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Evaluation of nuclear shell correction energies for realistic level schemes by temperature smearing method

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Abstract. Calculations of shell correction energies by the temperature smearing method for realistic single particle level schemes of finite depth potentials are described and discussed. It is found that the method provides unique values of the shell correction energies for the various shapes relevant in the fission of actinide nuclei including those shapes where breakdown of the usual Gaussian energy smearing procedure was observed.

Keywords. Nuclear shell correction energies; temperature smearing method; realistic level schemes.

1. Introduction

In the last few years several calculations of nuclear deformation potential energy surfaces have been carried out on the basis of the now well known macroscopic-microscopic approach (Strutinsky 1967, 1968) where the nuclear potential energy as a function of nucleon number and nuclear deformation is split into two components—a smooth part expressible in terms of the liquid drop model and a small fluctuating residue arising from nuclear shell effects. It has been shown by Strutinsky (1967) that the small fluctuating component, known as the shell correction energy, can be determined by considering the independent particle motion of nucleons in an appropriate one body potential well, as the difference between the sum of energies of the occupied single particle states and the corresponding quantity of a hypothetical system with suitably smoothed density of single particle energy states in which the shell structure has been washed out. In most calculations of nuclear potential energy surfaces, the equivalent smooth system is generated by the well known Strutinsky smearing procedure (Strutinsky 1967) where in the single particle spectrum each delta function in energy is replaced by an appropriate Gaussian function. An alternate approach for the calculation of the nuclear shell correction energies has been earlier suggested (Ramamurthy and Kapoor 1972), based on a study (Ramamurthy *et al* 1970) of the high temperature behaviour of the thermodynamic properties of nuclei. This method basically exploits the fact that at high temperatures, the smooth Fermi occupation factor of the single particle states in nuclei leads to a washing out of the influence of shell effects on the thermodynamic properties of nuclei. The method was earlier demonstrated (Ramamurthy and Kapoor 1972) for the single particle energy level scheme of Seeger and Perisho (1967) generated for a modified harmonic oscillator potential, where the calculated shell correction energies by the temperature smearing method were found to be in good agreement with those obtained by the Strutinsky smearing procedure. The general validity of this method and its basic equivalence to the Strutinsky method have been subsequently investigated (Bhaduri and Das Gupta 1973, Das Gupta and Radha Kant 1974) and some calculations of the deformation potential energy surfaces have also been reported (Bengtsson 1972) based on similar thermodynamic approach, but restricted to harmonic oscillator level schemes. However, so far no numerical calculations of the shell correction energies by this method have been reported for realistic single particle level schemes of finite depth potentials and it is not known as to whether this method can be successfully applied in those cases where the Gaussian energy smearing procedure has been found to have some difficulties.

In this paper, after a brief discussion of the present method of determination of the shell correction energy, typical results obtained by this method for a range of nucleon numbers and deformations for the realistic single particle levels schemes of Bolsterli *et al* (1972) generated for a folded-Yukawa potential are presented and discussed.

2. Outline of the method

On the basis of many numerical calculations (Ramamurthy *et al* 1970, Huizenga and Moretto 1972) starting from shell model single particle energy level schemes it is now well known that there is a rapid washing out of the influence of nuclear shell effects on the thermodynamic properties of nuclei with increasing temperature and a temperature of 2-3 MeV is sufficient to wipe out the shell effects in most medium and heavy nuclei. An important consequence of this behaviour of the thermodynamic properties of nuclei is that at sufficiently high temperatures, the entropy S and the total energy E of a nucleus become independent of the shell fluctuations inthe single particle level density and the following simple relations hold (Kapoor and Ramamurthy 1975).

