + Z)$ for a number of nuclei in the actinide region derived from the first chance anisotropy values given by Reising *et al* (1966) The open points refer to nuclei with non-zero target spin. The expected iso-spin dependence of ζ based on Pauli-Ledergerber (1971) and Myers–Swiatecki (1967) liquid drop parameters are also shown in the figure

become independent of the magnitude of the ground state shell correction energies (*see* figures (1) and (2)). An important implication of this result is that the entropies and the total energies calculated for any two single particle level schemes $G^1(\epsilon)$ and $G^2(\epsilon)$ having the same smooth components $g(\epsilon)$ but different local fluctuations $\delta g(\epsilon)$ and therefore different ground state shell correction energies, will become identical in the asymptotic high temperature region. That is, if E^1 and E^2 are the total energies for the two level schemes, calculated at any given temperature in the asymptotic high temperature region, one has

$$E^1 = E^2$$

i.e.,

$$E_g^1 + E_x^1 = E_g^2 + E_x^2$$

i.e.,

$$\begin{aligned} E_x^2 - E_x^1 &= E_g^1 - E_g^2 \\ &= (E_g^1 - \bar{E}_g) - (E_g^2 - \bar{E}_g) \\ &= \Delta_s^1 - \Delta_s^2 \end{aligned} \tag{9}$$

Here E_g^1 and E_g^2 are the ground state energies for the two level schemes, Δ_s^1 and Δ_s^2 are the respective ground state shell correction energies and $\bar{E}_g$ is the ground state energy of the hypothetical smooth system, assumed to be the same for both the level schemes. It is therefore seen that a plot of the calculated difference in excitation energies $(E_x^2 - E_x^1)$ versus temperature will approach an asymptotic constant value at high temperatures which is equal to the difference in the ground state shell correction energies for the two level schemes.

If however, small differences exist in the smooth component $g(\epsilon)$ of the two level schemes, the above simple relation between the calculated $(E_x^2 - E_x^1)$ and $(\Delta_s^1 - \Delta_s^2)$ is somewhat modified. It has been shown (Ramamurthy and Kapoor 1972, 1973) that in the asymptotic region of high temperatures, one can, in general, write

$$S = \sum_{i=1} a_i T^i \tag{10}$$

$$E_x = -\Delta_s + \sum_{i=1} \frac{i}{i+1} a_i T^{i+1} \tag{11}$$

for any level scheme where the coefficients a_i are characteristic of the overall behaviour of the level scheme. Therefore, for two level schemes, which have nearly the same overall behaviour,

$$S^2 - S^1 = \sum \delta a_i T^i \tag{12}$$

$$E_x^2 - E_x^1 = -(\Delta_s^2 - \Delta_s^1) + \sum \frac{i}{i+1} \delta a_i T^{i+1} \tag{13}$$

where δa_i are small. The value of $(\Delta_s^2 - \Delta_s^1)$ can therefore be obtained from either eq. (13) alone or a combination of eqs (12) and (13). The uniqueness of the value of $(\Delta_s^2 - \Delta_s^1)$ is determined by the fact that this is independent of the temperature range used in evaluating $(\Delta_s^2 - \Delta_s^1)$ provided all the coefficients δa_i which are important in that temperature range are included.

In earlier work (Ramamurthy and Kapoor 1972) it was shown that the ground state shell correction energies of nuclei can be obtained from an equation of the form of eq. (11), where the coefficients a_i are obtained by studying the asymptotic high temperature behaviour of the calculated entropy S of the nucleus, which was shown to be of the form of eq. (10). The equivalence of this thermodynamic method of determining the shell corrections with the Strutinsky smearing procedure has been discussed by several workers (Bhaduri and Das Gupta 1973, Das Gupta and Radhakant 1973). Here, we further point out that a calculation of the deformation potential energy surface where only relative shell correction energies with respect to deformation are of significance gets simplified with the use of eqs (12) and (13), where the temperature dependent terms appear only as small corrections. Figure 8 shows plots of the calculated excitation energy E_x versus temperature T for the two typical values of the deformation parameter $y = 0 \cdot 0$ and $0 \cdot 14$. Also shown in the figure is a plot of the differences in excitation energy versus temperature for the same two shapes. It can be seen that while E_x is strongly temperature dependent, the difference $E_x\,(y = 0 \cdot 14) - E_x\,(y = 0 \cdot 0)$ shows a weak dependence on the temperature, thus enabling a more

