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# ON THE UNCERTAINTIES IN THE *SHELL CORRECTION* BY STRUTINSKY SMEARING PROCEDURE FOR CERTAIN SHAPES RELEVANT IN FISSION

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## ABSTRACT

It is found that for level schemes obtained from a folded Yukawa potential, the Strutinsky smearing procedure for the evaluation of the shell correction to the total potential energy of nuclei does not lead to a unique value for nuclear shapes near and beyond the outer fission barrier deformations and consequently introduces uncertainties in the relative fission barrier heights.

# ON THE UNCERTAINTIES IN THE SHELL CORRECTION BY STRUTINSKY SMEARING PROCEDURE FOR CERTAIN SHAPES RELEVANT IN FISSION

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In the last few years numerous calculations of nuclear deformation potential energy surfaces have been carried out on the basis of the now well known macroscopic-microscopic approach developed by Strutinsky[1], which have been recently reviewed in references (2-4). In this approach, the total potential energy of the nucleus is assumed to consist of a major part which varies smoothly with respect to nucleon number and deformation, and a small residue called the shell correction energy term, whose value depends on the local fluctuations in the single particle energy level density near the Fermi level as calculated from a given shell model energy level scheme. The nuclear potential energy is therefore obtained by calculating the shell correction energy starting from a single particle level scheme for the relevant nuclear shape, and then adding this energy to the smoothly varying part calculated from a macroscopic model such as the liquid drop model. These calculations with suitably extrapolated single particle level schemes for deformed shapes, have led to the predicted existance of a secondary minima in the deformation potential energy for nuclei in the actinide region. These calculations have also predicted sizeable fission barriers for nuclei in the superheavy region due to the inclusion of shell correction energies.

Most of these calculations have been carried out on the basis of Strutinsky smearing procedure[1], for the calculation of the shell correction energy. This procedure involves the generation of a smooth single particle level density $\tilde{g}(\epsilon)$, from a discrete one:

$$g(\epsilon) = \sum_i \delta(\epsilon - \epsilon_i) \qquad (1)$$

by the following relation;

$$\tilde{g}(\epsilon) = \frac{1}{\sqrt{\pi}\,\gamma} \sum_i \exp - \left(\frac{\epsilon - \epsilon_i}{\gamma}\right)^2 f_p\left(\frac{\epsilon - \epsilon_i}{\gamma}\right) \qquad (2)$$

Where $\gamma$ is the smearing width, $\epsilon_i$ are the energy levels of the single particle spectra and $f_p(\epsilon - \epsilon_i/\gamma)$ is a polynomial of degree p (even only) which provides the curvature corrections.

Having obtained $\tilde{g}(\epsilon)$, the shell correction is obtained by the following relation:

$$\delta U(N,\delta) = \sum_{i=1}^{N} \epsilon_i(\delta) - \int_{-\infty}^{\lambda} \tilde{g}(\epsilon)\,\epsilon\, d\epsilon \qquad (3)$$

where '$\lambda$' is the Fermi energy which is determined by the nucleon number conservation:

$$N = \int_{-\infty}^{\lambda} \tilde{g}(\epsilon)\, d\epsilon \qquad (4)$$

and '$\delta$' is a suitable deformation parameter. In order that this method gives a unique value of the shell correction energy, it is required that the shell corrections be independent of the values of the non-physical parameters $\gamma$ and p over a suitably selected range of values of these parameters. This plateau condition has been shown to be satisfied for values of $\gamma$ around a value equal to the spacing between the major shells with a sixth order corrective polynomial for the cases of nuclear shapes in the neighbourhood of ground state deformations studied in detail by earlier workers[2,4], and the calculations of the potential energy in the past have therefore assumed the fulfilment of this condition as a general feature of the Strutinsky prescription[5]. It has however been found that in specific cases the above plateau condition is not satisfied[6,7]. Brack and Pauli have proposed an alternate stationary condition in its place which requires that the shell correction energy be evaluated at a value of $\gamma = \gamma_c$, such that

$$\frac{\partial}{\partial \gamma}\left(\delta u\right)_{\gamma=\gamma_c} = 0 \qquad (5)$$

where $\delta u$ is the shell correction energy.

The stationary condition also demands the stationarity with respect to the curvature correction order p, so that

$$\delta u\left(p, \gamma_c(p)\right) = \delta u\left(p+2, \gamma_c(p+2)\right) \qquad (6)$$

With these modifications the maximum uncertainty in the evaluated shell correction energy has been reported to be around $\pm$ 0.3 MeV[6].