$$S = S' \tag{1}$$

$$E = E' \tag{2}$$

$$E_x = E'_x - \Delta_s \tag{3}$$

where Δ_s is the ground state shell correction energy, and E_x is the excitation energy. The quantities S', E' and E'_x refer to an equivalent smooth system, stripped off its shell effects. The problem of calculation of the shell correction energy Δ_s is therefore reduced to that of determination of E'_x of the equivalent smooth system at temperatures sufficiently high to ensure disappearance of shell effects such that eqs (1-3) hold. It is known (Gilbert 1968) that the temperature dependence of the entropy S' for a smooth single particle level density can be expressed analytically as follows:

$$S' = \sum_{i=1,3,5,..} a_i T^i \tag{4}$$

and therefore

$$E'_x = \int T dS' = \sum_{i=1,3,5,\ldots} \frac{i}{i+1} a_i T^{i+1} \tag{5}$$

where the coefficients a_i are related to the single particle level density and its derivatives at the chemical potential. It is also known that the maximum value of i in eqs (4) and (5) is related to the highest non-vanishing derivative of the single particle level density. Combining eqs (3) and (5) one gets

$$E_x = \sum_{i=1,3,5,\ldots} \frac{i}{i+1} a_i T^{i+1} - \triangle_s \tag{6}$$

Equations (4) and (6) can be exploited in different ways to numerically calculate $\triangle_s$ from the calculated entropies and excitation energies at temperatures sufficiently high to ensure that eqs (1-3) hold. Calculations for a few typical cases using the modified harmonic oscillator level scheme of Seeger and Perisho (1967) were presented in an earlier work (Ramamurthy and Kapoor 1972). In these calculations, the quantities S and E_x were first numerically calculated as a function of temperature as described earlier (Ramamurthy *et al* 1970). Since in the asymptotic region of high temperatures $S = S'$, the calculated entropies in this region were used to evaluate the coefficients a_i in eq. (4) for a given order of the polynomial and the values of a_i were then used in eq (6) to determine $\triangle_s$. It was found that in all the cases, $\triangle_s$ could be determined to within 0·1 MeV by retaining terms up to $i = 3$ only in eqs (4) and (6), where the input values of the entropies in these equations corresponded to those calculated at temperatures above 3·0 MeV to ensure disappearance of shell effects. The observation that terms with $i > 3$ are not important is consistent with our a priori knowledge that for harmonic oscillator level schemes the average single particle level density is a second degree polynomial in energy and consequently has non-vanishing derivatives up to second order only. It may be pointed out here that for the same reason curvature corrections of higher orders were unimportant in the Strutinsky smearing procedure for this type of level scheme.

As different from the harmonic oscillator level scheme, for single particle energy level schemes based on realistic finite depth shell model potentials, no a priori knowledge exists regarding the functional form of the average single particle level density. It is therefore not known beforehand as to how many terms will be required in the polynomial expressions for the entropy and the excitation energy and what temperature range is approriate for the calculations of $\triangle_s$, so that the evaluated values of $\triangle_s$ satisfy the important requirement that these are insensitive to the temperature range and the number of terms chosen. We have examined these points in the following section and show that the shell correction energies can be uniquely determined by this method even for level schemes generated for finite depth potentials.

3. Typical numerical results for realistic single particle level schemes and discussion

We have used for the present investigations the level scheme of Bolsterli *et al* (1972) generated for a folded-Yukawa potential. This level scheme has in addition to the bound levels, a limited number of levels in the positive single particle energy region also up to single particle energies of about 20 MeV. Numerical calculations of entropy and excitation energy were first carried out for this level scheme as a function of the temperature T. In order to qualitatively infer as to how many significant terms will have to be retained in eqs (4) and (6) for the entropy and the excitation energy, we show in figure 1 a plot of the calculated (S/T) versus T^2 for the cases of single particle levels of protons and neutrons for a typical case of ^{240}Pu nucleus in its spherical shape. It is seen from the figure that for both neutron and proton levels, the asymptotic functional form of (S/T) versus T^2 deviates appreciably from a straight line implying that terms with $i > 3$ are significant for this type of level scheme, unlike the case of harmonic oscillator potential based level schemes. The

