DIFFERENCE OF THE AVERAGE SINGLE-PARTICLE ENERGY SUMS OBTAINED BY SMOOTHING IN ENERGY AND PARTICLE-NUMBER SPACE AS INDICATOR OF THE MAGIC SHELL STRUCTURE

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Abstract: Since more than 40 years the Strutinsky concept of the shell correction plays an important role in studying of the nuclear structure [1 – 2]. In this method the smooth energy of nucleus is obtained by folding of the single-particle (s.p.) energy density in the s.p. energy space (e-folding). An alternative way of obtaining of the smooth energy by folding of the single-particle energy sum in the particle number space ($N^{1/3}$-folding) was proposed in Ref. [3]. In both types of smoothing the same folding function was used: the Gauss function multiplied by a correctional polynomial. In each case the smearing width was obtained from the plateau condition. It was shown in [3 – 4] that for degeneracy of the s.p. spectra the both types of folding give the smooth energies which are close to each other. Completely another situation origins from the case of strongly degenerated spectra which appear at sphericity or in the region of shape isomers. The smooth energy obtained by the $N^{1/3}$-folding is a couple MeV larger than the traditional Strutinsky average energy. We are going to clarify this smooth energies difference and show that it can serve as a simple tool for searching the magic or quasi-magic structure in the s.p. spectra. I.e. it can be used to predict the shape isomers in the multidimensional deformation space.

1. Introduction

Investigation of the ground state equilibrium shapes, fission dynamics and saddle points of nuclear energy surface [5] demands the proper knowledge of the nuclear single-particle (s.p.) level structure dependent on deformation and temperature. We have investigated the s.p. levels density and disappearance of shell structure with temperature in various theoretical models an have got the best agreement of the nuclear density parameter with experimental data for the Yukawa folded single particle potential [6]. The evaluation of shell effects can be done by two ways. In the traditional Strutinsky method the levels were smoothed in the energy space (e-smoothing), what conserved only on average the nucleon number and brought the difficult sometimes problem of the choice of smoothing parameter fulfilling the plateau condition [1]. The method proposed in [3] - smoothing the s.p. levels sum in the nucleon number space (N-smoothing) allowed to avoid these problems, but has given much smaller (larger in absolute values) shell corrections for spherical case. The difference decreases with deformation. This effect is connected with the degeneration of s.p. levels which appears in the points of magic structure, closed subshells and "empty" places in the s.p. scheme. As these information is important especially for the new, unknown nuclei, as superhavies the idea of analysing the s.p. levels scheme by the difference of the both: e-smoothing and N-smoothing shell corrections seems to give the promising indicator of nuclear shells in dependence on deformation.

2. Nuclear energy

In the macroscopic-microscopic method the total energy of a nucleus in a given deformation point (def) can be calculated as a sum of macroscopic energy and corrections due to shell and pairing effects of protons and neutrons

$$E(def) = E_{macr}(def) + \delta E^{(p)}_{shell}(def) + \delta E^{(n)}_{shell}(def) + \delta E^{(p)}_{pair}(def) + \delta E^{(n)}_{pair}(def)$$

(1)

We are only interested in shell effects and the s.p. levels structure. The shell corrections can be obtained by subtracting the average s.p. levels sum from the real one. The averaging can be made in the energy space (e-smoothing), as in the traditional Strutinsky method [1] or in nucleon number space (N-smoothing) as proposed in [3]. Both methods give similar results for non degenerated levels schemes, but in the case of degeneration, which appears in magic places in deformation surface the differences between both shell corrections become large up to a few MeV. We can treat them as a good test of s.p. levels degeneration looking for the subshells in various deformation points. We define the difference of the smoothed energies in nucleon number (N) and energy (e) and space equal to the opposite difference of shell corrections:

$$dE^{q}(def) = \delta E^{(q)}_{shell}(def; e) - \delta E^{(q)}_{shell}(def; N) \tag{2}$$

where $q = \{p, n\}$ denotes protons or neutrons. The way of calculating the shell corrections will be described in section 4.