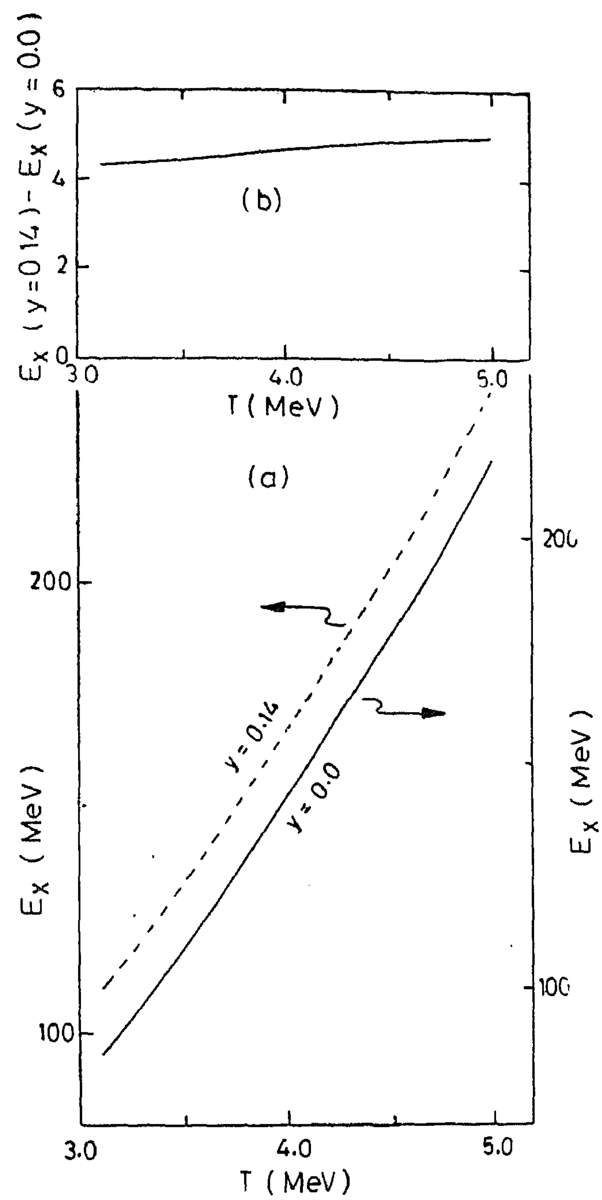

Figure 8. (*a*) Plots of the calculated excitation energy versus temperature for protons in ^{240}Pu for two values of the symmetric deformation parameter y. The single particle level scheme used for the calculations are those generated by Nix *et al* (1972) for a realistic folded Yukawa potential. (*b*) Plot of the calculated difference in excitation energies versus temperature for protons in ^{240}Pu for the same two values of the symmetric deformation parameter y as in (*a*).

accurate estimate of the zero temperature intercept which is equal to the relative shell correction energy $\triangle_s(y = 0\cdot 14) - \triangle_s(y = 0)$. Figure 9 shows the results of the shell correction energy for protons versus the deformation parameter y relative to spherical shape for the nucleus ^{240}Pu. The corresponding values obtained by the Strutinky smearing procedure with the smearing parameter $\gamma = 7$ MeV and the order of Hermite polynomial $p = 6$ are also shown for comparison. It should be remarked here that the disagreement of the values obtained by the Strutinsky procedure with $p = 6$ and $\gamma = 7$ MeV with the present values, is found to be due to the non fulfilment of the plateau condition in the Strutinsky method for higher deformations. Further details of these calculations and results will be discussed elsewhere our aim here was mainly to illustrate the principle of this method based on the washing out of the shell effects at high excitation energies.

5. Concluding remarks

An important conclusion arising from the present study of the washing out of shell effects with excitation energy and its implication on the fission of excited nuclei is as follows:

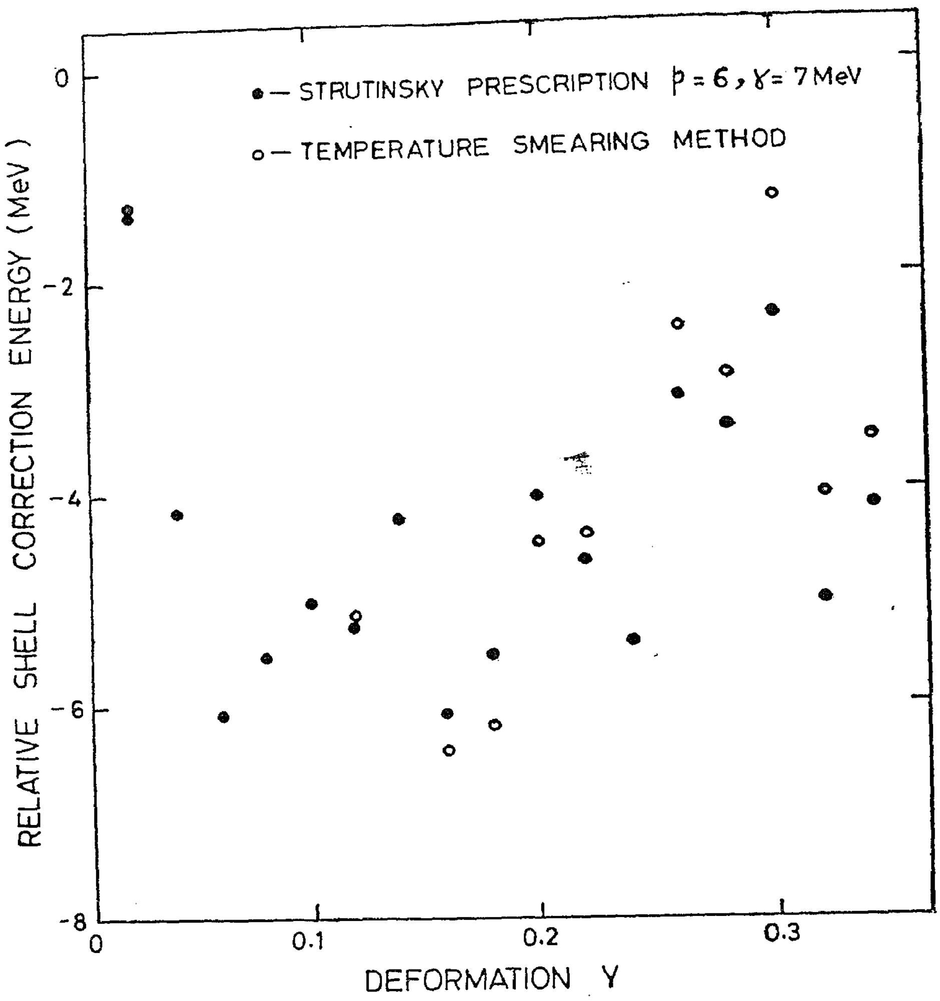

Figure 9. Calculated relative shell correction energies as a function of the symmetric deformation parameter y, by the temperature smearing method. The same quantities as calculated by the Strutinsky prescription are also shown for comparison.

Several recently discovered features arising from single particle corrections to the LDM potential energy surfaces, such as the existence of a double-humped fission barrier and an energetically preferred mass asymmetric outer barrier shape are shown to be of no relevance in the case of fission of a sufficiently excited nucleus due to the disappearance of shell effects. For example, it is shown that due to excitation energy dependence of shell effects a typical fissioning nucleus in the actinide region like ^{240}Pu which goes predominantly through a mass-asymmetric shape at the outer barrier in near threshold fission, goes over rapidly to a mass-symmetric shape with increasing excitation energy—a fact well known from experimental mass distribution studies. Similarly, the fragment angular anisotropy data in medium energy fission are shown to be characteristic of the LDM saddle point shapes. It is also shown as to how this excitation energy dependence of shell effects has been used to formulate a new method to determine the shell correction energies in the nuclear ground state.

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Appendix

For a given single particle level scheme the quantity $J_{\parallel}/\hbar^2$ versus excitation energy can be calculated numerically with eqs (1)–(4). Figure 10 shows the results of such calculations of the moment of inertia $J_0/\hbar^2$ versus excitation energy for a typical case of a spherical shape of ^{242}Pu. It is seen that, after the disappearance of shell effects, $J_0/\hbar^2$ asymptotically reaches a constant value which should be identified with the rigid body value. It is found that this asymptotic value in the present calculation corresponds to a radius parameter $r_0 = 1 \cdot 27$ fm which is also nearly equal to the sharp surface radius parameter of the potential used to generate the input single particle levels. This value of r_0, however, differs from the value $1 \cdot 16$ fm which is known to represent better the spatial properties of nuclei (Myers 1970). The above discrepancy arising from the non-self consistent nature of the shell model calculations of single particle levels shows that reliable calculations of moments of inertia based on shell model level schemes should incorporate a normalization procedure to ensure that the asymptotic values of $J/\hbar^2$ correspond to the rigid body values corresponding to the radius parameter $r_0 = 1 \cdot 16$ fm.

