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Remarks on the nuclear shell-correction method*

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Abstract. It is shown that the nuclear single-particle energy spectra obtained in the selfconsistent way obey similar particle number dependence as the spectrum of a pure 3D harmonic oscillator potential. This effect was used to improve the quality of evaluation of the shell correction energy in weakly bound nuclei. The magnitude of the traditional Strutinsky shell correction energy obtained by the smearing of the single-particle energy spectrum of light nuclei is compared with that obtained by the smoothing of the single-particle energy sums in the particle number space.

1 Introduction

The fifty years old macroscopic-microscopic model [1–4] in which one adds the shell and the pairing energy corrections to the macroscopic binding energy, evaluated *e.g.* using the liquid drop model, is still frequently used as an alternative to the time-consuming HFB calculations.

The shell correction method developed in ref. [5] offers an effective tool to extract the shell and pairing effects from the microscopic energy obtained in a selfconsistent way or by using a mean-field single-particle Hamiltonian, *e.g.* of the Saxon-Woods or Yukawa-folded type. Contrary to the traditional Strutinsky method [2–4], the shell energy is evaluated in ref. [5] by an averaging over the number of particles and not over the single-particle energies. This new approach is more consistent with the definition of the macroscopic energy. In addition, the smooth background was subtracted in [5] before averaging the sum of single-particle energies, which significantly has improved the plateau condition and has allowed to apply the method also for nuclei close to the proton or neutron drip lines.

A significant difference between the shell correction energy obtained with the traditional and the new method was found in particular for highly degenerated single-particle spectra (*i.e.* in magic nuclei) while for deformed nuclei, where the degeneracy is lifted to a large extent, both estimates are close to each other, except the region of super or hyper-deformed shape isomers. The difference between the smoothed energies evaluated using the traditional Strutinsky and the new method may be used as an effective tool for searching the quasi-magic numbers which may appear in deformed nuclei or in their shape isomers [6]. Our method allows also to extract the average smooth energy of a nucleus with pairing correlations [7] or from hot nuclei [8].

In the present paper we compare the estimates of the shell energy obtained in both methods using the single-particle spectra obtained within the selfconsistent HFB model with the Gogny D1S force.

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2 Harmonic oscillator spectrum

Let us begin with a recollection of some properties of the spherical harmonic oscillator (HO) Hamiltonian. Its eigenenergies

$$e_N = \left(N + \frac{3}{2}\right)\hbar\omega_0 \qquad (1)$$

are enumerated by the number of the oscillator quanta $N = 0, 1, 2, \ldots$ and its eigenstates are strongly degenerated

$$\deg_N = \frac{1}{2}(N+1)(N+2)\times 2\,, \qquad (2)$$

where factor two origins from the two orientations of spin. ω_0 is here the HO frequency. The total number of particles $n(N)$ which occupy all shells from 0 up to N is equal to

$$n(N) = \sum_{k=0}^{N} \deg_k = \frac{1}{3}(N+1)(N+2)(N+3)\,. \qquad (3)$$

The last equation can be approximated in the following way [9]:

$$n(N) \approx \frac{1}{3}\left(N+\frac{3}{2}\right)^3 = \frac{1}{3}\left(\frac{e_N}{\hbar\omega_0}\right)^3 . \qquad (4)$$

what leads to an approximative relation between the single-particle energy e and the number of particles which occupy all levels with energy smaller or equal to e

$$n(e) = \frac{1}{3}\left(\frac{e}{\hbar\omega_0}\right)^3 , \quad \text{or} \quad e(n) = (3n)^{1/3}\,\hbar\omega_0 . \qquad (5)$$

This equation leads to the well-known approximative expression for the density of the HO single-particle levels:

$$\rho_{\rm app} = \frac{\partial n}{\partial e} \approx \frac{e^2}{(\hbar\omega_0)^3} = \frac{(3\,n)^{2/3}}{\hbar\omega_0} . \qquad (6)$$