3. Yukawa folded mean field

The s.p. levels are obtained here by diagonalisation of the Yukawa folded mean-field hamiltonian [7] which potential part consists of the central V_{sp}, spin-orbit V_{so} and Coulomb V_{Coul} terms

$$V^{YF} = V_{sp} + V_{so} + V_{Coul} \tag{3}$$

The s.p. nuclear potential is given by the folding integral

$$V_{sp}(\vec{r}_1) = \int d^3 r_2 \; V(r_{12}) \, \frac{\rho_0(\vec{r}_2)}{\rho_0} \, ,$$

(4)

where the folding function $V(r_{12})$ has its origin in the finite range nucleon-nucleon interaction

$$V(r_{12}) = \frac{V_0^q}{4\pi\lambda^2} \, \frac{e^{-|\vec{r}_1 - \vec{r}_2|/\lambda}}{|\vec{r}_1 - \vec{r}_2|/\lambda} \, , \; r_{12} = |\vec{r}_1 - \vec{r}_2|$$

(5)

and the diffused density $\rho_0(\vec{r}_2)$ is obtained by folding the sharp density distribution ρ_0 over the deformed nuclear volume

$$\rho(\vec{r}_2) = \rho_0 \int_V d^3 r_1 \; g\,(|\vec{r}_1 - \vec{r}_2|) \, ,$$

(6)

where $g(|\vec{r}_1 - \vec{r}_2|)$ is the Yukawa function with the width parameter a

$$g(|\vec{r}_1 - \vec{r}_2|) = \frac{1}{4\pi a^2} \, \frac{e^{-|\vec{r}_1 - \vec{r}_2|/a}}{|\vec{r}_1 - \vec{r}_2|/a} \quad . \tag{7}$$

The Yukawa folding function is normalized to unity

$$\int g(r) \, d^3 r = 1 \; .$$

The Coulomb potential can be calculated with the charge density distribution of the nucleus in the form

$$V_{Coul}(\vec{r}_1) = e \int d^3 r_2 \, \frac{\rho(\vec{r}_2)}{|\vec{r}_1 - \vec{r}_2|} \; .$$

(8)

where e is the elementary charge.

The spin-orbit term of the total single-particle mean-field can be obtained from the central part as

$$V_{so} = i\lambda^q \left(\frac{\hbar}{2MC}\right)^2 \vec{\nabla} V_{sp} \cdot \left[\vec{\sigma} \times \vec{\nabla}\right], \qquad (9)$$

where $\vec{\sigma}$ is the vector of two dimensional Pauli matrices $(\sigma_x, \sigma_y, \sigma_z)$, M – nucleon mass, C – light velocity.

As the deformation points we use the modified Funny-Hills parameters: elongation c and neck parameter h proposed in [2].

We have used the following parametrization of the s.p. potentials for protons and neutrons [17]:

$$V_0^p = V_s + V_a\bar{\delta}, \qquad V_0^n = V_s - V_a\bar{\delta}, \qquad (10)$$

where

$$\delta = \left(I + \frac{3}{8}\frac{c_1}{Q}\frac{Z^2}{A^{5/3}}\right) / \left(1 + \frac{9}{4}\frac{J}{Q}\frac{1}{A^{1/3}}\right), \qquad I = (N-Z)/A,$$

$$\lambda^p = 6.0\left(\frac{A}{240}\right) + 28.0, \qquad \lambda^n = 4.5\left(\frac{A}{240}\right) + 31.5, \qquad (11)$$

Table 1. Yukawa folded potential parameters

constant	λ	a	V_s	V_a	J	Q	C_1	r_0
unit	fm	fm	MeV	MeV	MeV	MeV	MeV	fm
0.8	0.8	0.7	52.5	48.7	35.0	25.0	$\frac{3}{5}\frac{e^2}{r_0}$	1.16

4. Shell correction methods

The shell-correction energy can be expressed as the difference between the sum of s.p. energies and the corresponding smoothed energy.

$$\delta E_{shell}^{(q)} = \sum_{\nu_{occ}} e_{\nu}^{(q)} - \tilde{E}^{(q)} \quad , \tag{12}$$

We will discuss two methods of calculating these shell corrections: the traditional Strutinsky approach [1], consisting of a smearing of the s.p. energy spectrum in energy (e) space and the proposed in [3] smoothing in particle number (N) space.