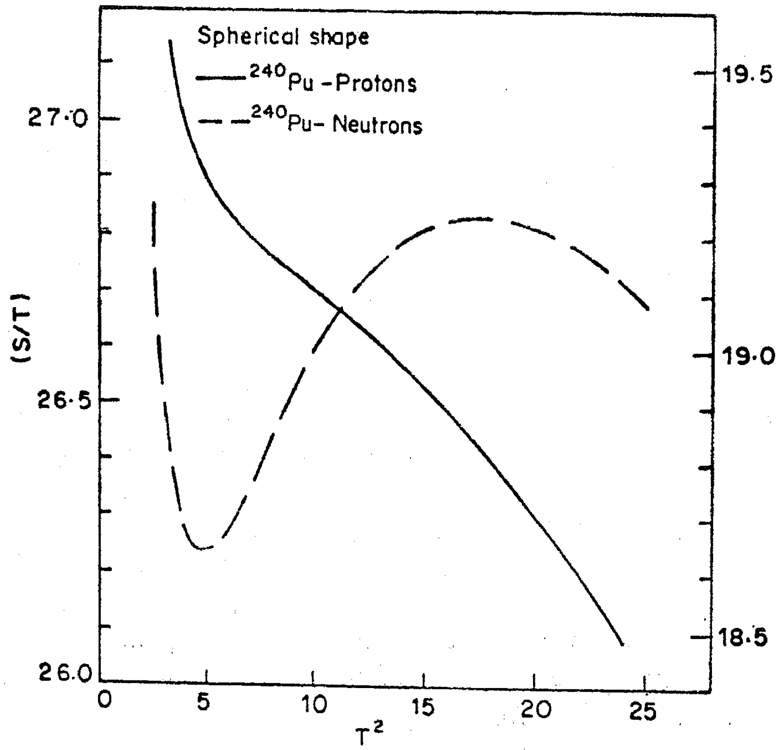

Figure 1. Plot of the calculated (S/T) versus T^2 for protons and neutrons in ^{240}Pu for the spherical shape.

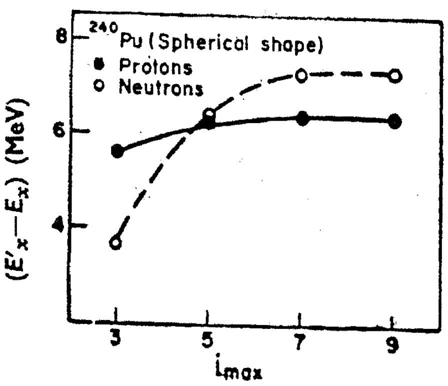

Figure 2. Calculated $(E'_x - E_x)$ versus i_{max} evaluated in the temperature range $T=4$ to 4·1 MeV for protons and neutrons in ^{240}Pu for the spherical shape.

shell correction energies are therefore to be calculated with the inclusion of terms with $i>3$ in eqs (4) and (6). We have examined the sensitivity of the calculated values of the shell correction energies with respect to the number of terms in eq. (4), when a temperature range of 4·0 to 4·1 MeV is used. Figure 2 shows these results for the cases of proton and neutron levels in ^{240}Pu nucleus in its spherical shape where the calculated shell correction energies are plotted as a function of i_{max}. It is seen that in both the cases four terms are sufficient in eq. (4) to ensure a constancy of the calculated shell correction energies with respect to the number of terms used. In order to bring out the sensitivity of the calculated shell correction energies on the temperature range used, we show in figure 3 for the same cases a plot of (E'_x-E_x) versus T obtained with four terms in eq. (4). The observed asymptotic constancy of (E'_x-E_x) in figures 2 and 3 show the validity of the method as applied to levels of finite depth potentials for the calculation of the shell correction energies. Similar calculations of Δ_s for a range of nucleon numbers and deformations for heavy nuclei corresponding to shapes relevant in fission were also carried out and results similar to those shown in figures 2 and 3 were obtained in all cases. It therefore follows that the thermodynamic method of calculation of Δ_s is applicable to any type of level scheme, with the requirement of a proper choice of i_{max} and temperature range.

A slightly different procedure, numerically simpler for routine calculations, has also been investigated by us. In this procedure, the calculation of the shell correction energy Δ_s was carried out on the basis of the function $(ST/2)-E_x$. From eqs (4) and (6) we have

$$\left(\frac{ST}{2}-E_x\right)=\Delta_s-\sum_i a_i\left(\frac{1}{2}-\frac{i}{i+1}\right)T^{i+1}. \tag{7}$$

