New method for calculating shell correction

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A new method is presented for the calculation of the shell correction with the inclusion of the continuum part of the spectrum. The smoothing function used has a finite energy range in contrast to the Gaussian shape of the Strutinski method. The new method is especially useful for light nuclei where the generalized Strutinski procedure cannot be applied.

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I. INTRODUCTION

Nuclei being far from the bottom of the stability valley are studied extensively at experimental facilities with radioactive beams. One of the fruits of this type of research is the production of light exotic nuclei. Let us refer to, for example, a recently identified new double-magic nucleus, ^{24}O [1], at the neutron drip line. The exact location of the particle drip lines limits the region for these studies and it is intensively investigated by both experimental and theoretical methods. Theoretical prediction of the drip lines is based on mass (binding energy) calculations because particle separation energies can be easily deduced.

There are two important theoretical frameworks for global mass calculations. Microscopic Hartree-Fock (HF) or Hartree-Fock-Bogoliubov (HFB) calculations with sophisticated effective density-dependent interactions are very successful in this field. In the best HFB mass formula so far [2] the rms error is 674 keV [3]. In earlier HF calculations [4,5] this number was somewhat larger, namely, 805 and 822 keV [3]. To achieve this improved fit a new parametrization of the effective nucleon-nucleon interaction has been introduced and the pairing interaction has been treated differently than in the earlier calculations.

Surprisingly a more simple alternative procedure in the framework of the so-called macroscopic-microscopic (MM) formalism can compete with the microscopic calculations in the calculation of the binding energies. The rms error in the MM calculation is 676 keV. We may say that the quality of the microscopic and MM methods are the same. Despite the almost identical global fits, however, the microscopic and MM methods show considerable differences when the neutron drip line is approached [3].

The key quantity of the MM calculations is the shell correction. The concept of the shell correction was suggested a long time ago by Strutinski [6,7] and it is still in use. For example, in a recent global mass calculation [8] the basic ingredient of the shell correction method, the smoothed single-particle density, is calculated in a semiclassical way by the Wigner-Kirkwood expansion. The other elements of the Strutinski method were not altered.

Since the invention of the shell correction there have been several refinements of the original method. In addition to the original energy averaging, a smoothing in the particle number space was introduced [9,10]. Even a combination of the two averaging spaces was considered [11]. The particle mean field, the simple harmonic oscillator, or the Nilsson potential was replaced in the calculations by more realistic phenomenological forms in which the spectrum has a continuum beside the discrete single-particle levels. The treatment of the single-particle level density due to the continuum was a long-standing problem [12,13] but an elegant solution was finally reached [14,15].

A large part of the uncertainty due to the proper choice of the technical parameters of the smoothing method has been removed by introduction of the generalized Strutinski procedure [15,16], which made it possible to calculate reliable shell correction values for medium and heavy nuclei, where the smoothed level density has a long region with linear energy dependence. As is discussed in Sec. IV, for lighter nuclei the length of the linear region is reduced due to the reduction of the number of the occupied shells and the increase of the shell gap. For light nuclei the lower and upper ends of the spectrum distort linearity; therefore the method is not appropriate for light nuclei.

The main goal of this work is to develop a new method that is free from this limitation and is applicable for the whole nuclear chart, even in the vicinity of the two drip lines. We solve this problem by introducing a finite-range smoothing instead of the infinite-range Gaussian smoothing used in the Strutinski method.

The article is organized as follows. In Sec. II we recapitulate the formalism of the calculation of the shell correction. In

Sec. III we describe the standard Strutinski method with the plateau condition. In Sec. IV we do the same with the generalized Strutinski procedure, what we want to replace in this work. In Sec. V we describe the new method with finite-range smoothing in details. In Sec. VI we apply the new method for several nuclei and calculate shell corrections for neutrons and protons. Finally in Sec. VII we end with the main conclusions of the article.

