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SHELL STRUCTURE FOR DEFORMED NUCLEAR SHAPES

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Eigenvalues for the harmonic oscillator without $\boldsymbol{l} \cdot \boldsymbol{s}$ or $\boldsymbol{l}^2$ terms suggest a defomed shell structure for nuclei with axes ratios 2 : 1 and deformation $\epsilon = 0.6$ with corresponding nucleon "magic numbers" 2, 4, 10, 16, 28, 40, 60, 80 110 and 140, subject to small modifications due to spin-orbit and other correction terms. Experimental evidence of reasonably stable highly deformed structures corresponding to nucleon numbers 16, 20, 28, 40 and 60 (64) is presented. Attempts to calculate the corresponding potential energy surfaces using the Strutinsky shell correction method are described.

The occurrence of shell structure in the spherical case for nuclei is associated with particular radial shapes in addition to angular symmetries. As pointed out first by Geilikman [1], later by Tsang et al. [2] and Bohr and Mottelson [3] shell structure can also occur for separable non-spherical systems such that the following condition on the energy eigenvalues is fulfilled:

$$a : b : c = \partial e/\partial n_a : \partial e/\partial n_b : \partial e/\partial n_c$$

where a, b and c are integer numbers and n_a, n_b and n_c three quantum numbers characterizing the eigenstates, e.g. in the harmonic oscillator case the cartesian nodal quantum numbers.

In the case of a pure harmonic oscillator the condition above is satisfied, with $a : b : c$ being $\omega_x : \omega_y : \omega_z$. We will here just discuss the rotation symmetric case with $\omega_x = \omega_y = \omega_\perp$. The well-known plot of corresponding eigenvalues is presented in fig. 1. As pointed out e.g. in ref. [3], the largest shell structure for deformed nuclei is found for $\omega_z : \omega_\perp = 2 : 1$ ($\epsilon = -0.75$) and $\omega_z : \omega_\perp = 1 : 2$ ($\epsilon = 0.6$) when we have 75 and 60% respectively of the shell gaps in the spherical case.

In the prolate 1 : 2 case the lowest quantum numbers are $N_{\mathrm{sh}}(1:2) = 2, 4, 10, 16, 28, 40, 60, 80, 110$ and 140. In fig. 2 the corresponding shell energies are shown.

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It has recently been suggested [3] that the quantum number $N = 140$ (or rather $N = 144–148$ due to the effect of spin orbit coupling, see below) is associated with the fission isomer minimum whose shell energy and deformation ($\epsilon = 0.6$) are now fairly well established [4].

Our interest here is somewhat arbitrarily centered

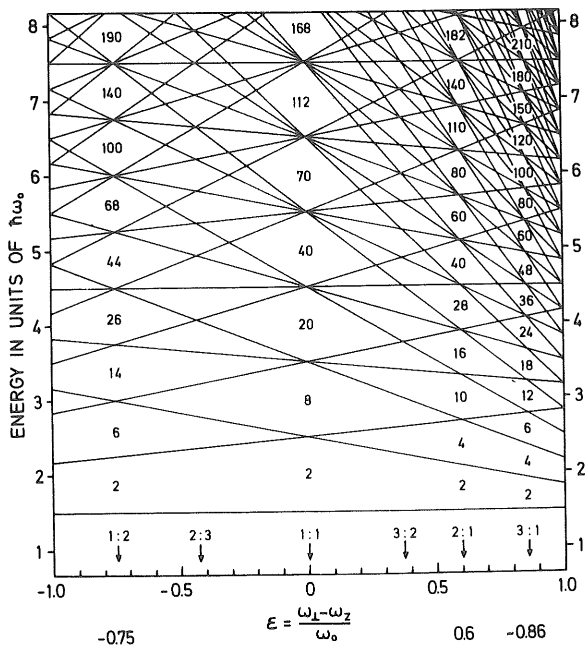

Fig. 1. Single-particle levels of the spheroidal oscillator as a function of $\epsilon = (\omega_\perp - \omega_z)/\omega_0$. Note in particular the shells at $\omega_z : \omega_\perp = 2:1$, $1:1$ and $1:2$ i.e. at $\epsilon = -0.75$, 0 and 0.6, respectively.

