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REMARKS ON THE NUCLEAR SHELL-CORRECTION METHOD

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The shell-correction energy is calculated using the single-particle levels obtained with the folded-Yukawa mean-field potential. Three different ways of evaluation of the shell-correction are compared: the traditional Strutinsky method, the modified prescription by the smearing of the total energy sum in the nucleon-number space, and by the smoothing of the single-particle energies of occupied states and summing them up. The dependence of these three energies on nuclear elongation is investigated.

1. Introduction

In spite of the great success of the selfconsistent models the macroscopic-microscopic method [1] of calculating the nuclear binding energies is still a powerful tool giving satisfactory results for nuclear masses, fission barriers heights and sizes of nuclei. The Lublin-Strasbourg-Drop (LSD) model [2] gives quite satisfactory description of the mentioned global properties of the nuclei when the appropriate microscopic shell and pairing corrections (taken from the tables [3]) are added to the macroscopic part composed of the volume, surface, curvature and Coulomb energy terms.

An alternative prescription to the traditional Strutinsky shell-correction method (I) [4] was proposed in. Ref. [5], where one performed the averaging of the single-particle energy sum in the nucleon number space (II). It turns out that the new shell-corrections evaluated for spherical nuclei are deeper (i.e. negative and larger in absolute value) as compared to the traditional Strutinsky results [4], while for the deformed isotopes the two estimates do not differ much. It was shown in Ref. [6] that the including of the collective zero-point vibrations could bring the value of the new shell energy towards the experimental estimates, which could mean that the new method can lead to a reasonable estimate of nuclear masses. Similarly as in Ref. [5] the averaging in the particle number space can also be applied to the BCS energy in order to obtain an estimate of the pairing correction [7].

Another way (III) of evaluating the shell-correction energy by summing up the smoothed single-particle energies is presented in this paper. All the three methods are compared for Ca and Sn isotopes.

2. Nuclear energy

In the macroscopic-microscopic method the binding energy E of a nucleus consists of the macroscopic part and the microscopic corrections for protons and neutrons

$$E = E_{\rm macr} + E_{\rm micr}^{\rm (p)} + E_{\rm micr}^{\rm (n)} \quad . \tag{1}$$

The microscopic correction due to the shell and pairing effects of protons (p) and neutrons (n) is

$$E_{\rm micr} = \delta E_{\rm shell}^{\rm (p)} + \delta E_{\rm shell}^{\rm (n)} + \delta E_{\rm pair}^{\rm (p)} + \delta E_{\rm pair}^{\rm (n)} \quad . \tag{2}$$

In this paper we are only interested in the shell-correction and its dependence on the nuclear elongation c [8]. The single-particle energies are obtained by the diagonalisation of the single-particle Hamiltonian with the mean-field given by the folded-Yukawa potential [9,8]. The shell effects in the nuclear energy are obtained by smoothing out the single-particle level scheme and subtracting this average value from the sum of the single-particle energies [4].

3. Shell-correction methods

The shell-correction energy can be expressed as the difference between the sum of the single-particle energies over occupied states and the corresponding smoothed energy

$$\delta E_{\rm shell}^{\rm (q)} = \sum_{\nu_{\rm occ}} e_\nu^{\rm (q)} - \widetilde{E}^{\rm (q)} = E^{\rm (q)} - \widetilde{E}^{\rm (q)} \quad , \tag{3}$$

where (q=p) for protons and (q=n) for neutrons.

We are going to discuss here the three ways of evaluating the shell-corrections: the traditional Strutinsky approach [4], consisting of a smearing of the single-particle energy spectrum in energy (e) space (I), the method proposed in Ref. [5] by smoothing in particle number ($\mathcal{N}^{1/3}$) space of the whole single-particle energy sum (II) and the new prescription to obtain the average single-particle energy by the summation of the previously smoothed in the $\mathcal{N}^{1/3}$ space energies of occupied single-particle states (III).