II. CALCULATION OF THE BINDING ENERGY BY USING THE SHELL CORRECTION

The binding energy of an atomic nucleus composed of $A = N + Z$ nucleons (N denotes neutrons and Z denotes protons) can be calculated in the microscopic-macroscopic model (MM) as

$$B(N, Z) = E_{\text{macr}}(N, Z) + \delta E(N, Z), \tag{1}$$

where $E_{\text{macr}}(N, Z)$ is the binding energy calculated in the macroscopic model (e.g., liquid drop or droplet model) and $\delta E(N, Z)$ is the shell correction. While $E_{\text{macr}}(N, Z)$ is a smooth function of the number of nucleons, the shell correction takes care of the shell fluctuations of the binding energy that is missing from the macroscopic model. Shell fluctuations are present in any microscopic model. For example, the shell correction can be calculated from single-particle energies of self-consistent HF and relativistic mean-field calculations [17,18]. In Ref. [18] shell corrections calculated on the single-particle energies were used to generate a smooth energy from the result of these microscopic calculations and the typical phenomenological parametrizations of the *microscopically calculated* macroscopic energy terms were analyzed.

In the present work we use the simplest, that is, the independent particle shell model to generate the single-particle energies in a phenomenological nuclear potential for the sake of simplicity only, because the smoothing procedure could be tested equally well on the result of this simple model. In this model we treat neutrons and protons separately. In this case the shell correction

$$\delta E(N, Z) = \sum_{\tau=\nu,\pi} \delta E_\tau(N_\tau) = \delta E(N) + \delta E(Z) \tag{2}$$

is the sum of the shell corrections $\delta E_\tau(N_\tau)$ calculated for neutrons, $\tau = \nu$ with $N_\nu = N$, and for protons, $\tau = \pi$ with $N_\pi = Z$. In what follows we discuss the calculation of the shell correction $\delta E_\tau(N_\tau)$ for a given type of nucleons only.

The shell correction can be estimated as the difference of the shell model binding energy E^τ_{sp} and its smoothed counterpart $\tilde{E}^\tau$ calculated also in the shell model:

$$\delta E_\tau = E^\tau_{\text{sp}} - \tilde{E}^\tau. \tag{3}$$

Here the shell model binding energy

$$E^\tau_{\text{sp}} = \sum_{j=1}^{N_\tau} E^\tau_j \tag{4}$$

is a sum of the single-particle energies E^τ_j of the lowest energy orbits, from E^τ_1 until the Fermi level. In the sum we can take into account the n_i-fold degeneracies of the shell model orbits and use only the different single-particle energies denoted by e^τ_i:

$$E^\tau_{\text{sp}} = \sum_i n_i e^\tau_i . \tag{5}$$

The key quantity of the MM model is the smoothed energy $\tilde{E}^\tau$; therefore, we have to give a unique definition for calculating it unambiguously. If we have the bound single-particle energies e^τ_i, the density of the bound nuclear levels is

$$g^\tau_{\text{d}}(E) = \sum_i n_i \delta\left(E - e^\tau_i\right). \tag{6}$$

The particle number as a function of the energy E of the single nucleon considered is an integral of the level density in Eq. (6); that is, it is equal to the following step function:

$$n^\tau(E) = \int_{-\infty}^{E} g^\tau_{\text{d}}(e) de = \sum_i n_i \Theta\left(E - e^\tau_i\right), \tag{7}$$

where $\Theta(x)$ is a Heaviside function of the form

$$\Theta(x) = \begin{cases} 0, & \text{if } x < 0 \\ 1, & \text{if } x \geqslant 0. \end{cases} \tag{8}$$

Because in the smoothing procedure we treat neutrons and protons on the same footing, we can drop the τ index for a moment. (We include it again later when it is needed to avoid ambiguity.) We can calculate the smoothed level density $\tilde{g}(E)$ from the level density in Eq. (6) by folding it with a properly selected smoothing function: $f_p(x)$. The smoothing function spreads the energy of a discrete level over a certain energy range characterized by the smoothing range parameter γ. Therefore, the smoothed level density is

$$\tilde{g}(E) = \frac{1}{\gamma} \int_{-\infty}^{+\infty} g(e) f_p\left(\frac{e - E}{\gamma}\right) de. \tag{9}$$

The smoothing function in Eq. (9) is usually a product of a weight function $w(x)$ and a polynomial $h_p(x)$ of degree p:

$$f_p(x) = w(x) h_p(x). \tag{10}$$

The latter is called a *curvature correction polynomial*. Because the smoothing function $f_p(x) = f_p(-x)$ is an even function of x, for an even weight function $w(x)$ the polynomial $h_p(x)$ should also be even and the coefficients of the odd terms in it should be equal to zero. Therefore, the curvature correction polynomial has the form

$$h_p(x) = \sum_{i=0,2,\ldots,p} c_i x^i . \tag{11}$$

The c_i coefficients of the curvature correction polynomial $h_p(x)$ are determined from the so-called *self-consistency condition* [19], which requires that the smoothing should reproduce the original function if it is a polynomial $g_n(x)$ with degree $n \leqslant p + 1$:

$$g_n(x) = \int_{-\infty}^{+\infty} g_n(x') f_p(x - x') dx'. \tag{12}$$

We calculate the smoothed energy by using the smoothed level density in Eq. (9):

$$\tilde{E} = \int_{-\infty}^{\tilde{\lambda}} \epsilon \tilde{g}(\epsilon) d\epsilon. \tag{13}$$