·• The traditional Strutinsky method gives the shell corrections through (12) with

$$\tilde{E}^{(q)}(def\,;e) = \int_{-\infty}^{\tilde{\lambda}_q} \tilde{g}(e)\; e\; de \;, \tag{13}$$

where the average Fermi energy $\tilde{\lambda}_q$ is fixed by the particle number condition while the function

$$\tilde{g}(e) = \frac{1}{\gamma_s} \int_{-\infty}^{\infty} g(e')\; j\left(\frac{e-e'}{\gamma_s}\right) de'$$

(14)

is obtained from the exact s.p. level density through smoothing procedure with a Gauss function multiplied by a 6^{th} order correctional polynomial [18]

$$j(u) = \frac{1}{\sqrt{\pi}}\, e^{-u^2} \left(\frac{35}{16} - \frac{35}{8}\, u^2 + \frac{7}{4}\, u^4 - \frac{1}{6}\, u^6\right) . \tag{15}$$

It can be shown [3] that the smoothed energy $\tilde{E}^{(q)}(def\,;e)$ calculated in this way is not the average sum of s.p. energies. The plateau condition usually taken at $\gamma_s = 1.2\,\hbar\omega_0$ is not very well fulfilled and difficult to establish.

• In the N-averaging method (more precisely one should speak about an averaging in the $N^{1/3}$ space) the smoothed energy $\tilde{E}^{(q)}(def\,;\,N)$ has, as function of the particle number N, the following form:

$$\tilde{E}^{(q)}(def\,;N) = \tilde{S}_N + \delta N^{1/3} + V_0 N \quad , \tag{16}$$

where $\tilde{S}_N$ is the average of the difference S_n between the sum of s.p. energies and the corresponding average global energy dependence of a harmonic oscillator potential subtracted only in order to smooth numerically the smaller quantity.

$$S_n = \sum_{v=1}^{n} e_v - b\, n^{4/2} - V_0\, n \;. \qquad (17)$$

The quantity $\tilde{S}_N$ be determined using a Gauss-Hermite folding procedure

$$\tilde{S}_N = \sum_{n=N_{\min}}^{N_{\max}} \frac{2}{3\mathrm{n}^{2/3}}\, S_n\, j\left(\frac{N^{1/2} - n^{1/2}}{\gamma}\right), \qquad (18)$$

where the weight function $j(u)$ is defined in (15) and $\gamma = 0.78$ is the smearing width [3], for which the plateau condition is always fulfilled. The parameters b and V_0 of Eqs. (6) and (7) are fixed by minimizing the mean-square deviations:

$$\sum_{n=N_{\min}}^{N_{\max}} S_n^2 = \min \;, \qquad (19)$$

with N_{min} and N_{max} given by $(N^{1/3} \mp 3\gamma)^3$. As opposed to the traditional procedure this new approach yields a smooth energy which is, indeed, the average of the s.p. energy sum in Eq. (12). The shell corrections estimated with both procedures turn out to be different for spherical, but almost the same for deformed nuclei.

5. Results

The calculations were performed for a few nuclei around ^{240}Pu and ^{264}108. In Fig. 3 we present the s.p. levels schemes in the three deformation points for protons of maximal *dEp* and neutrons dE_n seen in Figs. 1, 2. One can see the traditional magic numbers in the spherical point and some new subshells for maxima energies in of Figs. 1, 2 written in the breaks of the s.p. levels schemes. Our indicator has shown the magic structure properly.