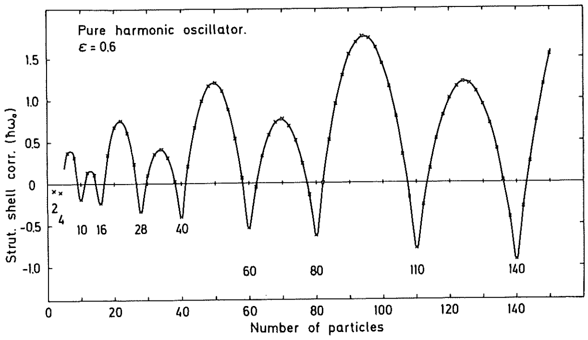

Fig. 2. The shell energies at $\epsilon = 0.6$ for the spheroidal oscillator as a function of particle number.

on the harmonic oscillator quantum numbers 16, 28, 40 and 60. The first concern is whether the modification due to spin-orbit and other correction terms to the harmonic oscillator can completely destroy the deformed shell structure. The spin-orbit term, absent in the level structure presented in fig. 1, energitically favours orbitals with large Λ and $n_\perp$ and with Λ and Σ parallel while disfavouring those with large n_z and and small Λ. For a more realistic single-particle potential we consider the following Hamiltonian [5, 6]

$$H = \mathrm{T} + \tfrac{1}{2}\hbar\omega_0\rho^2(1-\tfrac{2}{3}\epsilon P_2 + 2\epsilon_4 P_4)$$

$$-\kappa\hbar\mathring{\omega}_0(2\boldsymbol{l}_t\cdot\boldsymbol{s} + \mu(\boldsymbol{l}_t^2 - \langle \boldsymbol{l}_t^2\rangle_N)\,.$$

As the parameters κ and μ are unsatisfactorily known in the region under consideration (see e.g. discussion in ref. [7]), the effects on the harmonic oscillator gaps are shown in figs. 3 and 4 as a function of κ for given μ, approximately valid in the $A \approx 25$ and the $A \approx 100$ case, respectively. In these figures we compare the level schemes for $\epsilon_4 = 0$ and 0.08, the latter being the value which approximately corresponds to the liquid drop valley for the nuclei under consideration. In the lower part of the figures we also show some corresponding shell energies. It is immediately obvious from fig. 3 that for $\mu = 0$ the 16 nucleon gap will not be destroyed by either $\boldsymbol{l}\cdot\boldsymbol{s}$-coupling or ϵ_4-deformation. It is also of interest that for $\epsilon_4 = 0.08$, a 20 nucleon gap is developed which is further augmented if an $\boldsymbol{l}^2$-term is added.