The smoothed Fermi-level $\tilde{\lambda}$ is calculated from the condition that the number of neutrons and protons, that is, the particle number, is given by

$$N = \int_{-\infty}^{\tilde{\lambda}} \tilde{g}(\epsilon) d\epsilon. \tag{14}$$

The smoothed Fermi-level $\tilde{\lambda}$ is different from the Fermi-level λ because the level density has been modified by the smoothing.

III. STANDARD STRUTINSKI METHOD WITH PLATEAU CONDITION

Strutinski [6,7] used a smoothing function with the Gaussian weight function

$$w(x) = \frac{1}{\sqrt{\pi}} \exp(-x^2), \tag{15}$$

and it can be shown that the curvature correction polynomials for a weight function of Gaussian shape are the associated Laguerre-polynomials:

$$h_p(x) = L_{p/2}^{1/2}(x^2). \tag{16}$$

Therefore, in the standard Strutinski method the smoothing function is

$$f_p(x) = \frac{1}{\sqrt{\pi}} \exp(-x^2) L_{p/2}^{1/2}(x^2). \tag{17}$$

For nuclei lying on the bottom of the stability valley the single-particle potential can be approximated by a simple harmonic oscillator (h.o.) form. For a nucleus with mass number A the distance of consecutive shells can be expressed by the well-known rule [20]

$$\hbar\Omega_0 = 41 A^{-1/3} (\text{MeV}). \tag{18}$$

The shell structure of this simple h.o. model is modified by the presence of the spin-orbit interaction and also by the nonspherical shape of deformed nuclei but the quantity in Eq. (18) is still serves as a reasonably good measure for the shell structure. An attractive feature of the h.o. potential is that the shell correction $\delta E(\gamma, p)$ as a function of the smoothing range γ shows a wide plateau in which the

$$\frac{\partial \delta E(\gamma, p)}{\partial \gamma} = 0 \tag{19}$$

plateau condition is fulfilled. More precisely, the fulfillment of the plateau condition is valid if at the same time the values belonging to the plateau are practically independent of the p value used. It has been observed that the plateau condition is fulfilled for the h.o. potential. Because γ and p are technical parameters of the smoothing procedure and they have no physical meaning, it is natural to expect that the definition of the smoothed quantities should not depend strongly on these values. Therefore, the shell correction calculated for the h.o. potential is well defined. This nice feature of the h.o. potential is related to the fact that this potential has only bound states (even at high positive energy values). For potentials that are similar to the harmonic oscillator potential, for example, the Nilsson potential, we can always find regions for γ where the plateau condition is fulfilled [12,21]. Because these potentials have only bound states (infinitely many) and no continuum, the ending of the bound states does not spoil the picture.

IV. GENERALIZED STRUTINSKI PROCEDURE FOR SPECTRA WITH THE CONTINUUM

However a more realistic single-particle potential has a discrete spectrum with a finite number of bound states, $e_i < 0$, and a continuum of scattering states with $E > 0$ energy. The full level density in this case is a sum of the level densities of the discrete states $g_d(E)$ and that of the scattering states $g_c(E)$ forming the continuum

$$g(E) = g_d(E) + g_c(E). \tag{20}$$

Now the smooth level density has to be calculated again with the prescription of Eq. (9). It was realized by Brack and Pauli [21] that for this case the plateau condition cannot be satisfied because the $\delta E(\gamma, p)$ curves, what we call *plateau curves*, do not have wide plateaus, where Eq. (19) is fulfilled. They searched for the minima $\delta E(\gamma_p, p)$ of the plateau curves for each p value and introduced the concept of *local plateau condition*. At the minima, that is, at $\gamma = \gamma_p$, Eq. (19) is certainly satisfied. An additional requirement of the local plateau condition is the approximate p independence of the $\delta E(\gamma_p, p)$ values, which is satisfied if the variation of the $\delta E(\gamma_p, p)$ values are small.

