NUCLEAR SHELL ENERGY OBTAINED BY AVERAGING IN PARTICLE-NUMBER SPACE* **

K. Pomorski

Theoretical Physics Department
Maria Curie-Skłodowska University, Lublin, Poland

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A revised version of the shell-correction method, based on a new way of evaluating the smooth part of the total single-particle energy, is proposed. The folding of the sum of nucleon energies is performed in the particle-number space, not in the energies of individual nucleons, as was done in the old Strutinsky method.

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The macroscopic–microscopic method of evaluating the binding energy of nuclei was proposed by Myers and Świątecki [1] and Strutinsky [2] and despite of tremendous progress of the self-consistent models it still remains one of the most important tools. In this approach the microscopic energy corrections consisting of shell and pairing parts are added to the binding energy described by the liquid drop (see *e.g.* [3]) or other macroscopic model.

The prescription for the evaluation of the shell energy by smoothing the single-particle energy spectra was first given in Ref. [2] and then improved in Refs. [4,5]. This Strutinsky method is still widely used up to now, in spite of its known problems arising for nuclei close to the proton and neutron drip lines, but also more generally for any finite-depth (selfconsistent or model) nuclear mean-field potential.

By definition the shell energy $E_{\rm shell}$ is the sum of the proton and neutron contributions, which for one kind of particles are equal to the difference:

$$E_{\rm shell} = \sum_{i=1}^{\mathcal{N}} e_i - \tilde{E}(\mathcal{N})\,. \tag{1}$$

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Here $\mathcal{N}$ is the number of particles in the system and $\tilde{E}$ the smooth part of the total single-particle energy.

In the Strutinsky approach one evaluates first the smooth single-particle level density $\tilde{g}(e)$ by folding the discrete spectrum of the eigenstates e_i and then the smoothed energy $\tilde{E}$ is obtained by the integral

$$\tilde{E}_{\rm Str} = \int\limits_{-\infty}^{\lambda} e\,\tilde{g}(e)\,de\,, \tag{2}$$

where λ is the Fermi energy of the system without the shell structure. It is worthwhile to notice that the above definition of the smoothed energy $\tilde{E}_{\rm Str}$ does not necessarily correspond to the average sum of single-particle energies and that it conserves the number of nucleons on the average only.

Another method free from the above mentioned deficiencies was recently proposed in Ref. [6]. The new prescription is similar to the one of Strutinsky but smoothing is performed in the particle number space, not over the single-particle energies. The new prescription for $\tilde{E}$ is the following:

- one defines a discrete sample S_n of data by summing the single particles energies up to a given number n of nucleons

$$S_n = \sum_{i=1}^{n} e_i\ , \tag{3}$$

- then one performs the Gauss–Hermite folding in the $n^{1/3}$-space and one obtains the smoothed energy in the form [6]

$$\tilde{E}(\mathcal{N}) = \frac{1}{\gamma} \sum_{n=2,4}^{\mathcal{N}_{\rm max}} \frac{2}{3\,n^{2/3}}\, S_n\ j_k \left(\frac{\mathcal{N}^{1/3} - n^{1/3}}{\gamma} \right)\,, \tag{4}$$

  which corresponds to the average of S_n when the folding width γ is comparable with the distance between the major shells in the $n^{1/3}$ coordinates[1].

The proton shell-correction energy for ^{208}Pb evaluated using a Saxon–Woods central potential [7] and Eqs. (1) and (4) for different order of the correction polynomial in the folding function j_k [4]:

[1] In order to increase the accuracy of the method for finite depth potentials, it is recommended (see Ref. [6]) to subtract from the S_n, Eq. (3), before folding the average energy $\bar{E}(n)$ given by the harmonic-oscillator sum rule.

$$
\begin{aligned}
j_2(x) &= \frac{1}{\sqrt{\pi}} e^{-x^2} \left(\frac{3}{2} - x^2 \right), \\
j_4(x) &= \frac{1}{\sqrt{\pi}} e^{-x^2} \left(\frac{15}{8} - \frac{5}{2} x^2 + \frac{1}{2} x^4 \right), \\
j_6(x) &= \frac{1}{\sqrt{\pi}} e^{-x^2} \left(\frac{35}{16} - \frac{35}{8} x^2 + \frac{7}{4} x^4 - \frac{1}{6} x^6 \right), \\
j_8(x) &= \frac{1}{\sqrt{\pi}} e^{-x^2} \left(\frac{315}{128} - \frac{105}{16} x^2 + \frac{63}{16} x^4 - \frac{3}{4} x^6 + \frac{1}{24} x^8 \right),
\end{aligned} \tag{5}
$$

is plotted in Fig. 1 as function of the smearing width γ. It is seen that for $k = 6$ and $\gamma \approx 0.75$ one obtains already a very good plateau of the function $E_{\rm shell}(\gamma)$. The next order $k = 8$ does not change much, what proves the accuracy of the new method. The quality of this plateau is better than that usually obtained using the traditional Strutinsky method [6].