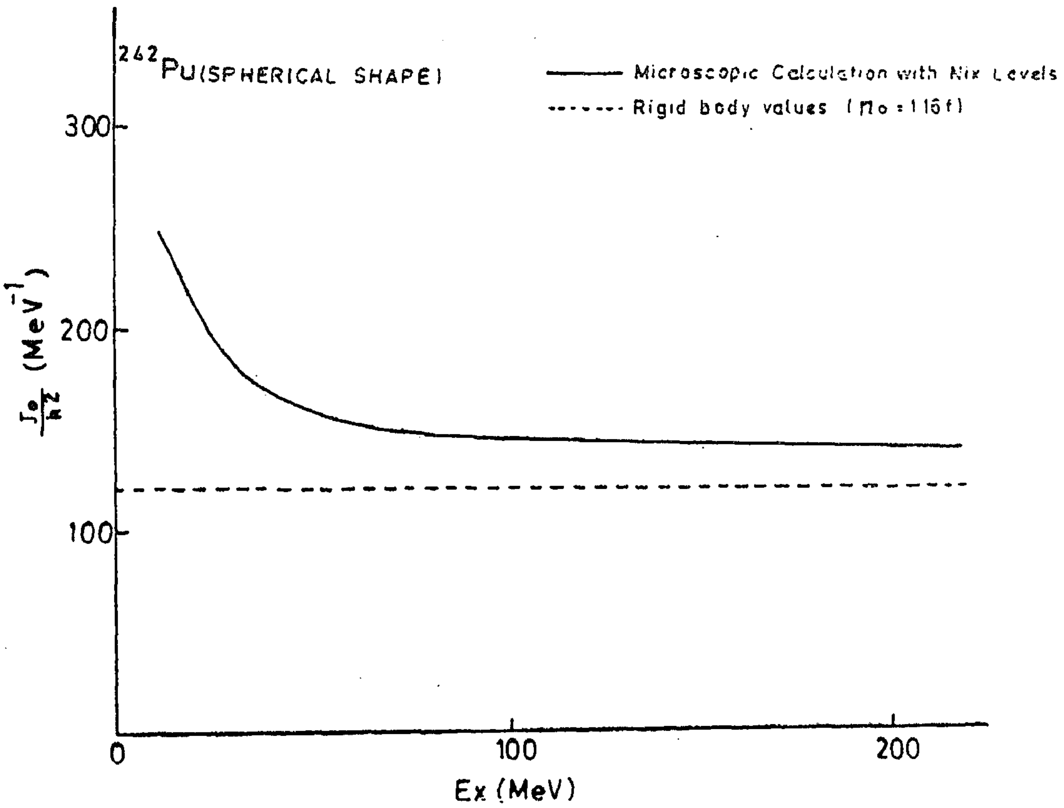

Figure 10. Results of the numerical calculations of the moment of inertia $J_0/\hbar^2$ versus the excitation energy for a typical case of spherical shape of ^{242}Pu. The dotted line represents the corresponding rigid body value with $r_0 = 1 \cdot 16$ fm for the radius parameter.

However, such a normalization procedure is useful only if the normalization constant is independent of nuclear deformation. Figure 11 shows the results of calculations of $J_{\|}/\hbar^2$ as a function of deformation for the same nucleus ^{242}Pu for the single particle levels of Nix and co-workers (Bolsterli *et al* 1972) and also for the modified harmonic oscillator levels of Seeger and Perisho (1967) along with the rigid body values for $r_0 = 1 \cdot 16$ fm. It can be seen that, for both the level schemes, the quantity $J_{\|}/\hbar^2$ exceeds the rigid body esimates and these differences can be directly traced to the different $\langle r \rangle^2$ of the single particle potentials in the two cases. However, it is seen that the normalization factor $C = (J_{\|})/(J_{\|})_{\text{rigid}}$