It was shown in Ref. [15] that sometimes even the local plateau condition might not be fulfilled and the smoothing procedure of the standard Strutinski method might not able to furnish us with well-defined smoothed energy. A typical nucleus for which the local plateau condition fails if the continuum part of the spectrum is taken into account is ^{146}Gd, as one can see in Fig. 1. Although one can find minima for each plateau curve, the shell correction values at these minima vary too much (even an approximate p independence does not hold). Therefore it is not surprising that the $\delta E(\gamma_p, p)$ values deviate considerably from the semiclassical values.

To address this difficulty, in Ref. [15] a *modified plateau condition* was suggested. In the modified plateau condition the plateau condition in Eq. (19) is replaced by the requirement that in a certain energy region the smoothed level density should be fit well by a straight line.

The shell correction $\delta E(\gamma_p, p)$ for a given p should be calculated with those γ_p values for which the smoothed level density can be fit best by a linear function, $y(E) = aE + b$ in a certain energy range, $[e_l, e_u]$. So we should find the minimum of the function in the variable γ for each p value by

$$\chi^2(\gamma, p) = \sum_{i=1}^{n_u} [\tilde{g}(q_i, \gamma, p) - y(q_i)]^2. \tag{21}$$

Here q_i for $i = 1, .., n_u$ is a mesh of the energy interval $[e_l, e_u]$ used, and γ_p is the value where the function χ^2 has its minimum at a given p value. To get rid of the shell fluctuations the length of the interval must be larger than the estimated shell gap:

$$e_u - e_l = 1.5\hbar\Omega_0. \tag{22}$$

Having selected the proper γ_p value for a set of p values between $p_{\min} = 6$ and $p_{\max} = 14$, the mean value and the variation of the corresponding $\delta E(\gamma_p, p)$ values must be calculated as follows:

$$\delta E = \frac{2}{(p_{\max} - p_{\min} + 2)} \sum_{p=p_{\min}, p_{\min}+2,\ldots,p_{\max}} \delta E(\gamma_p, p), \tag{23}$$

$$\sigma = \sqrt{\frac{2}{(p_{\max} - p_{\min} + 2)} \sum_{p=p_{\min}, p_{\min}+2,\ldots,p_{\max}} [\delta E(\gamma_p, p) - \delta E]^2}. \tag{24}$$

Because in Ref. [15] this variation was reasonably small for most of the nuclei, the mean in Eq. (23) was used to define the shell correction, and the variation in Eq. (24) was considered as an uncertainty of the method. The procedure described previously was called as a *generalized Strutinski procedure*.

To illustrate the use of the modified plateau condition we present the smoothed level densities for the ^{146}Gd nucleus in Fig. 2. The lower and upper ends of the energy interval in which the best linear fit of the $\tilde{g}(E)$ is required are shown by solid triangles on the E axis. Practically no p dependence of the $\tilde{g}(E)$ curves can be observed in the $[e_l, e_u]$ interval where $\tilde{g}(E)$ apparently behaves as a linear function of E. Some p dependence can only be observed at around $E \approx -10$ MeV, being a bit above the $\tilde{\lambda}$ value, and at higher energy in the $E = 0$ MeV region, which has no influence on the shell correction. The large bump of the smoothed level density around $E = 0$ MeV is the effect of the higher end of the spectrum. In the positive part of the spectrum only a few neutron resonances contribute to the level density and their effect is smoothed by the smoothing parameters, which are the abscissas of the solid circles in Fig. 1. These γ_p values are between 10 and 15 MeV; therefore the end effect is spread well below the threshold. The effect of the lower end is less pronounced but can be seen at $E < -35$ MeV. Here the derivative of $\tilde{g}(E)$ with respect to E changes and at $E < -45$ MeV $\tilde{g}(E)$ goes below zero for a while. The main feature of the $\tilde{g}(E)$ is that the linearity required in Eq. (1) holds only at a certain distance from the lower and upper ends of the spectrum.