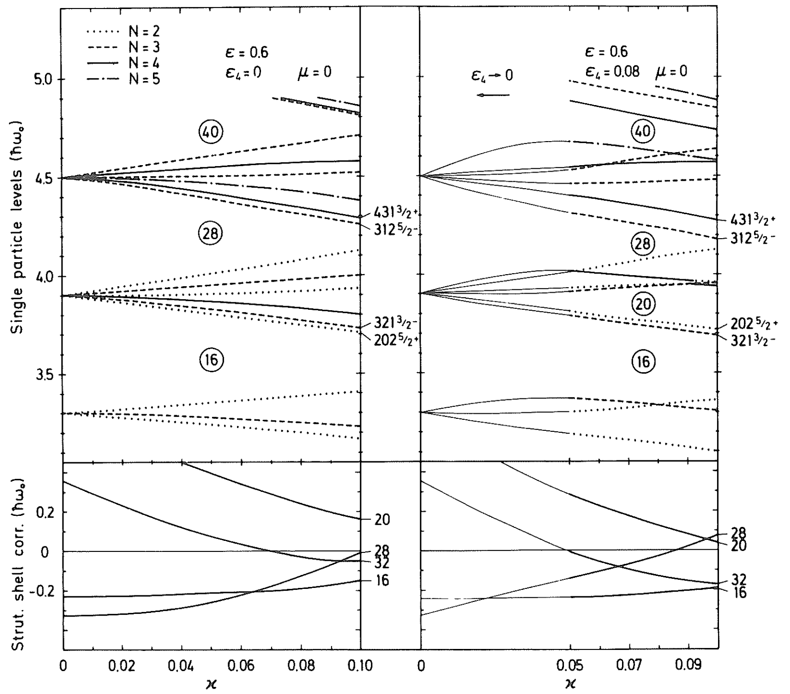

Fig. 3. Single-particle energies at $\epsilon = 0.6$, for $\epsilon_4 = 0$ and 0.08 in the left and right half of the figure, respectively, for nucleon numbers below 40. The corresponding spherical shell quantum number is denoted by the character of the lines. The $\epsilon = 0.6$ shells ($\kappa = \mu = \nu$) are shown to the left in each figure half. The lower part of the figure presents the Strutinsky shell corrections for the indicated neutron numbers.

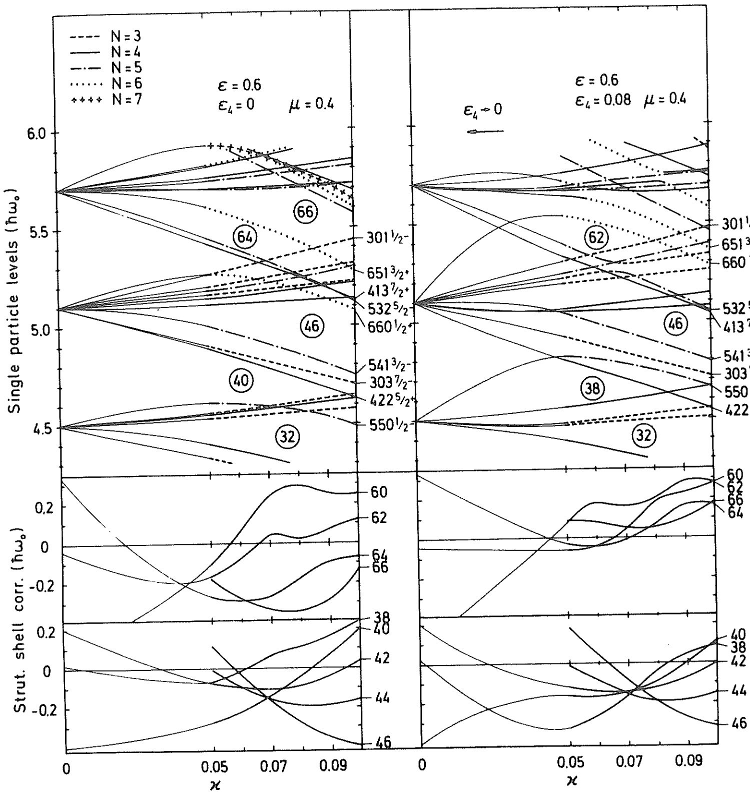

Fig. 4. Same as fig. 3 for orbitals relevant to A = 100 region or $Z \approx 40, N \approx 60$. The effect of ϵ_4 to lift orbitals of type [660 1/2], [550 1/2] etc. relative to the pure oscillator case is here apparent. Correspondingly an increase in κ lowers orbitals with large Ω and Λ as [422 5/2], [303 7/2], [413 7/2] etc. The influence on the 40–46 and 60–66 regions is seen to be critical to the choice of κ and μ.

In the other cases studied, i.e. N_{sh} = 28, 40 and 60, we have similar situations. Two or three levels come down into the gap from the levels above, while one level (with $n_z = 0$), at least if ϵ_4 is included, comes up from the levels below. We thus see that the regions 28–32, 38–46 and 62–66 have low level density. The details of these figures may be changed somewhat for different radial shapes and with a modification of the spin-orbit term. The general trend will, however, remain for reasonable changes.