(**I**) In the traditional Strutinsky method [4] one defines the averaged, in the energy, density of the single-particle states

$$\widetilde{g}(e) = \int\limits_{-\infty}^{\infty} g(e')\, j\!\left(\frac{e-e'}{\widetilde{\gamma}}\right) de' \tag{4}$$

through the smoothing procedure of the exact single-particle level density g with the Gauss function multiplied by a $M^{\rm th}$ order correctional polynomial (see e.g. Ref. [5]) which in the case of $M=6$ has the form

$$j(u) = \frac{1}{\sqrt{\pi}\,\widetilde{\gamma}}\, e^{-u^2} \left(\frac{35}{16} - \frac{35}{8}u^2 + \frac{7}{4}u^4 - \frac{1}{6}u^6\right) \quad . \tag{5}$$

The smooth energy $\widetilde{E}^{(\mathrm{q})}$ is obtained by the integration of the average density of the single-particle states over energy from $-\infty$ to $\tilde{\lambda}_{\mathrm{q}}$, where $\tilde{\lambda}_{\mathrm{q}}$ is the average Fermi energy fixed by the particle number conservation.

$$\widetilde{E}^{(\mathrm{q})} = \int_{-\infty}^{\tilde{\lambda}_{\mathrm{q}}} \widetilde{g}(e)\, e\, de \ , \qquad \int_{-\infty}^{\tilde{\lambda}_{\mathrm{q}}} \widetilde{g}(e)\, de = N \ . \tag{6}$$

It was shown in Ref. [5] that the smoothed energy $\widetilde{E}^{(\mathrm{q})}$ calculated in this way did not always coincide with the averaged sum of the single-particle energies which could be visible for near spherical nuclei [10,5].

(**II**) In the $\mathcal{N}^{1/3}$-averaging method the smoothed energy $\widetilde{E}^{(\mathrm{q})}$ is approximated by the following form:

$$\widetilde{E}^{(\mathrm{q})}(N) = \widetilde{S}_N + b\, N^{4/3} + V_0\, N \ \ , \tag{7}$$

where $\widetilde{S}_N$ is the average of the difference S_n between the sum of the single-particle energies and the corresponding global energy sum dependence as in the harmonic oscillator potential

$$S_n = \sum_{\nu=1}^{n} e_\nu - b\, n^{4/3} - V_0\, n \ \ . \tag{8}$$

A quantity $\widetilde{S}_N$ can be determined using a Gauss-Hermite folding procedure

$$\widetilde{S}_N = \sum_{n=N_{\mathrm{min}}}^{N_{\mathrm{max}}} \frac{1}{3\, n^{2/3}}\, S_n\, j\left(\frac{N^{1/3} - n^{1/3}}{\gamma}\right) \ \ , \tag{9}$$

where the weight function $j(u)$ is defined by (5) with γ instead of $\tilde{\gamma}$. The parameter γ is the smearing width, for which the plateau condition of $\widetilde{S}(\gamma)$ is fulfilled. For heavier nuclei γ is of the order $0.5 - 1.0$. The parameters b and V_0 of Eq. (8) are fixed by minimizing the mean-square deviations:

$$\sum_{n=N_{\mathrm{min}}}^{N_{\mathrm{max}}} {S_n}^2 = \mathrm{min} \ \ , \tag{10}$$

where N_{max} and N_{min} given by $\left(N^{1/3} \pm 3\gamma\right)^3$ respectively. Contrary to the traditional procedure this new approach yields a smooth energy which is, indeed, the average of the single-particle energy sum in Eq. (3). The shell-corrections estimated with procedure (II) turn out to be smaller (larger absolute value) for spherical nuclei, but almost the same for deformed nuclei as compared to those evaluated using the method (I).

(**III**) One can also introduce an alternative way of defining of the smoothed single-particle sum. First, one averages the single-particle energies by folding in the particle number space ($\mathcal{N}^{1/3}$-space)

$$\widetilde{e}_n^{(\mathrm{q})} = \sum_{\nu} e_\nu^{(\mathrm{q})} j\left(\frac{n^{1/3} - \nu^{1/3}}{\gamma}\right) \tag{11}$$

and then evaluates the sum of the smoothed energies

$$\widetilde{E}^{(\mathrm{q})}(N) = \sum_{n=1}^{N} \widetilde{e}_n^{(\mathrm{q})} \quad . \tag{12}$$

Such a smoothed energy still gives the average estimate of the single-particle energy sum and conserves exactly the nucleons number, not only on the average as it was in the case of the traditional Strutinsky method (I). The results of method (II) and (III) are almost the same which proves that the type of averaging in nucleon number space is not so important.