In Fig. 1 the solid circles on the different p curves show the $[\gamma_p, \delta E_n(\gamma_p, p)]$ points where the γ_p values are those where the function in Eq. (21) has its minimum. One can see from the circles that these shell correction values have a much smaller variation (σ) than the shell correction values at the minima of the curves. Moreover the mean of the $\delta E_n(\gamma_p, p)$ values denoted by circles is in good agreement with the dotted line showing the semiclassical value. In Ref. [15] it was found that this situation is quite typical and the generalized Strutinski

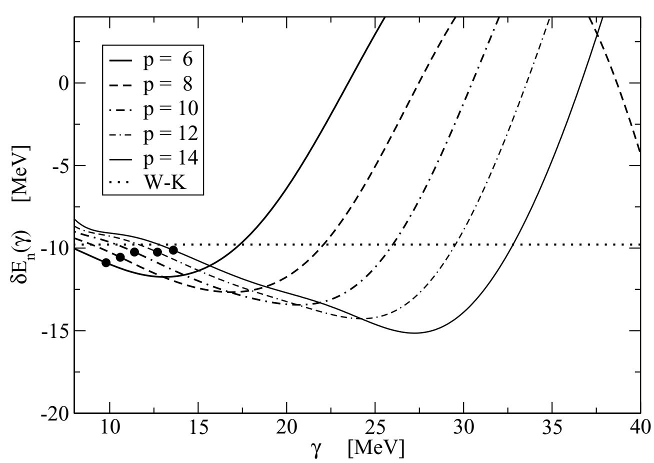

FIG. 1. Neutron shell correction $\delta E_n(\gamma, p)$ for the nucleus ^{146}Gd as a function of the smoothing range γ calculated for $p = 6, .., 14$ by using the Gaussian weight function for the smoothing functions f_p. Solid circles on the different curves denote the $[\gamma_p, \delta E_n(\gamma_p)]$ points, where γ_p values belong to the minima of the function in Eq. (21) and the $\delta E_n(\gamma_p, p)$ values are the results of the generalized Strutinski procedure. The dotted horizontal line shows the value of the semiclassical value $\delta E_{sc} = E_{sc} - E^n_{sp}$.

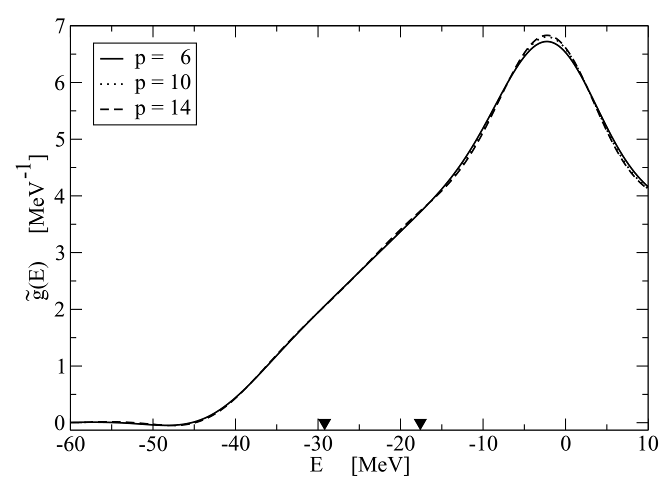

FIG. 2. Energy dependence of the smoothed level densities calculated in the generalized Strutinski procedure for $p = 6, 10, 14$ by using a Gaussian weight function for the smoothing functions f_p for the nucleus ^{146}Gd. The lower and upper ends of the interval $[e_l, e_u]$ in which the condition of the best linear fit is applied are shown by triangles on the E axis.

procedure gave values similar to the result of the semiclassical averaging based on the Wigner-Kirkwood expansion [21–27] in those cases in which the latter could be applied. Moreover the generalized Strutinski procedure gave results similar to those of the standard one for all cases where the plateau condition was fulfilled. But it gave a well-defined value for the smoothed energy even in cases like ^{146}Gd where we cannot really speak about plateau.

It turned out only later, in Ref. [16] where the generalized Strutinski procedure was used for deformed nuclei, that the function in Eq. (21) might have more than one minimum in γ. It was concluded in Ref. [16] that the minimum at the smaller γ value should be selected.

An uncertainty of the generalized Strutinski smoothing procedure is that the results are slightly dependent on the position of the $[e_l, e_u]$ energy interval used. For medium and heavy nuclei the uncertainty of the generalized Strutinski procedure was always below 250 keV. To get this small variation, the energy interval $[e_l, e_u]$ was adjusted to the smoothed Fermi level, and the upper end of the energy interval was $e_u = \tilde{\lambda} - \hbar\Omega_0$. If the interval was shifted up to have $e_u = \tilde{\lambda}$ and the length was kept the same as in Eq. (22), a variation of the shell correction by around 400 keV was observed. This uncertainty was still reasonably small and it was comparable to the typical deviation from the semiclassical result.