The sum E of single-particle energies of all occupied levels up to the shell N

$$E = \hbar\omega_0 \sum_{k=0}^{N}\left(k+\frac{3}{2}\right)(k+1)\,(k+2) \qquad (7)$$

can be approximated by the following expression [5]:

$$\overline{E} = \frac{1}{4}(3n)^{4/3}\hbar\omega_0 . \qquad (8)$$

The difference $\delta E = E - \overline{E}$ between the exact sum of the HO single-particle levels E and its approximation $\bar{E}$ is plotted in fig. 1 as a function of the particle number $n^{1/3}$. The deep minima in this difference correspond to the closed HO shells. Using the approximation (4) one can show that asymptotically the distance in the $n^{1/3}$ coordinate between the subsequent closed shells goes to $\gamma_0 = 3^{-1/3}$. This result suggests that one can apply the Strutinsky procedure [2–4] to evaluate the smoothed part of the single-particle energy sum not only by smearing in the s.p. energies but also in the particle number coordinate $n^{1/3}$ [5].

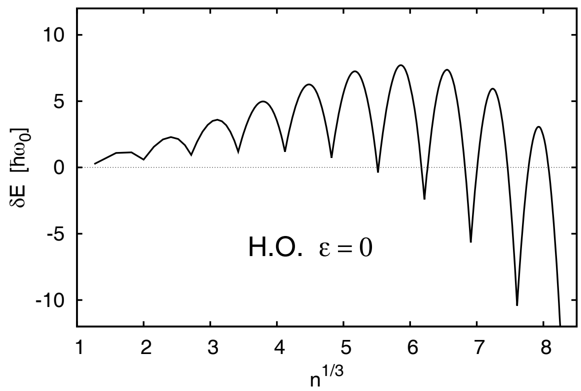

Fig. 1. Sum of the spherical HO single-particle energies after subtracting its average dependence as a function of $n^{1/3}$, where n is the particle number.

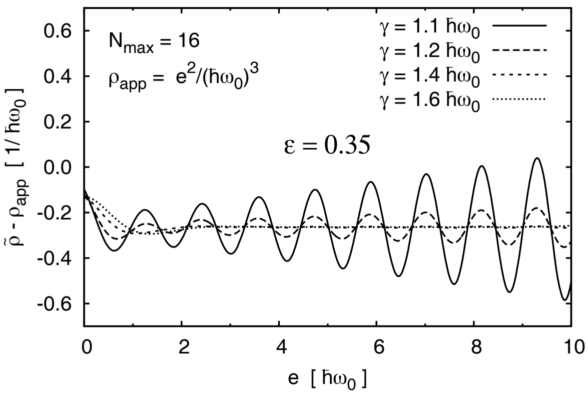

Fig. 2. Deviation of the single-particle density smoothed with different smearing parameters γ from its approximative behaviour ($\rho_{\rm app}$) as a function of the single-particle energy. The plot is made for the anisotropic harmonic oscillator spectrum at the deformation parameter $\varepsilon = 0.35$.

3 Strutinsky smoothing of the single-particle energy spectrum

Strutinsky has proposed to wash out the shell effects by using the folding function in the form of the Gauss function multiplied by the so-called correctional polynomial [10]:

$$\xi(x) = \frac{1}{\sqrt{\pi}} e^{-x^2} \sum_{k=0,2}^{2m} a_k H_k(x) , \qquad (9)$$

where $H_k(x)$ are the Hermite polynomials and $2m$ is the order of the correction polynomial. The coefficients a_k, where $k \geq 2$, are given by the following recurrence relation:

$$a_k = -\frac{1}{2k}\,a_{k-2} \quad \text{with} \quad a_0 = 1 . \qquad (10)$$

In the most applications of the Strutinsky method one uses the correction polynomials of the 6th or 8th order.