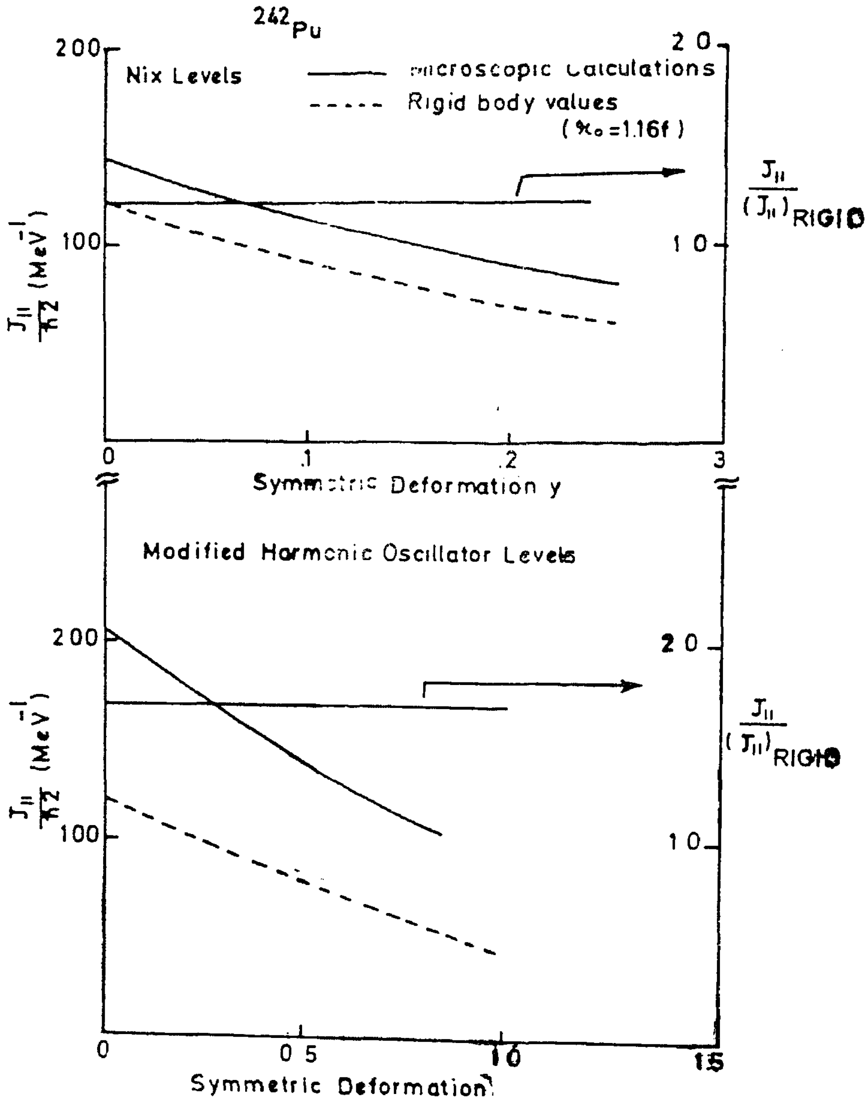

Figure 11. Results of calculations of $J_{\|}/\hbar^2$ as a function of deformation for the nucleus ^{242}Pu. The calculations have been carried out for the single particle levels of Nix (1972) and for the modified harmonic oscillator levels of Seeger and Perisho (1967). The dotted lines represent the corresponding rigid body values with $r_0 = 1 \cdot 16$ fm. Also shown in the figure is the ratio $J_{\|}/(J_{\|})_{\text{rigid}}$ as a function of the deformation for both the level schemes.

is almost independent of the deformation, although the magnitude of C is itself different in the two cases. The calculated values of $J_{\parallel}/\hbar^2$ versus the excitation energy E_x for any deformation should therefore be divided by the factor C to ensure the correct asymptotic value of the quantity $J_{\parallel}/\hbar^2$. Similar renormalization will also be required in the calculations of moments of inertia, $J_{\perp}/\hbar^2$, perpendicular to the nuclear symmetry axis.

For the same reasons as mentioned above, the level density parameter a derived from the asymptotic values of the calculated thermodynamic quantities needs to be normalized to a value corresponding to the radius parameter $r_0 = 1 \cdot 16$ fm, which can be done on the basis that a is proportional to $\langle r_0^2 \rangle$. Since the parameter K_0^2 characterizing fragment anisotropies is given by

$$K_0^2 = (J_{\text{eff}}/\hbar^2)\, T \simeq (J_{\text{eff}}/\hbar^2)\,(E_x/a)^{\frac{1}{2}}$$

it follows that a microscopic calculation of K_0^2 will be nearly proportional to the input radius parameter $\langle r^2 \rangle^{\frac{1}{2}}$ of the potential used to generate the single particle levels, and therefore needs to be normalized to the radius parameter r_0 of the actual nucleon density distribution. Without incorporating the above normalization procedure, then microscopic calculations could lead to a significant overestimate of K_0^2, which when compared with "experimental" values of K_0^2, might result in misleading conclusions regarding the transition state shape.

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