The dependence on the position of the interval become stronger for light nuclei. If the mass number A is reduced, the distance of the shells estimated in Eq. (18) increases and the length of the interval in Eq. (22) also increases. We should use larger and larger γ values for smoothing the shell fluctuations. However, the region in which $\tilde{g}(E)$ is linear becomes shorter and shorter because the effect of the lower end shifts higher and that of the higher end shifts lower. Therefore, for small A there is not enough space where the required linear region could develop. The linearity of the $\tilde{g}(E)$ function is spoiled by the end effects. This explains why the generalized Strutinski procedure breaks down for light nuclei.

Therefore, in this work our goal is to find a new smoothing procedure that is less sensitive to the end effects, but still keeps the advantages of the generalized Strutinski procedure; that is, the shell correction is practically independent of the p values (σ is small). An additional requirement is that $\tilde{E}$ resulting from the new procedure should not be too different from the result of the semiclassical procedure (Wigner-Kirkwood method) if the latter approach can be applied.

V. NEW SMOOTHING PROCEDURE

A disadvantage of the smoothing procedures used so far is that the Gaussian weight function $w(x)$ used has an infinite range; therefore, the effect of the energy e_i is smeared to the whole energy axis from $-\infty$ to ∞. Therefore, the effect of the lower and upper ends of the spectrum influences the whole region of the smoothed level density and also the shell correction δE. In this work we try to reduce the end effects in these quantities by using weight functions that have only a finite range. One possible candidate for a weight function with finite range is the shape

$$w(x) = \begin{cases} ke^{-\frac{1}{1-x^2}}, & \text{if} \quad |x| < 1 \\ 0, & \text{if} \quad |x| \geqslant 1. \end{cases} \tag{25}$$

The value of the normalization constant k should be chosen from the condition

$$1 = \int_{-1}^{+1} w(x)dx. \tag{26}$$

One advantage of the form in Eq. (25) is that all derivatives of that function are continuous at $|x| = 1$, so the weight function continues smoothly to the regions where it is equal to zero. The effect of the smoothing with this form is localized to the $x \in [-1, 1]$ interval. To use the new smoothing function we have to recalculate the curvature correction polynomials $h_p(x)$ in Eq. (11) for the new weight function [in Eq. (25)]. The recalculated polynomials $h_p(x)$ will be different from the one in Eq. (16) and they should satisfy the self-consistency condition in Eq. (12), with the finite-range weight function. As was shown in Ref. [19], the coefficients c_i of the curvature correction polynomials in Eq. (11) are solutions of the system of linear equations

$$\sum_{i=0}^{p} c_i a_{i+j} = \delta_{j,0}, 0 \leqslant j \leqslant p, \tag{27}$$

where the coefficients a_l are the integrals:

$$a_l = \int_{-1}^{1} w(x)x^l dx. \tag{28}$$

The integration is over the interval where the weight function $w(x)$ is different from zero.

We present the coefficients c_i for the $p \in \{0, 2, 4, 6\}$ values in Table I for illustration purposes. In Fig. 3. we present the shape of the smoothing function $f_p(x)$ for a few p values and the finite-range weight function in Eq. (25) $w(x) = f_0(x)$. To show the difference from the standard Gaussian case, we present similar curves with the Gaussian weight function in Fig. 4. For both weight functions, for $p > 0$ the curvature correction polynomials $h_p(x)$ have $p = 2m$ zeros:

$$h_p\big(x_j^{(p)}\big) = 0, \quad j = \pm 1, \ldots, \pm m, \quad x_{-j} = -x_j. \tag{29}$$

One can observe the positions of the roots $x_j^{(p)}$ of Eq. (29) in Figs. 3 and 4. For a fixed p value it is convenient to arrange the positive roots of Eq. (29) so that they form a monotonous series:

$$0 < x_1^{(p)} < x_2^{(p)} < \cdots < x_m^{(p)}. \tag{30}$$

TABLE I. Coefficients of the curvature correction polynomials for the lowest p values corresponding to the finite-range weight function in Eq. (25).

p	c_0	c_2	c_4	c_6
0	1	0	0	0
2	1.8934	−5.6506	0	0
4	2.7492	−20.62052	28.52324	0
6	3.5866	−48.45461	155.33082	−136.79695