In the Strutinsky shell correction method one evaluates first the smooth single-particle level density $\widetilde{g}(e)$ by folding the discrete spectrum of eigenstates of a single-particle Hamiltonian e_i

$$\rho(e) = \sum_i \delta(e-e_i) , \qquad (11)$$

with a smoothing function (9)

$$\widetilde{\rho}(e) = \int_{-\infty}^{\infty} \xi\left(\frac{e-e'}{\gamma}\right)\rho(e')\mathrm{d}e' = \sum_i \xi\left(\frac{e-e_i}{\gamma}\right) . \qquad (12)$$

Here γ is the smearing width which should be comparable with the major shell distance in the harmonic oscillator. The influence of the smearing width on the smooth single-particle level density can be seen in fig. 2. The HO level density evaluated using four different values of γ is plotted as a function of the energy. All single-particle levels of the deformed HO ($\varepsilon = 0.35$) from the major shell up

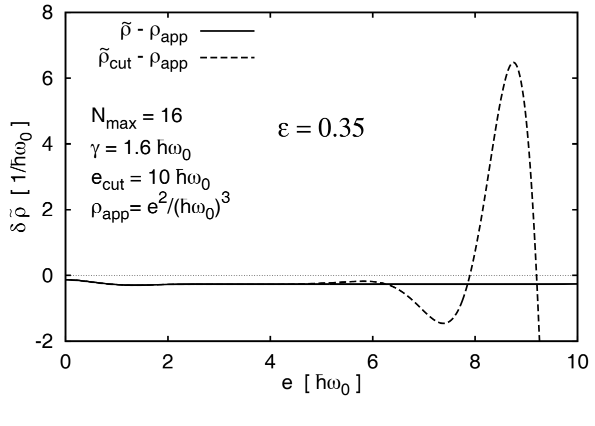

Fig. 3. Smoothed single-particle level density ($\tilde{\rho}$) of the deformed HO compared to its approximation ($\rho_{\rm app}$) and the smooth density ($\tilde{\rho}_{\rm cut}$) obtained with the truncated energy spectrum at the cut-off energy $e_{\rm cut} = 10\,\hbar\omega_0$.

to $N_{\max} = 16$ were taken into account in the calculation. The approximative value of the density (6) was subtracted from the smoothed density $\tilde{\rho}$ in order to see its tiny oscillations which appear when $\gamma < 1.4\,\hbar\omega_0$. Note that at $e = 0$ the smoothed density $\tilde{\rho}(0) \neq 0$.

In practical applications of the Strutinsky smoothing method one has to work with single-particle spectra which are well defined up to a given energy, which one calls usually the cut-off energy $e_{\rm cut}$. The influence of the value of the cut-off energy on the smooth single-particle level density $\tilde{\rho}$ is presented in fig. 3, where the density evaluated with the infinite spectrum of the deformed HO ($\tilde{\rho}$, solid line) and the density ($\tilde{\rho}_{\rm cut}$, dashed line) obtained with the artificially cut of the HO spectrum at the energy $e_{\rm cut} = 10\,\hbar\omega_0$ are plotted as functions of the energy e. The smoothing width $\gamma = 1.6\,\hbar\omega_0$ is taken here. We have subtracted the average HO density ρ_{app} from both densities in order to observe better the cut-off effect. The effect of the cut-off is visible already at energies higher than $e_{\rm cut} - 3\gamma$. The large sensitivity of the smooth density on the cut-off energy is one of the weak points of the traditional Strutinsky shell correction method and it makes problems when one applies this method to weakly bounded nuclei near the proton or neutron drip lines.

According to the Strutinsky prescription [2–4] the smoothed energy sum of the occupied single-particle levels ($E^{\rm old}_{\rm Str}$) is given by the integral

$$E^{\rm old}_{\rm Str} = \int_{-\infty}^{\lambda} 2\, e\, \widetilde{g}(e)\, {\rm d}e\,, \qquad (13)$$

where λ is the position of the Fermi energy given by the particle number conservation condition

$$\mathcal{N} = \int_{-\infty}^{\lambda} 2\, \widetilde{g}(e)\, {\rm d}e\,. \qquad (14)$$

Here the average number of particles $\mathcal{N}$ is equal to Z for protons or N for neutrons. The factor two in the above equations reflects the spin degeneracy of the single-particle levels.