We have carried out a detailed study of shell corrections obtained by the Strutinsky method in order to examine the uncertainties in the calculated shell corrections for all the nuclear shapes relevant for fission barrier calculations. The single particle level schemes used are those of Nix and co-workers[6] calculated for the folded-Yukawa potential for various nuclear shapes represented by the symmetric deformation parameter "Y" and the mass-asymmetric parameter "$\alpha_2$" which are defined in ref.[8]. These level schemes in addition to the bound levels include levels in the continuum upto single particle energies of 18-19 MeV, the total number being one hundred and forty six in the case of protons and two hundred and fifty in the case of neutrons. The numerical calculation of the shell correction energy was carried out by the Strutinsky smearing method for values of $\gamma$ in the range of 2 to 20 MeV and for p = 4, 6 and 8. The results of these calculations for the single particle proton and neutron levels in $Pu^{240}$ are shown in Figs. 1 and 2 respectively for the various nuclear shapes represented by the symmetric deformation parameter Y. Figs. 3 and 4 show the results of calculations for the same values for the proton and neutron levels corresponding to the outer barrier deformation for various mass asymmetric shapes $\alpha_2$. Also shown in the figures by vertical lines are the values of the shell correction energy corresponding to $\gamma$ = 7 MeV and p = 6, which have been used earlier[8] for the calculation of fission barriers. The results of the present calculations for $\gamma$ = 7 MeV and p = 6 are found to be in complete agreement with those of ref.[8], providing a check on our computer-programme.

It is seen from Figs. 1-4 that the plateau is not fulfilled for several nuclear shapes in the region of outer barrier deformation. It is to be further noted that the stationary condition suggested by Brack et al[6] also does not lead to a unique value of the shell correction energy in most of these cases. In the framework of the Strutinsky procedure, neither the plateau condition nor the stationary condition leads to a unique value of the shell correction energy for the cases of symmetric proton levels corresponding to $Y = 0.22$ to 0.30, symmetric neutron levels corresponding to $Y = 0.22$ and $Y = 0.24$, for asymmetric proton levels corresponding to $\alpha_2 = 0$ to 0.20, and for asymmetric neutron levels corresponding to $\alpha_2 = 0$ to 0.40. In all these cases, the density of the single particle levels near the Fermi level is significantly higher than the average, and therefore the failure of (both) the plateau condition and the stationary condition to give a unique value of the shell correction energy appears to be related with this strong bunching of levels near the Fermi level.

We have also carried out the above calculations for different nucleon numbers at a few typical deformations near the symmetric second barrier. Fig. 5 and 6 show these results for the proton numbers Z = 84 to 102 and neutron numbers N = 136 to 154 for the deformation characterised by Y = 0.24 and $\alpha_2 = 0$. Figs. 7 and 8 show similar results for the deformation characterised by Y = 0.26 and $\alpha_2 = 0$. It is seen that the failure of the plateau condition and the stationary condition is not limited to the specific case of $_{94}Pu^{240}$, but is a general feature for all nucleon numbers in this region.

It is seen that whenever the shell correction is negative or near zero, the plateau criterion can be successfully applied and a unique value of the shell correction can be obtained. However for large positive shell corrections, the failure of both the plateau condition and the stationary condition is marked and no unique value of the shell correction can be obtained. This feature is clearly evident from Fig. 8, where with increasing nucleon numbers the shell correction can be seen to slowly go over to large positive values where the failure is particularly marked.

On the basis of these calculations, we emphasize that for any quantitative calculations of the fission barrier heights it is necessary to establish the uncertainty in the shell corrections obtained by the Strutinsky method for all relevant shapes. It is further pointed out, that for the level scheme used in this work, the height of the outer for mass-symmetric nuclear shapes is not uniquely determined by the Strutinsky smearing procedure, with the result that one cannot draw definite conclusions regarding the relative heights of the mass-symmetric and the mass asymmetric barriers at the outer barrier shapes. These uncertainties may become critical in any dynamic calculation involving the full deformation potential energy surface.