The zero temperature intercept of $(ST/2)-E_x$ is the shell correction energy while the leading term in temperature is T^4. For harmonic oscillator potential based level schemes, the terms higher than T^4 in eq. (7) are absent and, consequently, determination of Δ_s in this case is straightforward through a straight line extrapolation to zero temperature. Even for realistic single particle level schemes, which have non-vanishing higher order terms, the extrapolation to zero temperature of $(ST/2)-E_x$ is more reliable and accurate since in this case the T^2 term is totally absent and the coefficients of the higher order terms are considerably reduced. Figures 4(a) and 4(b) show plots

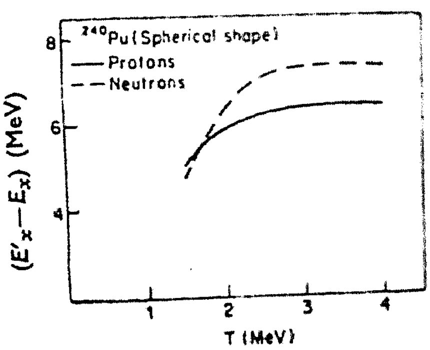

Figure 3. Calculated (E'_x-E_x), versus temperature evaluated with $i_{max}=7$ for protons and neutrons in ^{240}Pu for the spherical shape.

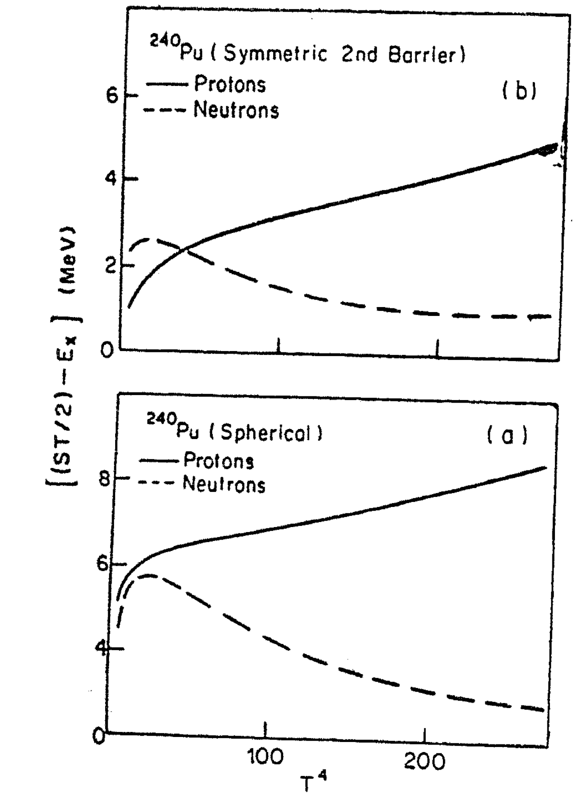

Figure 4. Plot of the calculated $(ST/2)-E_x$ versus T^4 for protons and neutrons in ^{240}Pu (a) for the spherical shape and (b) for the second symmetric fission barrier shape.

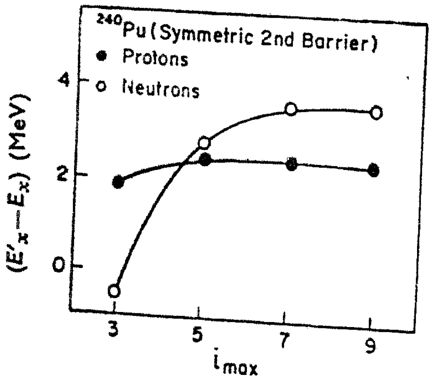

Figure 5. Calculated (E'_x-E_x) versus $i_{\max}$ evaluated in the temperature range T=4 to 4·1 MeV for protons and neutrons in ^{240}Pu for the second symmetric fission barrier shape.