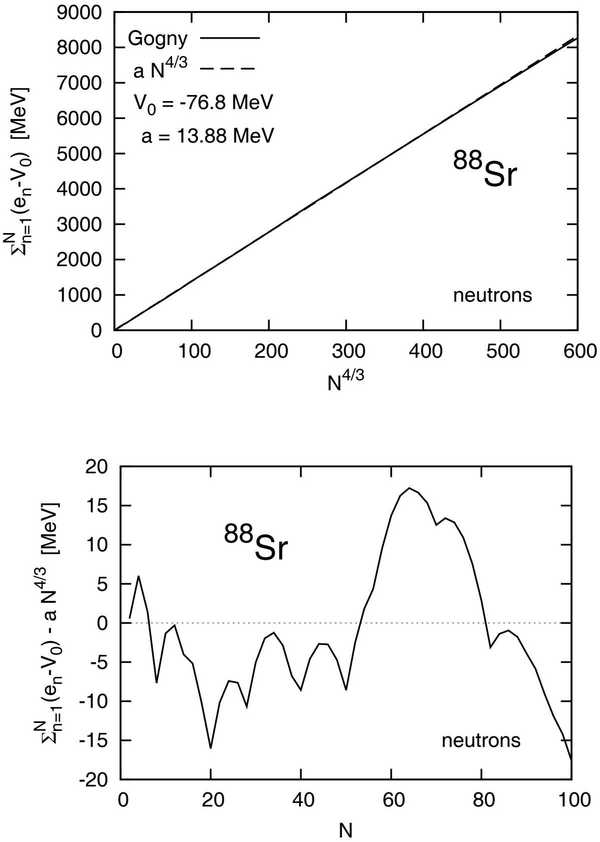

Fig. 4. Sum of the Gogny neutron single-particle energies of ^{88}Sr as a function of particle number $N^{4/3}$ (upper panel). The straight dashed line corresponds to the HO approximation (15). The deviation of the single-particle energies sum from its HO approximation is plotted in the bottom panel as a function of the neutron number N.

4 Smoothing in the particle number space

An alternative way of obtaining of the smooth single-particle energy sum is the folding in the particle number space, namely in the $n^{1/3}$ coordinate [5]. Let us take a discrete sample of data S_n defined as the difference between the sum of the n occupied single-particle energies and the background energy $\overline{E}(n)$, obtained using a generalisation of the HO average energy formula (8):

$$S_n \equiv \sum_{i=1}^{n} e_i - \overline{E}(n) = \sum_{i=1}^{n} (e_i - V_0) - a\, n^{4/3}\,. \qquad (15)$$

The parameters a and V_0 are determined by the least square fit

$$\sum_{n=1}^{\mathcal{N}_{max}} S_n^2 = \min\,, \qquad (16)$$

where $\mathcal{N}_{max}$ can be chosen, *e.g.*, as the double number of occupied levels in the single-particle energy spectrum. The quality of the approximation (15) can be visible in fig. 4, where the sum of the Gogny single-particle energies of ^{88}Sr (solid line) is compared with the $N^{4/3}$ function