The empirical evidence for especially stable nuclear structure in deformed as well as spherical nuclei is scattered broadly throughout the nuclear periodic table and will be the subject of a more comprehensive paper. Here we have chosen to concentrate on a relatively small region of medium light nuclei with $32 \leqslant A \leqslant 110$. Among recent experimental studies we mention here only the decisive efforts of Cheifetz

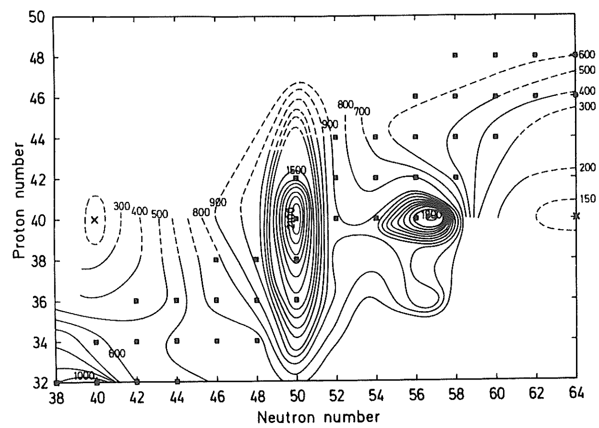

Fig. 5. Contour plot of the experimental energy of the lowest 2^+ state given in keV as a function of N and Z. Stable isotopes are indicated by solid black squares. Most of the data are taken from the compilation of ref. [22]. Note "hills" and "valleys" associated with Z = 40.

et al. [8] on the neutron rich side produced as fission fragments and the work of Nolte and collaborators [9] on neutron deficient nuclei following heavy ion bombardment. Historically the energy of the lowest 2^+ state has been used as an especially simple criterion for deformation and sphericity. Accordingly a contour plot of the lowest 2^+ state as a function of N and Z is presented in fig. 5 for masses between 70 and 110. It is immediately obvious that $Z = 40$ (Zr) plays a decisive "chameleon" role (adjusting dramatically to the neutron number). Thus it has not only the highest peaks at ${}^{90}_{40}Zr_{50}$ and ${}^{96}_{40}Zr_{56}$ corresponding to the