of $(ST/2)-E_x$ versus T^4 for proton and neutron levels in ^{240}Pu nucleus for its spherical shape and for the shape corresponding to symmetric second barrier, where it can be seen that the significance of terms higher than T^4 has been considerably reduced as expected. It therefore follows that in all cases $(ST/2)-E_x$ is a more suitable function for the determination of Δ_s by extrapolation to zero temperature. Figure 5 shows the results for typical cases of proton and neutron levels in ^{240}Pu nucleus for its symmetric second barrier shape, where the values of Δ_s obtained by extrapolating the function $(ST/2)-E_x$ to zero temperature with terms up to $i_{\max}$, and a temperature range of 4 to 4·1 MeV are plotted against $i_{\max}$. It is seen that well defined values of the shell correction energies Δ_s can be obtained in both the cases with $i_{\max}=7$. Figure 6 shows for the same two cases, plots of the values of Δ_s obtained by extrapolating the function $(ST/2)-E_x$ to zero temperature with terms up to $i_{\max}=7$ versus the average of the temperature range used in the calculations. The asymptotic constancy of Δ_s for temperatures $T>3$ MeV is evident in both cases, leading to unique values of shell correction energies. Similar results have been obtained for other nuclear shapes and

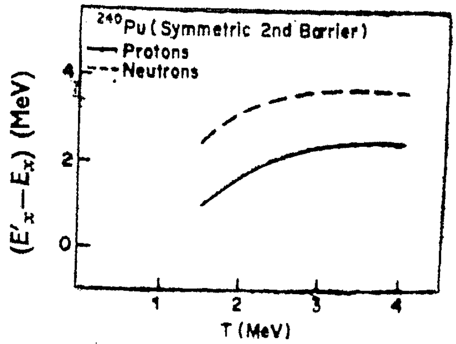

Figure 6. Calculated (E'_x-E_x) versus temperature evaluated with $i_{max}=7$ for protons and neutrons in ^{240}Pu for the second symmetric fission barrier shape.

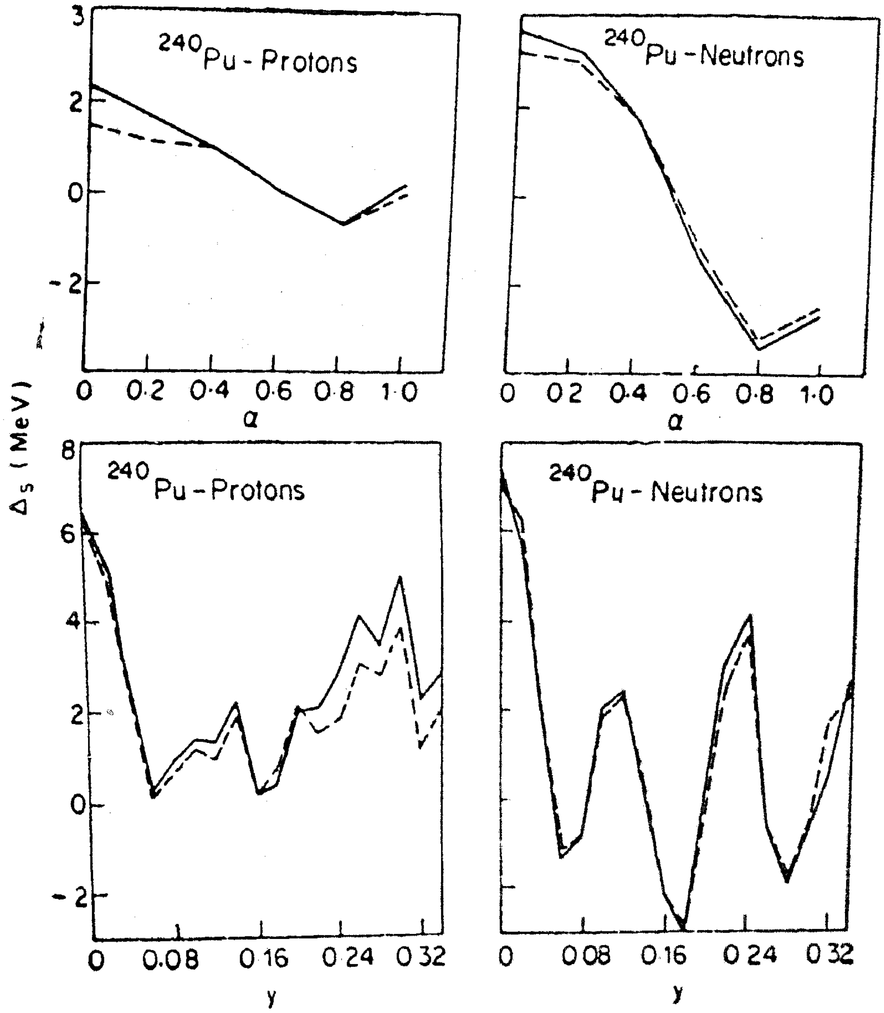

Figure 7. Calculated shell correction energies versus the mass asymmetric deformation parameter α and the symmetric deformation parameter y for proton and neutrons in ^{240}Pu. The dashed line represents the results obtained using the Strutinsky smearing procedure with $\gamma=7$ MeV and $p=6$.