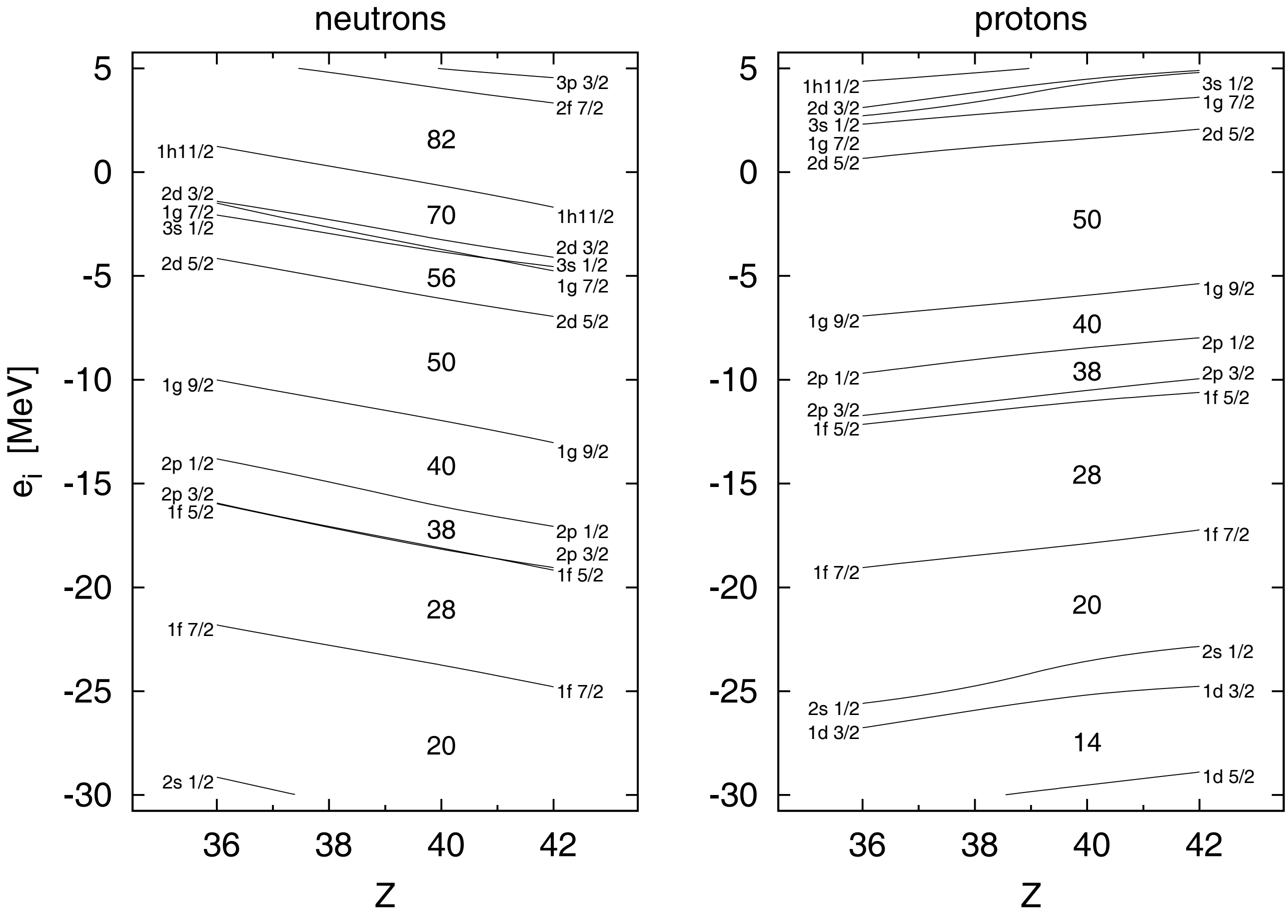

Fig. 5. Neutron and proton single-particle energy levels as a function of the proton number Z. The levels are obtained for the neutron number $N = 50$ within the HFB calculation with the Gogny D1S force.

characteristic for the HO energy spectrum. The deviation S_n (15) is plotted in the bottom panel as a function of the neutron number N.

Using the Strutinsky folding function (9) one can evaluate the smooth value of S_n corresponding to $\mathcal{N}$ nucleons

$$\widetilde{S}_{\mathcal{N}} = \frac{1}{\gamma} \sum_{n=1}^{\mathcal{N}_{max}} \frac{1}{3\,n^{2/3}}\, S_n\, \xi\left(-\frac{\mathcal{N}^{1/3} - n^{1/3}}{\gamma}\right) \tag{17}$$

The folding is performed here in the cubic root of the particle number n since the distance between the major harmonic oscillator shells is constant in $n^{1/3}$ and approximately equal to 0.7 as has been shown above. The factor $3n^{2/3}$ in the denominator of eq. (17) is the direct consequence of the transformation $n \to n^{1/3}$.