The proper quantitative results now demand a new fit of the macroscopic model parameters and of the pairing strength to the experimental masses. Appropriate calculations are in progress (now). We can expect that the new methods (II) or (III) will show new features of the nuclear energy surface: stronger binding of spherical nuclei, new shape isomers or higher spontaneous fission barriers.

4. Results

Fig. 1 shows the results obtained with the folded-Yukawa mean-field level scheme of ^{40}Ca using the $\mathcal{N}$-smoothing of the individual single-particle energies method (III).

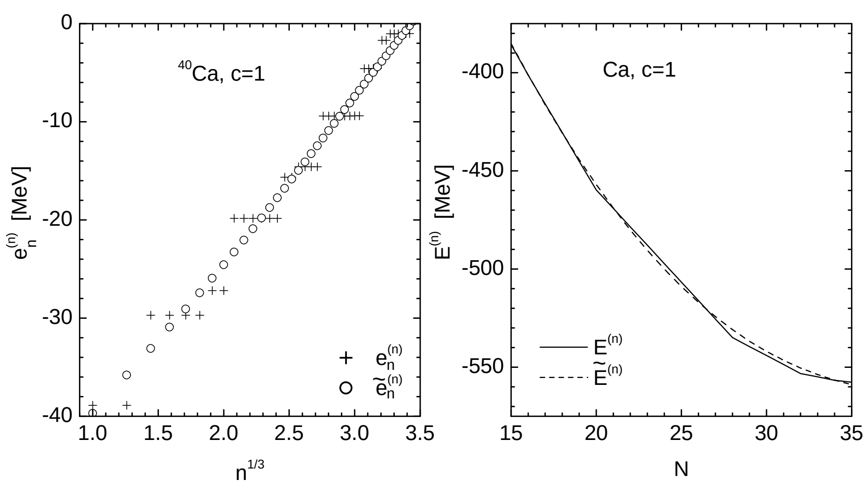

Fig. 1. Single-particle levels scheme of neutrons for spherical ^{40}Ca (l.h.s. panel) obtained with the folded-Yukawa mean-field potential (crosses) compared with the smoothed single-particle energies (Eq. (11)-open circles). (R.h.s.): The sums of the exact (solid line) and the smoothed (Eq. (12)-dashed line) neutron single-particle energies for a few Ca isotopes.

In the left panel of Fig. 1 the neutron single-particle energies $e_n^{(\mathrm{n})}$ (crosses) are shown as a function of $n^{1/3}$ at the spherical shape ($c = 1$) [8]. The smoothed single-particle energies $\widetilde{e}_n^{(\mathrm{n})}$ (11) are marked with open circles. In Fig. 1 they are shown for