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REFERENCES

(1) V.M. Strutinsky, Nucl. Phys. A95 (1967) 420

(2) J.R. Nix, Ann. Rev. Nucl. Sci. 22 (1972) 65

(3) M. Brack, J. Damgaard, A.S. Jensen, H.C. Pauli, V.M. Strutinsky and C.Y. Wong, Rev. Mod. Phys. 44 (1972) 320

(4) P. Moller and J.R. Nix, Proc. IAEA Symp. Phys. Chem. Fission, 3rd Rochester, 1973 Vol I, 103, IAEA, Vienna

(5) P. Moller and J.R. Nix, Proc. IAEA Symp. Phys. Chem. Fission, 3rd Rochester, 1973, Vol I, P 141, IAEA, Vienna (Discussion)

(6) M. Brack and H.C. Pauli, Nucl. Phys. A207 (1973) 401

(7) R.R. Chasman, Phys. Rev. Lett. 33 (1974) 544

(8) M. Bolsterli, E.O. Fiset, J.R. Nix and J.L. Norton, Phys. Rev. 05 (1972) 1050. J.R. Nix (Private Communication, 1971).

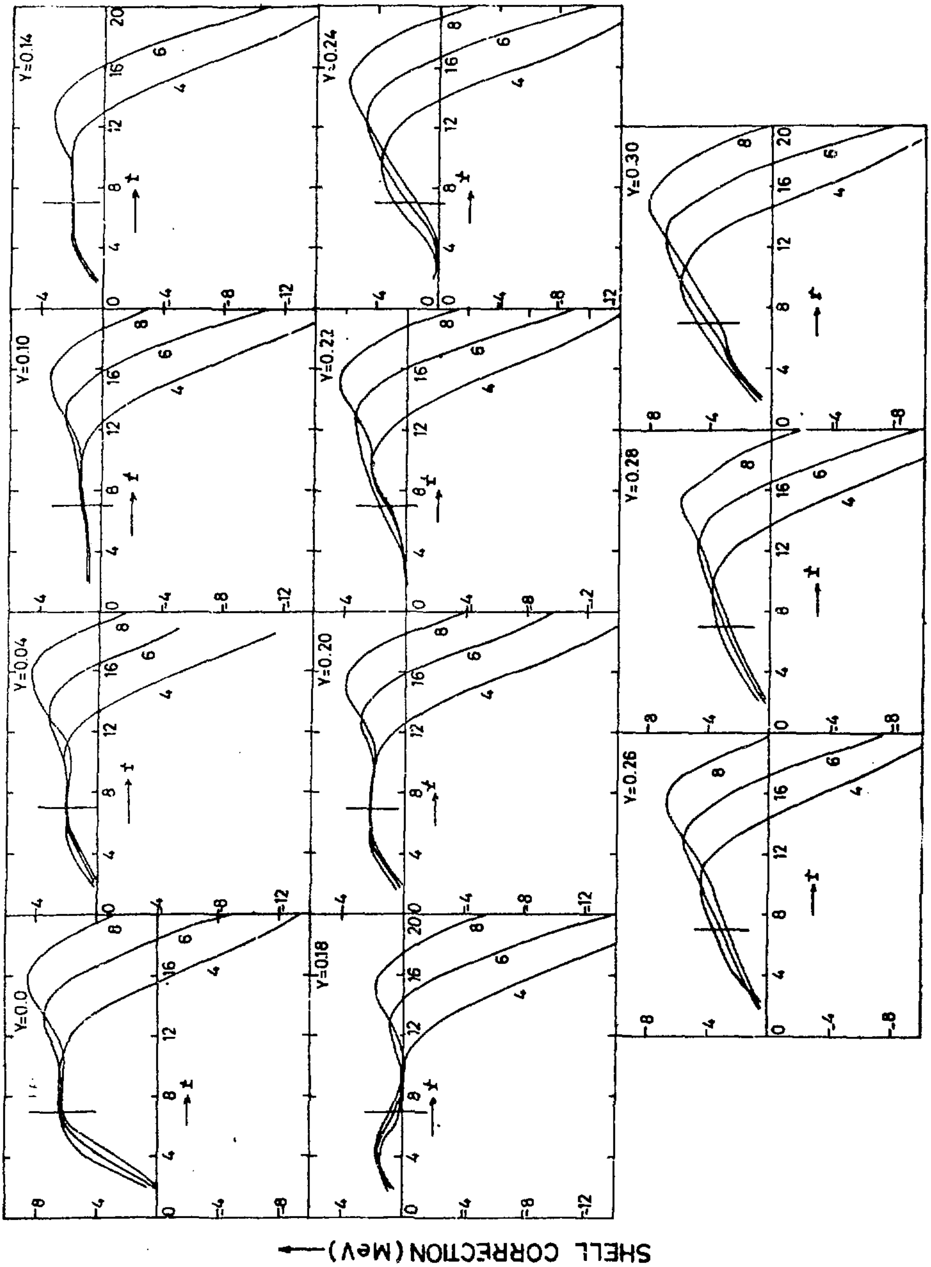



Fig. 1. Calculated shell corrections "$\delta u$" for protons in $_{94}Pu^{240}$ as a function of the smearing parameter ' $\gamma$ ' and order of polynomial 'p'. Results are shown for different values of the mass symmetric deformation parameter 'Y'. The levels used are those generated by Nix for a realistic folded Yukawa potential.

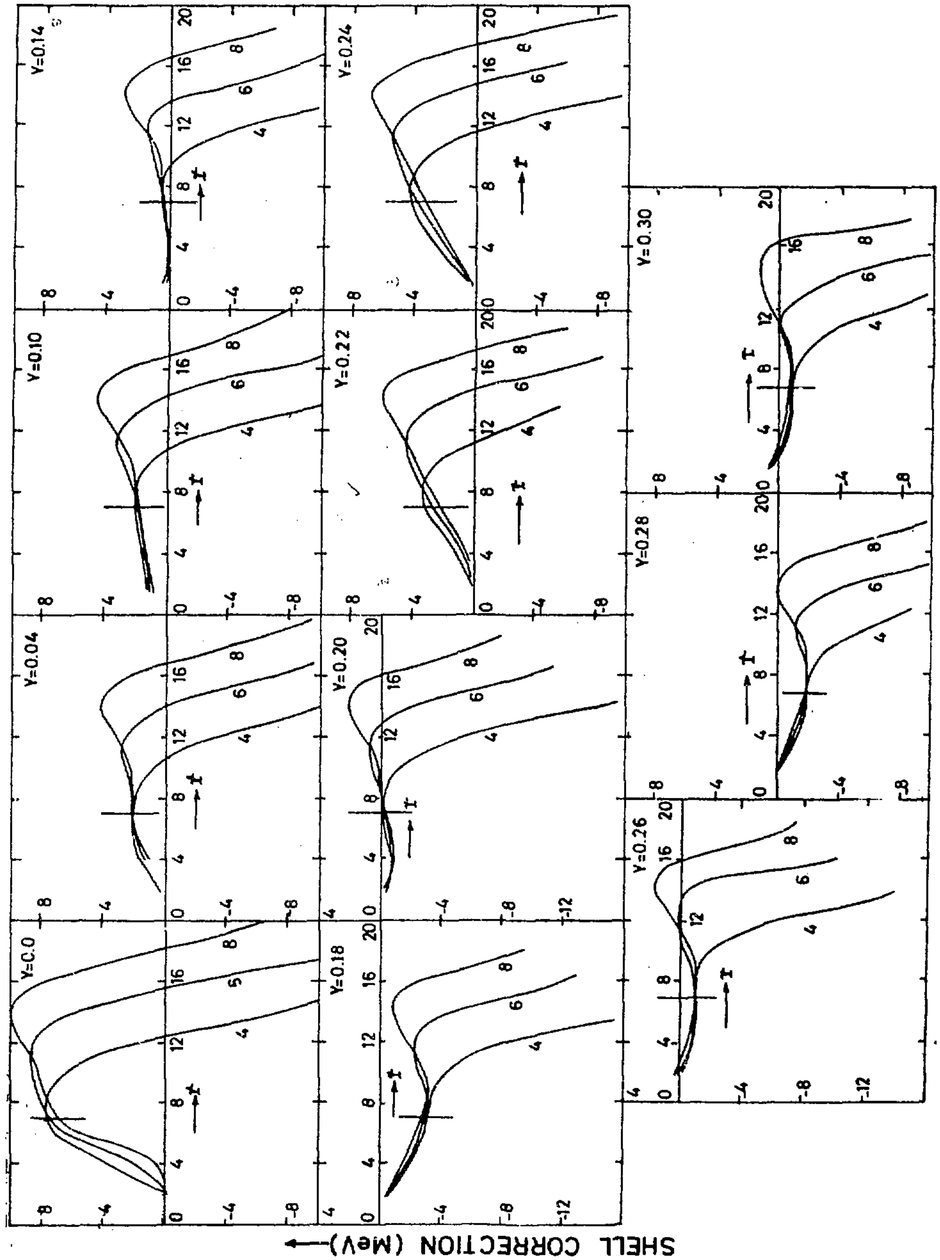



Fig.2. Calculated shell corrections "$\delta u$" for neutrons in $_{94}Pu^{240}$ as a function of the smearing parameter ' $\gamma$ ' and order of polynomial 'p'. Results are shown for different values of the mass symmetric deformation parameter 'Y'.