The smoothed energy obtained in this new way for even or odd $\mathcal{N}$ systems reads

$$E_{\rm Str}^{\rm new} = \widetilde{S}_{\mathcal{N}} + a\mathcal{N}^{4/3} + V_0\mathcal{N}\,, \tag{18}$$

where we have restored the background energy $\overline{E}(\mathcal{N})$, which has been subtracted before the folding from the single-particle energy sum in eq. (15).

One has to note that the subtracting of $\overline{E}(n)$ in (15) increases significantly the accuracy of evaluating the smoothed part ($E_{\rm Str}^{\rm new}$) of the energy as the deviations S_n are 2 to 3 orders of magnitude smaller than the value of $\overline{E}(n)$. The smoothed energy obtained in this way is also less sensitive to the energy cut-off of the single-particle spectrum, which is important for evaluating the shell energy of nuclei close to the proton or neutron drip lines.

5 Comparison of the both methods

It was already shown in ref. [5] that the traditional Strutinsky method based on the smoothing energies of the single-particle level density (old) and that alternative one which applies the Strutinsky smearing directly to the sum of the single-particle energies (new) lead to different estimates of the shell correction energies of spherical nuclei while both estimates are close to each other when a nucleus is deformed. The difference between both shell corrections is due to the large degeneracy of the single-particle levels which appears in spherical nuclei or in the shape isomers [5].

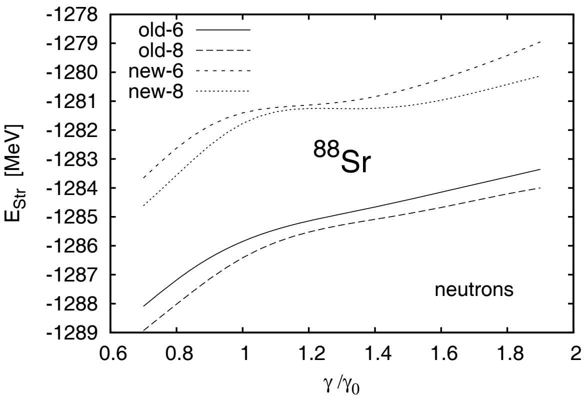

Fig. 6. Old and new Strutinsky smoothed energies of neutrons evaluated with the Gogny neutron single-particle energies of ^{88}Sr using the correction polynomials of the 6th and 8th order as functions of the smearing parameters γ. Here γ_0 is the distance between the HO shells.

Now, we would like to compare both shell correction methods in the region of light nuclei. The calculation was done using the single-particle energy spectra obtained within the HFB theory with the Gogny D1S force for a few spherical nuclei having the magic number $N = 50$ of neutrons. The neutron and proton single-particle energy spectra are shown in fig. 5 as functions of the proton number Z. The magic and semi-magic particle numbers corresponding to the close orbitals are marked in the plots. The first step, necessary in the Strutinsky method, is to check the so-called plateau condition, *i.e.* the independence of the smothed energy on the smearing width γ (see eqs. (12) and (17)). In fig. 5 the smoothed sum of the neutron single-particle energies E_{Str} of ^{88}Sr obtained using the traditional prescription (old) and the new method (new) are plotted as functions of γ/γ_0. Here γ_0 is the distance between the major HO shells equal to $\hbar\omega_0 = 41/A^{1/3}\,\mathrm{MeV}$ when the smearing is performed in the single-particle energies or $\gamma_0 = 3^{-1/3} \approx 0.7$ when one smoothes in the $n^{1/3}$ coordinate. The results are obtained using the correction polynomials of the 6th and 8th order in the folding function (9). A nice plateau in E_{Str} around $\gamma \neq 1.15\gamma_0$ is visible in fig. 6 when the new method of smoothing is applied while the plateau is not so well defined when the smoothed energy is obtained in the traditional (old) way. A similar situation occurs when the smoothed proton energy is discussed or when one applies both smearing methods to nuclei from other mass regions [5].