nucleon numbers. Figure 7 shows a plot of the calculated shell correction energies for proton and neutron levels in the nucleus ^{240}Pu for its various shapes of interest in fission. These shapes are represented by the symmetric deformation parameter

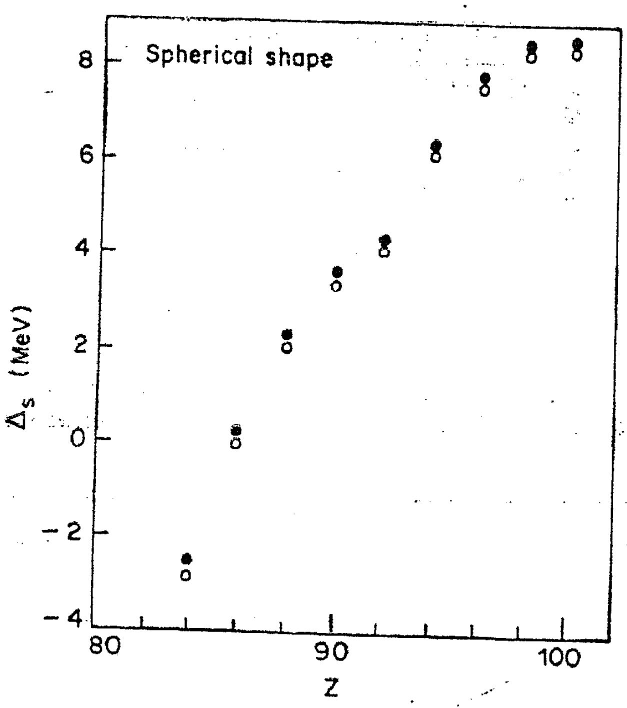

Figure 8. Calculated shell correction energies versus nucleon number for spherical shape of the nucleus. The dots represent the results obtained by the present method while the open circles represent the results obtained by the Strutinsky smearing procedure.

y and the mass asymmetric deformation parameter α corresponding to the second barrier as defined in the paper of Bolsterli *et al* (1972). The values of Δ_s calculated using the Strutinsky smearing procedure with smearing parameter corresponding to Gaussian smearing width $\gamma=7$ MeV, and a sixth order polynomial ($p=6$), are also shown in figure 7, as dashed curves. Figure 8 shows a similar plot of the calculated shell correction energies versus nucleon number for the spherical shape along with the values of Δ_s obtained with the Strutinsky smearing procedure. It can be seen from figures 7 and 8 that although the values of the shell correction energies obtained by the present method are generally in good agreement with the values obtained by the usual Gaussian energy smearing procedure of Strutinsky, significant differences of the order of 1 MeV or more are encountered in specific cases, particularly for protons in the region of symmetric second barrier shapes. It may be remarked here that with the same level schemes for the same shapes close to the second symmetric fission barrier, the Strutinsky procedure for the evaluation of Δ_s has been found (Ramamurthy *et al* 1976) to break down as it fails to give an unique value of the shell correction energy. No such breakdown has been encountered in the present method, as for example, seen from figures 5 and 6 for the specific cases where the Strutinsky procedure does not yield unique values. This difference between the two methods, in spite of their basic equivalence, appears to be related to the relative importance of the higher order curvature correction terms in the two methods. In particular, the use of two thermodynamic variables in the present method, namely E_x and S, seems to provide partial curvature corrections of all orders, as compared to the Strutinsky procedure where only energy smearing is used.

In conclusion, the temperature smearing method is shown to give unique values of shell correction energies of nuclei for any type of single particle level scheme including realistic level schemes of finite depth potentials. No breakdown of the method is encountered, while applying the method to calculations of shell correction energies of actinide nuclei for various shapes of interest in fission.

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