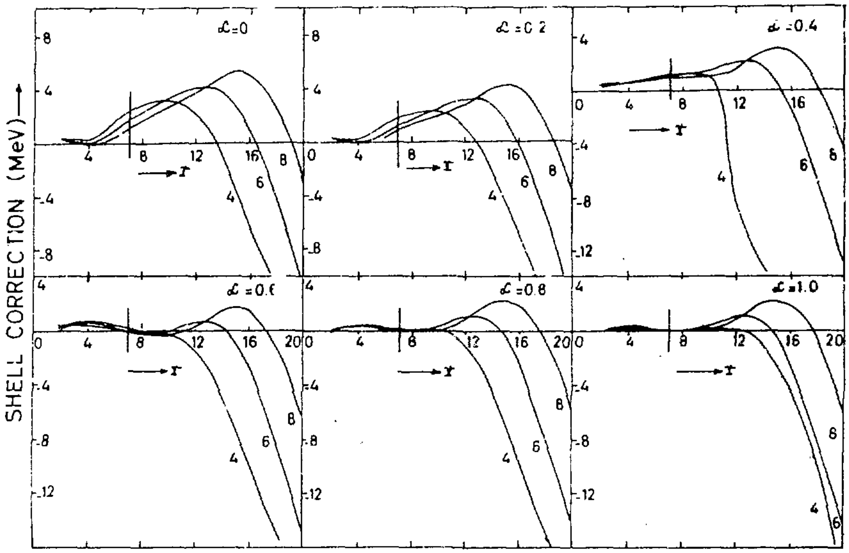



Fig. 3. Calculated shell corrections "$\delta u$" for protons in ${}_{94}Pu^{240}$ as a function of smearing parameter '$\gamma$' and order of polynomial 'p'. Results are shown for different mass asymmetric deformation parameter '$\alpha_2'$'.

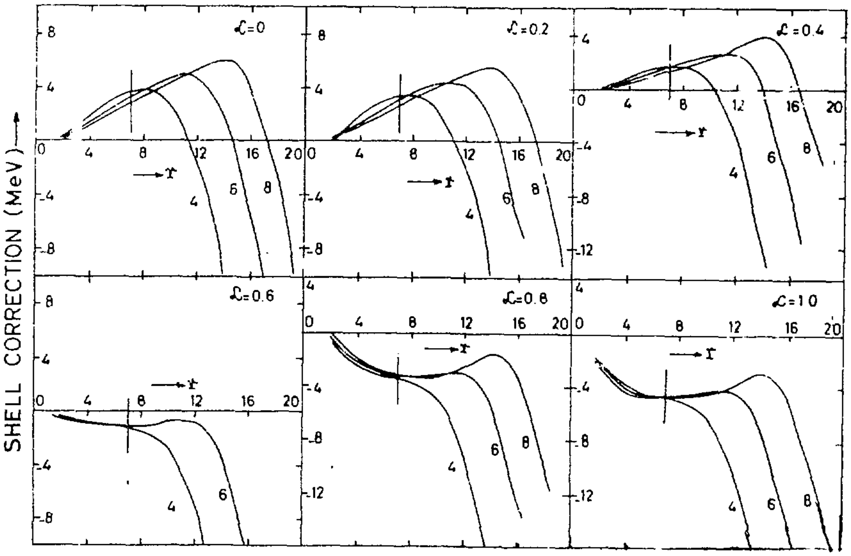



Fig. 4. Calculated shell corrections "$\delta u$" for neutrons in ${}_{94}Pu^{240}$ as a function of smearing parameter '$\gamma$' and order of polynomial 'p'. Results are shown for different mass asymmetric deformation parameter '$\alpha_2'$'.