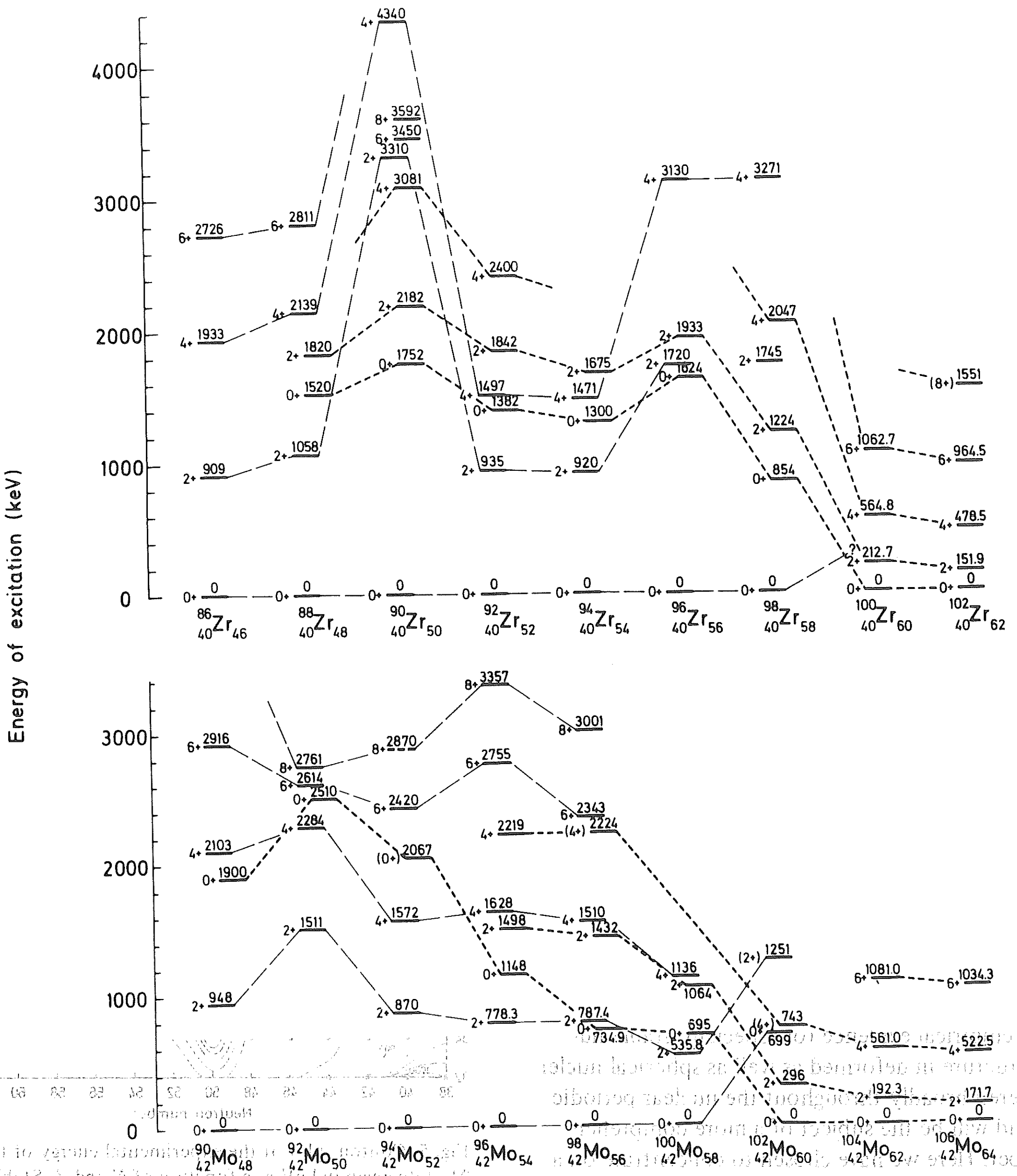

Fig. 6. Detailed spectroscopy of the low-lying positive parity states of the Zr and Mo nuclei drawn in such a way as to emphasize the possible shape isomerism. All low-lying positive parity states have been plotted with the exception of a 2^+ state (847.2 keV) in ^{102}Mo which is believed to be the gamma vibration of the ground state band. Data are from refs. [10, 22].

closed 50 neutron shell and 56 neutron subshell respectively, but also appears to be associated with the deepest holes at ${}^{80}_{40}Zr_{40}$ and ${}^{104}_{40}Zr_{64}$ (marked with an X in fig. 5). Since neither ^{80}Zr nor ^{104}Zr is known, their discovery and study represent an exciting experimental challenge within the reach of today's experimentalists. Of decisive importance is the measured energy and lifetime of the first 2^+ state in ^{102}Zr. The energy, 151.9 keV, is by far the lowest in this region and lower than any other below the deformed rare earth region. The measured lifetime significantly corresponds to $\epsilon \approx 0.6$ which is the deformation of maximal shell structure.

In view of the important role of the Zr nuclei in this region, fig. 6 presents the positive parity states for a sequence of even Zr and Mo nuclei. The spectrum for each nucleus is arranged in two different sequences to emphasize the possible existence of shape isomerism. The $0^+ - 2^+$ energy spacing of the shape isomers indicates that it might be associated with a highly deformed secondary minimum which moves down in energy with increasing N and becomes the ground state minimum at $N = 60, 62, 64$ in both Zr and Mo nuclei. We suggest that this secondary minimum is associated with the 40 proton (42 proton in the case of Mo) deformed shell structure with axes ratio 2 : 1 and deformation $\epsilon = 0.6$ and that when it is stabilized by the corresponding deformed neutron shell structure with neutron numbers 60, 62 and 64 it becomes the ground state. As suggested in fig. 5 we believe a similar sequence should be observed for the Zr and Mo isotopes with neutron numbers 40 and 42. The transition in shapes in the Mo isotopes at neutron number 60 is strongly supported in (t, p) and (p, t) studies [10, 11] in analogy with similar reaction cross section systematics for the transitional Sm isotopes.