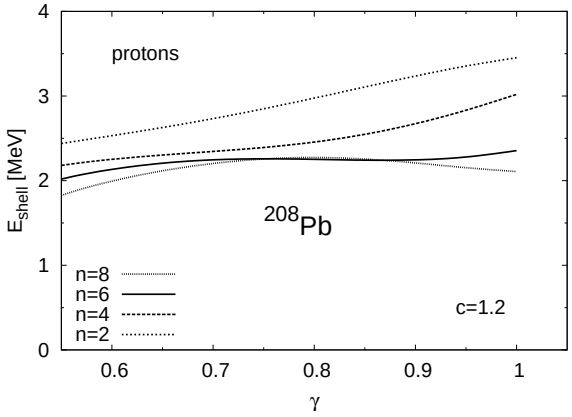

Fig. 1. Proton shell-correction energy of ^{208}Pb evaluated for different orders of the correction polynomial as function of the folding width γ.

It is seen in Fig. 2 that for spherical nuclei the new shell energy is systematically pushed down by a few MeV with respect to the old one, while for deformed systems the both energies are close to each other as demonstrated in Fig. 3. The deformation parameter c used in Figs. 1 and 3 is the relative elongation of the nucleus as defined in Ref. [5].

One could be concerned about the systematic difference between $E_{\rm shell}$ evaluated using both method which one observes for spherical nuclei. This difference has an important physical meaning as was pointed by Werner *et al.* in Ref. [8], who have shown that the particle–phonon coupling reduces the

shell corrections for spherical nuclei by several MeV and keeps it almost unchanged in the case of deformed shapes. This effect is ignored in a majority of papers in which the traditional Strutinsky shell correction method is used.

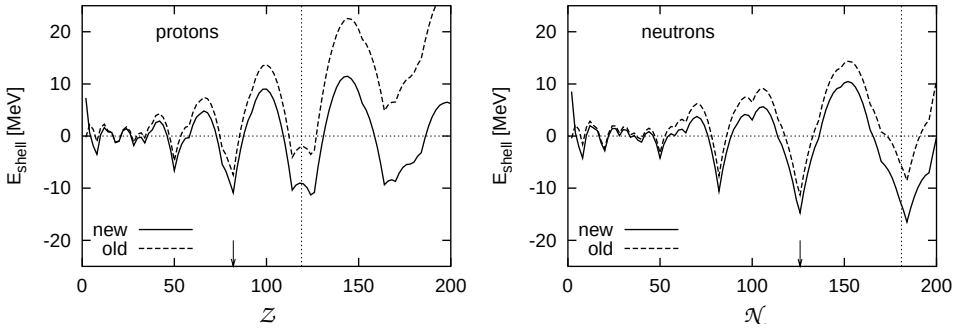

Fig. 2. Proton (l.h.s.) and neutron (r.h.s.) shell-correction energies ($E_{\rm shell}$, Eq. (1)) obtained with the Saxon–Woods spectrum of spherical ^{208}Pb as function of the nucleon number. The smooth part of the energy is evaluated by folding in the $\mathcal{N}$-space (new, Eq. (4)) as well as using the traditional Strutinsky e-averaging method (old, Eq. (2)). The arrows indicate the positions of the Fermi level and the vertical lines mark the end of the bound spectra.

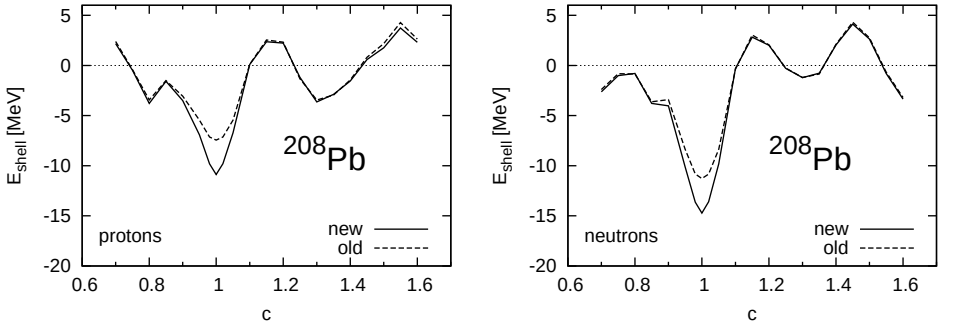

Fig. 3. Deformation dependence of the proton (l.h.s.) and neutron (r.h.s.) shell energy of ^{208}Pb obtained with the traditional (old) and modified in Ref. [6] (new) Strutinsky method as function of the elongation parameter c.

The new method of folding in the $\mathcal{N}$-space is more consistent than the old one with the definition of the macroscopic energy which represents the average dependence on Z and A of the nuclear binding energy. In addition it corresponds to a well defined number of nucleons what it is not the case in the traditional Strutinsky approach in which the number of particles was only conserved on the average.

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