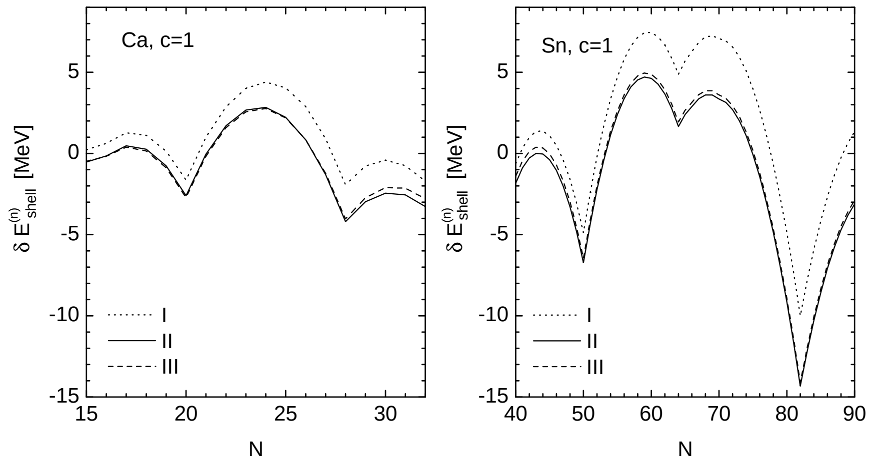

Fig. 2. The neutron shell-corrections of Ca (l.h.s) and Sn (r.h.s) isotopes obtained by methods (I), (II) and (III) as functions of neutron number N.

discrete values of n (which are necessary in order to calculate the smoothed energy (12)), though Eq. (11) defines $\widetilde{e}_n^{(\mathrm{n})}$ for any continuous values of n). The right panel of Fig. 1 shows the sum $\widetilde{E}^{(\mathrm{n})}$ (see Eq. (12)) of the smoothed neutron energies of spherical Ca isotopes with $15 \leq N \leq 35$ (dashed line) compared with the sum $E^{(\mathrm{n})}$ of the exact single-particle energies (Eq. (3)-solid line).

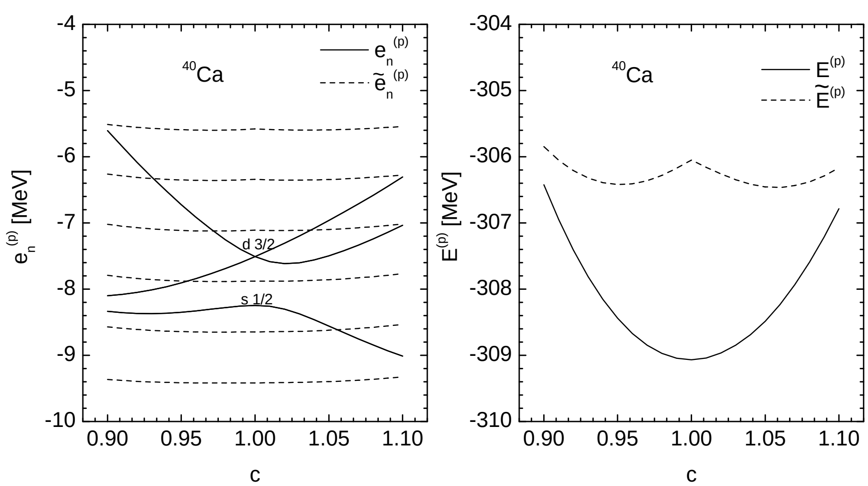

Fig. 3. (L.h.s.) - Smoothed (dashed lines - $\widetilde{e}_n^{(\mathrm{p})}$) and sharp (solid lines - $e_n^{(\mathrm{p})}$) single-particle levels of 6 protons closest to Fermi surface of ^{40}Ca as functions of the nuclear elongation c. (R.h.s.) - The sum of the proton single-particle levels (solid line - $E^{(\mathrm{p})}$) and the energy smoothed by the (III) method (dashed line - $\widetilde{E}^{(\mathrm{p})}(20)$) in function of elongation c.

As one can see from the right side of Fig. 1, the difference between $E^{(\mathrm{n})}$ and $\widetilde{E}^{(\mathrm{n})}$ is very small in comparison to the energies themselves. To represent this difference (the shell-correction) better, we show it in Fig. 2 as a function of the neutron number for a few Ca (l.h.s) and Sn (r.h.s.) isotopes. For a better comparison the shell-corrections obtained by methods (I) and (II) are also shown. The magic numbers N=20, 50, 82 are nicely reproduced by all the three methods. One can see that the methods (II, III) lead to almost identical values of the shell-correction. At the same time this values remain several MeV smaller than these obtained by the energy-averaging method (I).

The deformation dependence of the smoothed single-particle energies (11) is also worth investigating, see Fig. 3. Although the smoothed levels seem to be the regular functions of the deformation, a tiny pick around the spherical shape ($c = 1$) is still visible, which (after summation over the occupied states) leads to the maximum in the smoothed single-particle energy sum seen in the right panel of Fig. 3. This effect makes the shell-corrections shown in Fig. 4 smaller (dashed line - III) than in the Strutinsky estimates (dotted line - I).