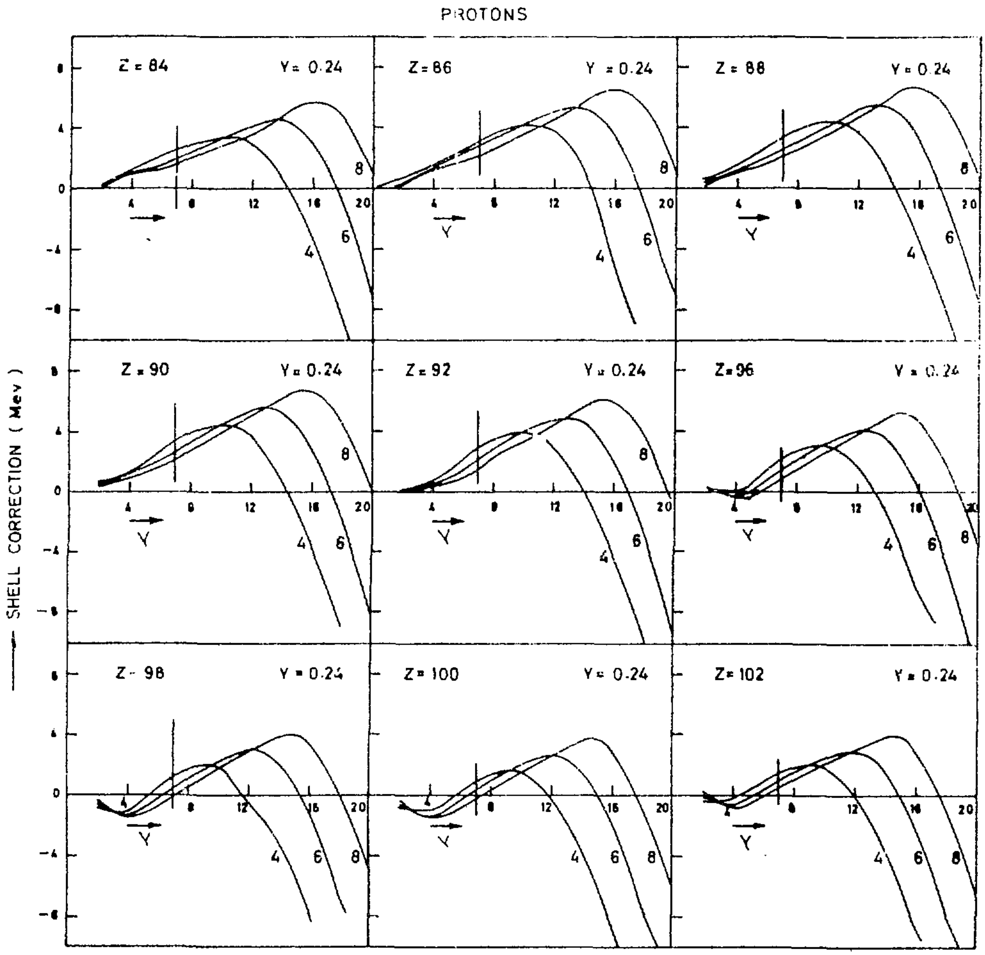
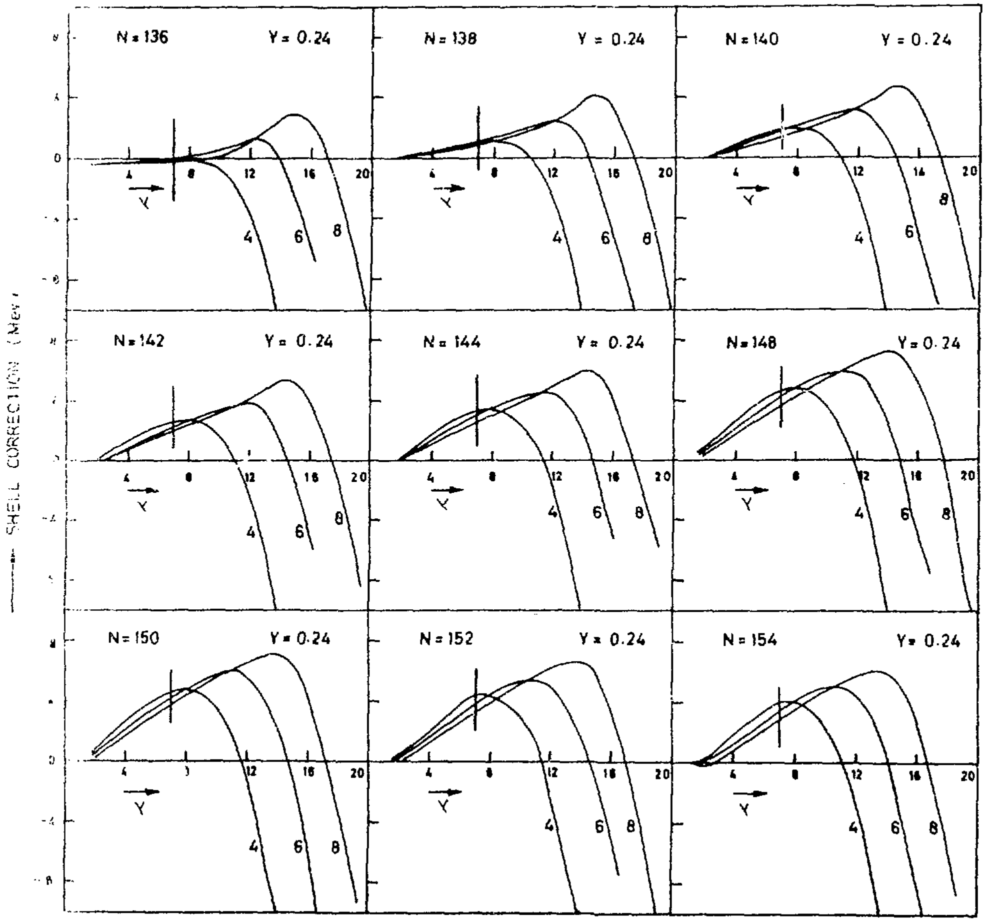