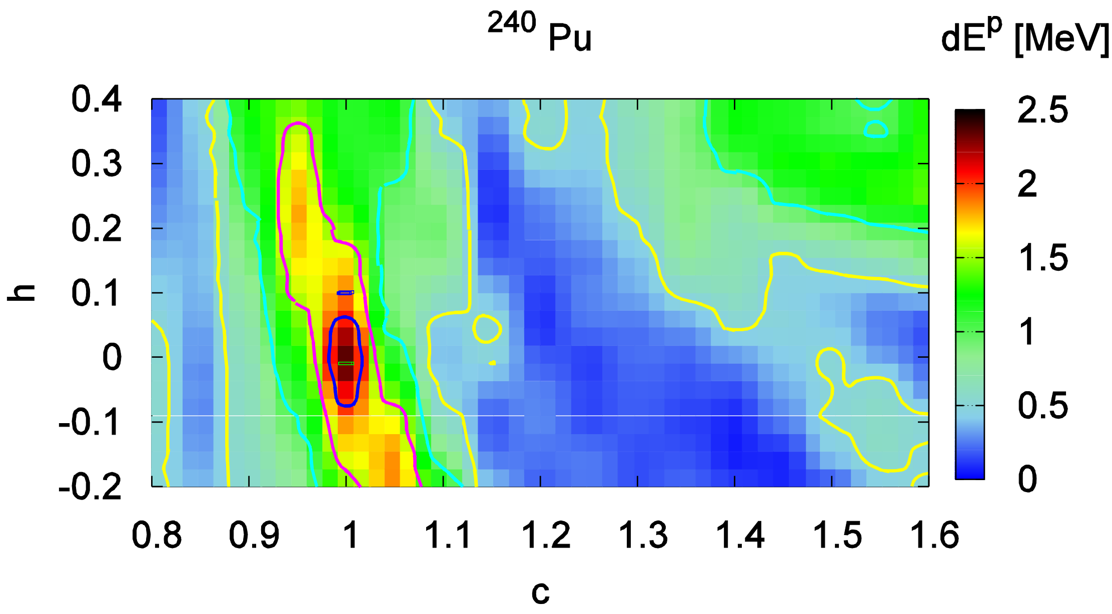

Fig. 1. Difference dE^{p} between the proton energies in ^{240}Pu smoothed in energy (*e*) and nucleon number space as function of elongation *c* and neck parameter *h* obtained with theYukawa folded mean field.

In Figs.1, 2 the maps of smoothed energies difference of protons (dE^{p}) and neutrons (dE^{n}) for ^{240}Pu on (*c,* h) plane are shown. One can see the strong pick in spherical point: $c = 1$, $h = 0$ and the sign of magic structure for the top of the fission barrier: $c = 1.6$, $h = 0.3$. There is also the "suspected" deformation point for neutrons in $c = 1.3$, $h = 0.2$.