The proton and neutron shell energies obtained in both methods as functions of the particle number are presented in figs. 7 and 8, respectively. The constant values of the smearing width equal to $\gamma = 1.2\,\hbar\omega_0 = 11\,\mathrm{MeV}$ (or $\gamma = 0.8$) were used when the old (or new) smoothing procedure was applied. In both cases the 6th order correction polynomial was used in the folding function (9). One can learn from both figures that the proton and neutron shell energies corresponding to the magic numbers obtained by the smoothing in the particle number space (new) are shifted down by a few MeV with respect to those evaluated in the traditional way (old).

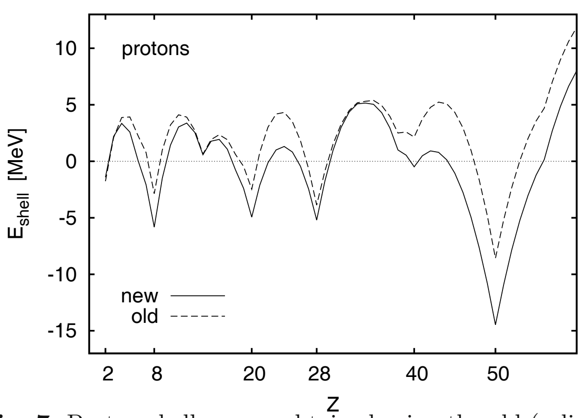

Fig. 7. Proton shell energy obtained using the old (solid line) and new (dashed line) Strutinsky smoothing procedure as functions of the proton number.

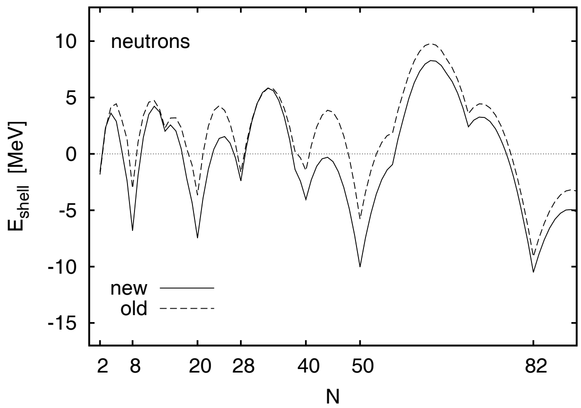

Fig. 8. The same as in fig. 7 but for neutrons.

These results mean that the new shell correction method predicts that the spherical magic nuclei, due to the large degeneracy of the single-particle levels, are more bound than it was estimated using the macroscopic-microscopic model with the traditional Strutinsky shell correction.

6 Summary and conclusions

The Strutinsky smearing method was applied to evaluate the smoothed single-particle energy sum. Two smearing methods: i) in the single-particle energies (e-folding) and ii) in the particle number space ($n^{1/3}$-folding), were used to evaluate the shell corrections.

In addition the average dependence on the particle number of the single-particle energy sum (seen in the HO energy spectrum) was subtracted form the single-particle energy sum before performing the $n^{1/3}$-folding. This subtraction increases the accuracy of the estimates for weakly bound nuclei in which the Fermi level is close to the positive part of the single-particle energy spectrum and leads to a better smoothed energy plateau with respect to the smearing width.

One has also shown that the shell correction energy evaluated using the $n^{1/3}$-folding is deeper by a few MeV than that obtained with the e-folding in the case of the magic nuclei which are spherical. This effect can be important in future calculations of the nuclear masses as both shell corrections are comparable in the deformed nuclei [5].

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