We now attempt to indicate very briefly that this observation is by no means an isolated phenomenon. Fig. 7 presents the low lying positive parity spectra of ${}^{32}_{16}S_{16}$, ${}^{40}_{20}Ca_{20}$ and ${}^{56}_{28}Ni_{28}$. The spectra are again divided into sequences possibly indicative of separate structures and potential energy minima. In the case of ^{32}S (level scheme as in fig. 7a) the 2^+ and 4^+ levels at 2.232 and 4.461 MeV respectively with the E_{4^+}/E_{2^+} ratio 2.23 are what one expects for a near spherical vibrator. A second set of 0^+ and 2^+ states is observed at 3.775 and 4.280 which we suggest is associated with a prolate isomeric minimum with $\epsilon = 0.6$. The

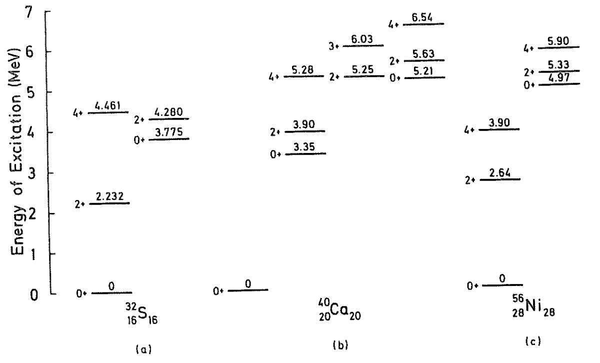

Fig. 7. Spectra of ^{32}S, ^{40}Ca and ^{56}Ni. One should in particular note the high-lying bands at 3.78, 5.21 and 4.97 MeV with $3\hbar^2/J$ equal to 0.505, 0.42 and 0.36 MeV, respectively. Data are taken from ref. [22].

$0^+ - 2^+$ energy spacing is consistent with this interpretation. Unfortunately no transition is observed between these states from which a B(E2) value would provide further information.

The spectrum of ^{56}Ni (fig. 7c) has a very high energy first 2^+ state at 2.64 MeV and only a slightly higher 4^+ state at 3.90 MeV as expected for a double closed shell spherical nucleus. However, a new spectral sequence begins with 0^+, 2^+ and 4^+ states at 4.97, 5.33 and 5.99 MeV. The moment of inertia implied by this band is consistent with a prolate isomeric minimum with $\epsilon = 0.6$. The fact that the E_{4^+}/E_{2^+} ratio, 2.58, is considerably less than the expected 3.33, may reflect on the interaction of the 4^+ state at 5.99 with a second 4^+ state at 6.38 MeV.

In the spectrum of ^{40}Ca (fig. 7b) there are two rotational bands with E_{4^+}/E_{2^+} ratios of 3.45 (lower band) and 3.17. Again the moments of inertia inferred from the $0^+ - 2^+$ spacing is large, particularly that of the third band. In this case the simple harmonic oscillator (fig. 1) does not predict deformed shell structure but the modified oscillator (fig. 3) does.

In summary, the experimental evidence strongly supports deformed shell structure for nucleon numbers 16, 20, 28, 40 and 60 (64). The question then arises whether it is possible to reproduce theoretically the potential energy surfaces suggested by the experimental spectra.

Instead of summing single-particle energies as a function of distortion Swiatecki and Strutinsky have advocated a normalization of the average behaviour of the nuclear potential energy surface to that of the liquid-drop model. Following Strutinsky [12] we calculate the shell energy

$$E_{sh} = \sum e_v - \sum e_v$$

and the pairing and liquid-drop energies according to Myers and Swiatecki [13]. Pairing is calculated as described in Nilsson et al. [6] and more specifically for the Zr-region Ragnarsson [14].