The comparison of the deformation dependence of the shell-corrections calculated by all the three methods is shown in Fig. 4 for ^{40}Ca (top panel) and for ^{132}Sn (bottom panel). It turns out the results of methods (II) and (III) remain very close to each other. At the same time the shell-corrections (II) and (III) around the spherical shape are larger (by absolute value) as compared with (I). This means that in the new approaches (II) and (III) spherical nuclei and near- spherical nuclei are calculated to be more bound than what is obtained in the traditional Strutinsky method.

The difference between the energy smoothing (I) and the particle number smoothing (II) was discussed in earlier works [11,5]. This difference is caused by the degeneration of the single-particle states and is especially large in the (magic) particle numbers or deformations where the shell effects have the largest magnitude.

5. Conclusions

The estimate of the average single-particle energy by the sum (III) of the smoothed single-particle energies in the particle number space is similar to that evaluated by the $\mathcal{N}^{1/3}$-averaging procedure of the single-particle energy sum (II). Both methods lead to the deeper shell-corrections for spherical nuclei than the traditional Strutinsky result. The difference between the three estimates of the shell-corrections becomes smaller with the developing nuclear deformation.

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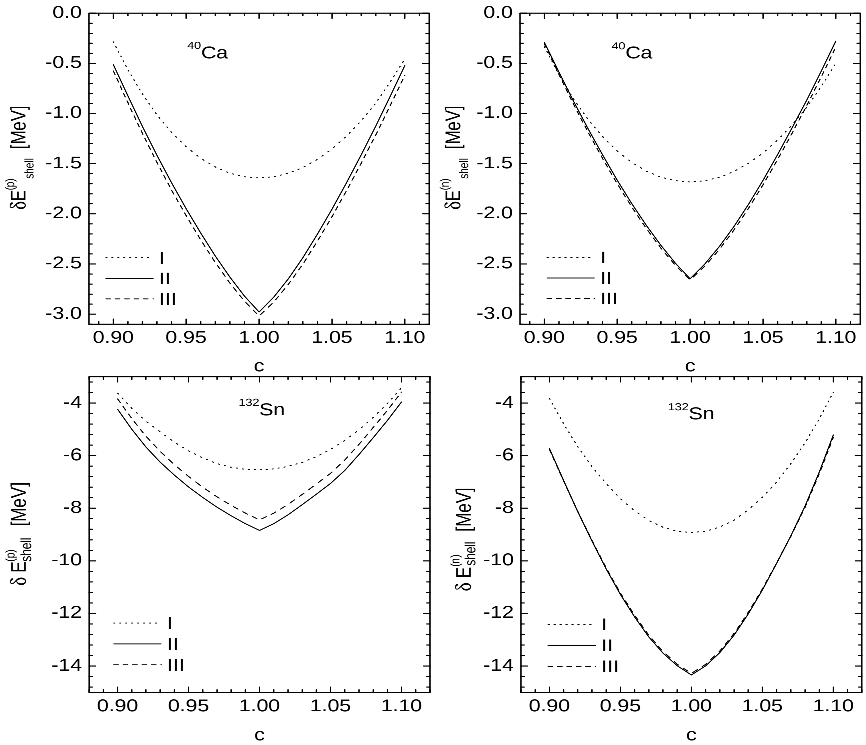

Fig. 4. Proton (l.h.s.) and neutron (r.h.s.) shell-corrections obtained by Strutinsky method (dotted lines - I), the averaging of single-particle sum in nucleon number space (solid lines - II) and the summing of the smoothed single-particle energies (dashed lines - III) for ^{40}Ca (top) and ^{132}Sn (bottom) as function of the nuclear elongation c. Averaging parameters are: $\tilde{\gamma} = 7$ MeV, $\gamma = 0.5$ (top), $\tilde{\gamma} = 10$ MeV, $\gamma = 0.75$ (bottom).

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