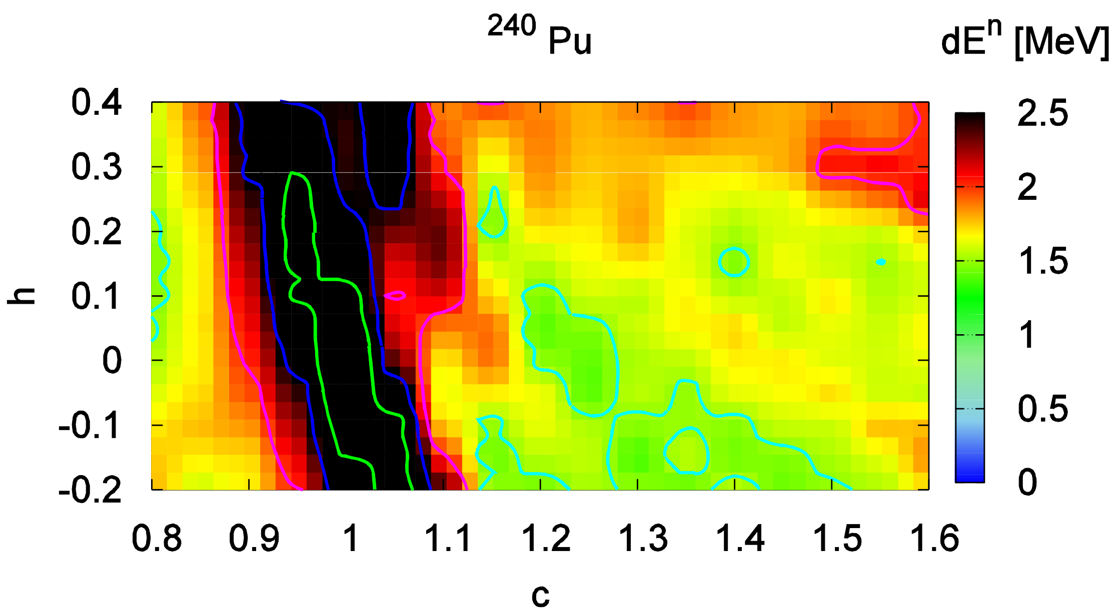

Fig. 2. Difference dE^{n} between the neutron energies in ^{240}Pu smoothed in energy (*e*) and nucleon number space as function of elongation *c* and neck parameter *h* obtained with the Yukawa folded mean field.

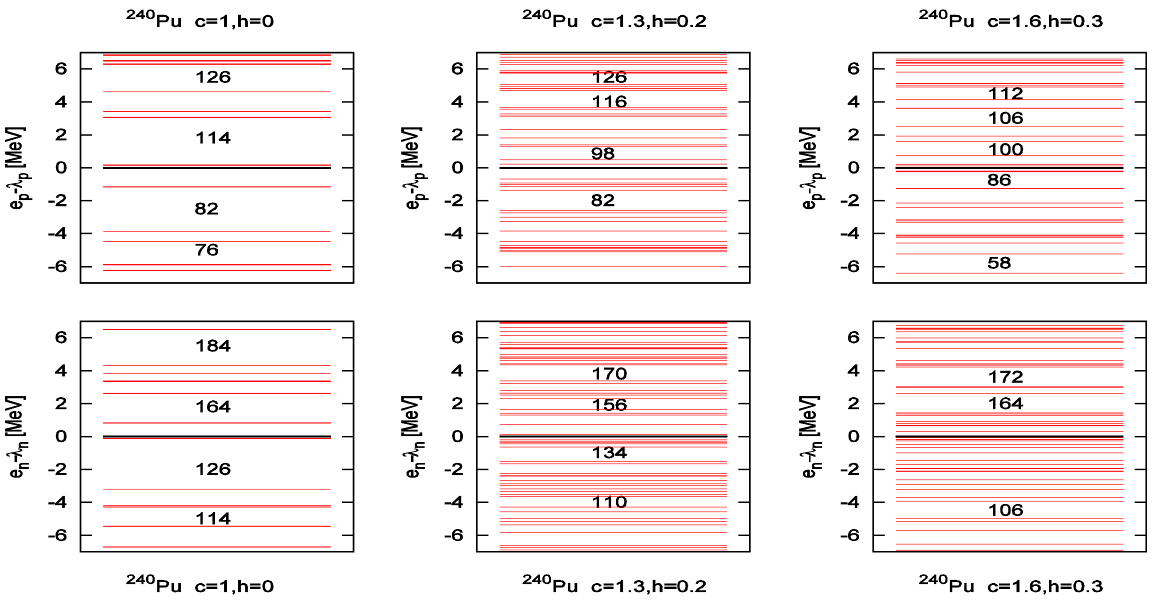

Fig. 3.Single particle levels schemes of ^{240}Pu for protons (upper row) and neutrons (lower row) in the magic points of deformation *c, h* obtained with the Yukawa folded mean field .

6. Conclusions

The following conclusions can be drawn from our analysis:

1. The Strutinsky shell-correction obtained by the e-smearing are in magic places up to 10 MeV higher than those by the new N-folding procedure.
2. Shell corrections obtained by smoothing the s.p. energies in the nucleon number space fulfill the plateau condition better than those calculated traditionally in energy space.
3. The nucleon number is exactly conserved in the s.p. levels smoothing in the N-folding while only on average in the e-folding procedure
4. The large differences in shell corrections calculated in *e* and N space show the deformation points with strong magic shell structure .

In order to test the single particle levels structure in various deformation points we are going to perform calculations for superheavy nuclei [19].

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