For nuclei with $Z, N \approx 20$, pairing has completely been neglected. For the κ and μ-values we have assumed [15] $\kappa_p = \kappa_n = 0.08$, $\mu_p = \mu_n = 0$. The resulting total energy for ${}^{32}_{16}S_{16}$ is shown in fig. 8 as are the liquid-drop and the shell energies. The calculations in this case appear to bear out the empirically founded suggestions in the preceding section. Just as expected we have a secondary minimum a little less than 4 MeV above the ground state at a corresponding deformation of $\epsilon \approx 0.6$ ($\epsilon_4 \approx 0.10$).

Turning to ${}^{40}_{20}Ca_{20}$ (fig. 7b) we find that with the parameters above there is no secondary minimum at prolate deformations smaller than $\epsilon = 0.7$. For $\epsilon = 0.6$ there is just an inflection point about 20 MeV up in energy. The main reason is that with these κ- and μ-values, fitting the $A \approx 25$ region, the spherical 20 nucleon gap comes out much too large, and this means

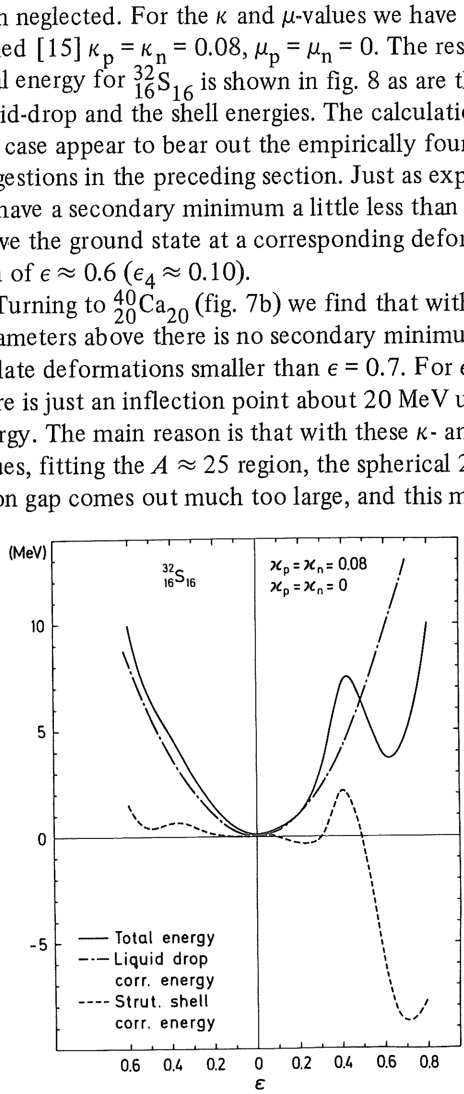

Fig. 8. Liquid-drop, shell correction and total energies as a function of ϵ for ^{32}S. The shape parameter ϵ_4 has been included and the total and liquid-drop energies have been minimized with respect to ϵ_4 for each ϵ. The shell correction has been drawn for the same ϵ_4-values as the total energy.

that the very deep spherical minimum is too dominating. If we consider instead the somewhat differer ly parameterised modified oscillator used in the calc lations of Metag et al. [16], a secondary minimum f ^{40}Ca is obtained at about the right energy. The parameterisation involves $l \cdot s$ coupling (which is differ ent for different spherical shells) and a finite l^2 term This makes the spherical 20 nucleon gap much smaller. Metag et al. obtain their secondary minimu for ^{40}Ca for a deformation corresponding to $\epsilon = 0.4$ however, their shell correction energy has its minim at $\epsilon = 0.6$. It is just the competition between the liq uid-drop and the shell correction which places the t tal energy minimum at a smaller deformation. Using the parameter of Metag et al. we calculate a secondary minimum for ^{32}S at $\epsilon = 0.6$ while maximal shell correction occurs at $\epsilon = 0.7$. However, for this parameter choice the minimum is calculated about 6.5 MeV above the ground state which is somewhat less consistent with experiment. Probably a third set of (κ, μ)-values could combine the advantages of the (κ, μ)-values of these calculations with those of Met et al.