Fig.5. Calculated shell corrections "$\delta u$" as a function of smearing parameter ' $\gamma$ ' and order of polynomial 'p'. Results are shown for different proton numbers at the mass symmetric deformation parameter Y = 0.24.

NEUTRONS




Calculated shell corrections "$\delta u$" as a function of smearing parameter '$\gamma$' and order of polynomial 'p'. Results are shown for different neutron numbers at the mass symmetric deformation parameter Y = 0.24.

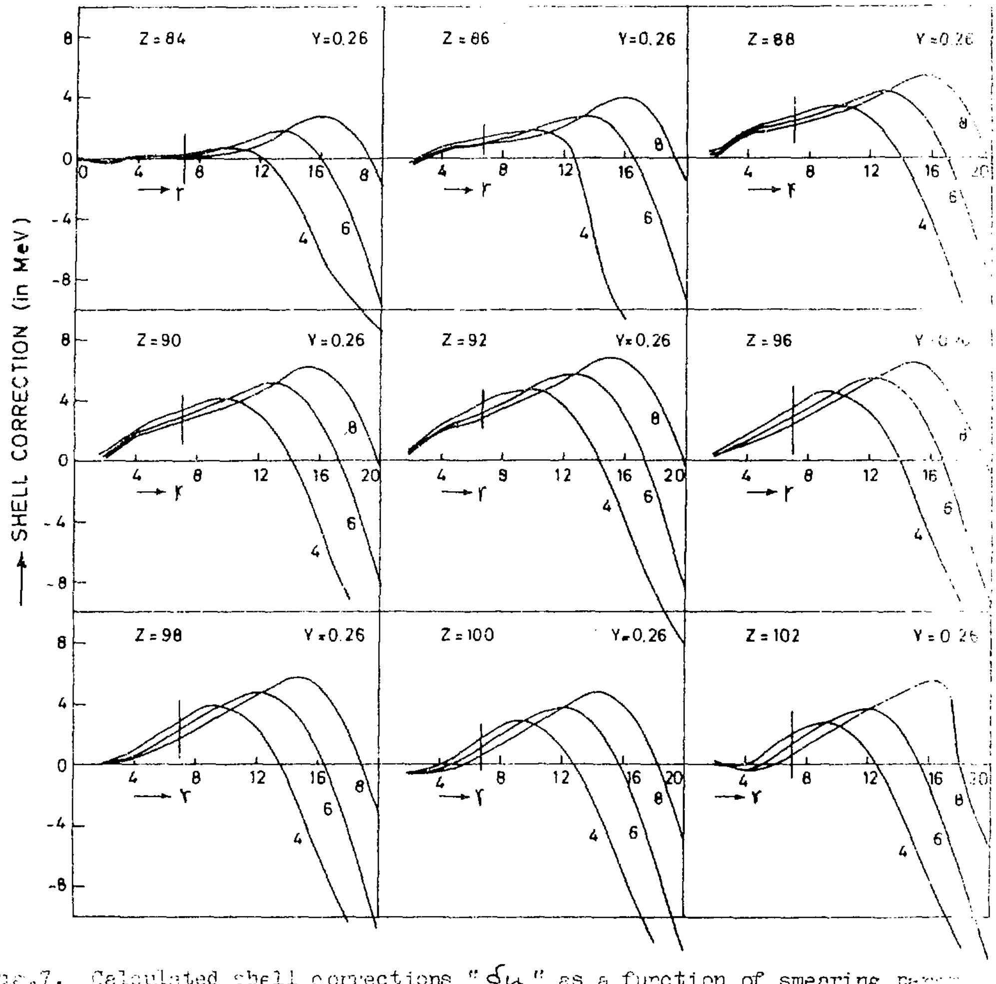



Fig.7. Calculated shell corrections "$\delta u$" as a function of smearing para- ' $\gamma$ ' and order of polynomial 'p'. Results are shown for different proton numbers at Y = 0.26.

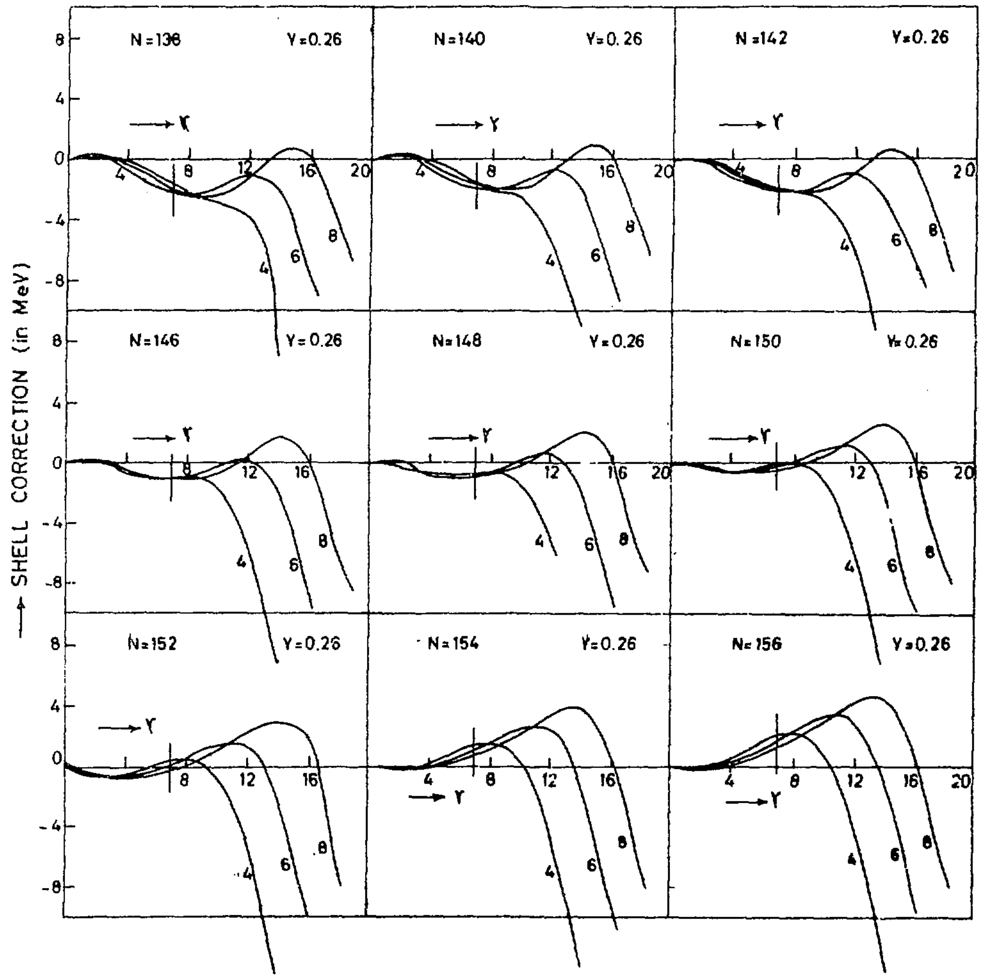



Fig. 8. Calculated shell corrections "$\delta u$" as a function of smearing parameter '$\gamma$' and order of polynomial 'p'. Results are shown for different neutron numbers at Y = 0.26.