No calculations of the total energy have been made for ^{56}Ni and we therefore turn immediately t the Zr- and Mo-isotopes. It should be said at once, that we have not succeeded in getting the energy su faces suggested by the above interpretation of the d ta and the simple harmonic oscillator scheme ($\kappa = \mu$ The main difficulty is that the liquid-drop energy su face rises too steeply for the larger deformations fo this region of nuclei to allow any secondary minima Indeed the liquid-drop energy is about 17.5 MeV fo $\epsilon = 0.6$, $\epsilon_4 = 0$ and 14.5 MeV for $\epsilon = 0.6$, $\epsilon_4 = 0.08$ an about 4.0 MeV for $\epsilon = 0.3$, $\epsilon_4 = 0$.

This implies that, if we expect to get the ground state at a deformation $\epsilon = 0.6$ for neutron excess Zr and Mo nuclei, then shell energies must be greater than 10–12 MeV (assuming a small negative shell c rection of about 2–4 MeV for approximately spher cal shapes). However, fig. 2 indicates that for 40 pro tons and 60 neutrons the shell energies cannot be greater than ~4 and ~6 MeV respectively, and, in fact, with realistic single-particle potentials like tho of figs. 3 and 4 will always be less than this. A great deal of effort has gone into the problem of maximizing shell energies for Zr and Mo isotopes. For ex ample, comparison of $\epsilon_4 = 0$ and $\epsilon_4 = 0.08$ in fig. 4

suggests that for ϵ_4 slightly larger than the 62 nucleon gap considerably increases in size. The possibilities of shell effects from ϵ_3 and ϵ_5 deformation and of somewhat smaller ϵ-deformation have also been considered. In the end we can hardly avoid the conclusion that using the Strutinsky method and the liquid-drop as presently formulated it is impossible to obtain two sets of minima – a ground state minimum at $\epsilon \approx 0.6$ and an isomeric minimum at $|\epsilon| \leqslant 0.3$ for any nuclei in the vicinity of $^{100}_{40}$Zr.

This dilemma would appear to present a considerable challenge to nuclear theory and perhaps requires a drastic solution. We have not mentioned the possibility that the Strutinsky method gives a large systematic error particularly for lighter nuclei. In view of the success in other regions and of the good agreement with shell energies for $100 \leqslant N \leqslant 140$ with the temperature method [17], this possibility seems somewhat remote.

A second drastic possibility is that the liquid-drop energy must be considerably altered. For a low-lying secondary minimum to occur in this region, a much weaker liquid-drop energy would be required. Indeed, the gamma induced fission experiments of Methasiri and Johansson [18] may be taken to indicate a reduction relative to theoretical predictions in liquid-drop barrier heights in the A = 50–140 region by 20 MeV or more. This suggests a modification in the liquid-drop parameters that goes far beyond the recent suggestions [19, 20], of a change in the charge radius and surface symmetry coefficient of the Myers-Swiatecki liquid-drop parameters. The lâtter modifications would affect the barrier by at most 1 MeV each at ϵ=0.6. Johansson [21] suggests on the basis of the results of ref. [18] a considerable lowering of the total surface energy term, emphasising that the deformation dependent surface energy term, which is the "true" surface energy, might differ substantially, particularly as to its isospin dependent part, from the $A^{2/3}$ term in the semi-empirical mass formula.

We believe that the experimental evidence for deformed shells at ϵ = 0.6 is compelling, that potential energy surface calculations following the conventionally used shell correction method support this eicidence for A = 32 to 40 regions but their failure in the Zr and Mo regions stands as a considerable theoretical challenge.

We are grateful to Professors Aage Bohr and Ben Mottelson for use prior to publication of Vol. II of their book, Nuclear Structure, and for discussions which have been so instrumental in the conduct of the research. Of equal stimulation has been the exchange of ideas with Professor Sven Johansson on the applicability of the liquid-drop model in the mass region in question. The superb draftmanship of Mr. Lennart Nilsson is highly appreciated. One of us (R.K.S.) is grateful for the award of a Nordita Professorship and the hospitability of the Department of Mathematical Physics of the Lund Institute of Technology and Nordita in Copenhagen.

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