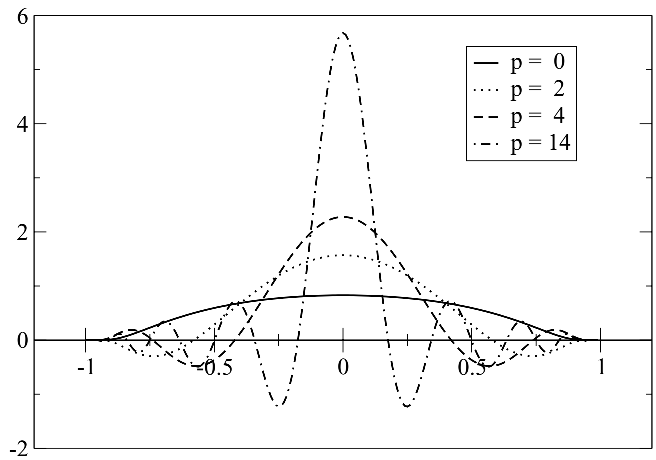

FIG. 3. Shapes of the finite-range smoothing function $f_p(x)$ for $p = 0, 2, 4, 14$. Note that $f_0(x) = w(x)$.

In the smoothing function $f_p(x)$ in Eq. (10) the most important part of the smoothing is produced by the central region in $h_p(x)$: $x \in [-x_1^{(p)}, x_1^{(p)}]$, determined by the first root $x_1^{(p)}$. One can see in the figures that for $p > 0$ values, $x_1^{(p+2)} < x_1^{(p)}$; that is, the value of $x_1^{(p)}$ decreases when p increases.

The finite-range smoothing has the advantage that the effect that a certain single-particle energy, e_i, vanishes beyond the interval $E \in [e_i - \gamma, e_i + \gamma]$. Therefore, the smoothed level density becomes exactly zero for energies lying below $(e_1 - \gamma)$, while the Gaussian oscillates around zero. This oscillation character appears at any value of the smoothing parameter.

If we go to higher E values, we can smooth the oscillatory character of $\tilde{g}(E)$ if we use large enough γ values in the smoothing function with Gaussian weight function. This is not the case, however, if we smooth with finite-range weight function, where some undulation in $\tilde{g}(E)$ remains even if we use large smoothing range parameters. Therefore, it cannot be well approximated by a straight line as it was in the generalized Strutinski procedure.

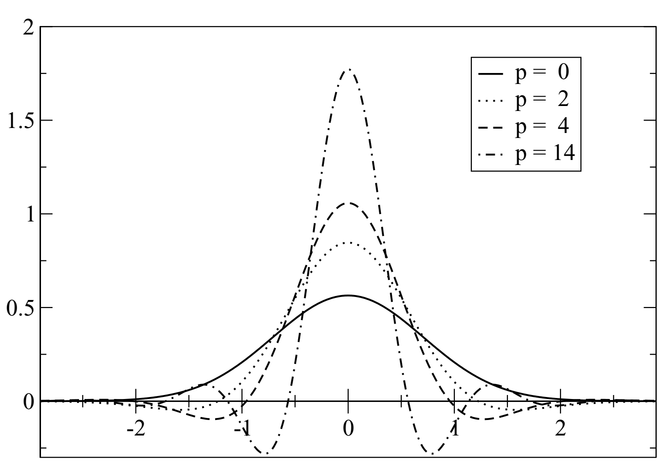

FIG. 4. Shapes of the smoothing function $f_p(x)$ with Gaussian weight function for $p = 0, 2, 4, 14$. Note that the Gaussian weight function is $f_0(x) = w(x)$.

This seems to be an important difference between the smoothed level densities calculated by using Gaussian or finite-range smoothings.

We calculate the smoothed energy in Eq. (13) by using the finite-range smoothing functions for a range of $\gamma \in [\gamma_{\min}, \gamma_{\max}]$ and $p \in \{p_{\min}, p_{\min} + 2, \ldots, p_{\max}\}$ values. This allows us to study the plateau curves. For $p = 0$ the plateau curve is a monotonously increasing function; therefore, neither the plateau condition in Eq. (19) nor the local plateau condition can be applied. (There is no γ value where the derivative is zero.) This result shows the necessity of using curvature correction polynomials.

For $p > 0$, plateau curves have minima (and maxima) where the plateau condition in Eq. (19) is fulfilled locally. However the plateau curves might have several minima and we must find the proper one among those minima. A necessary condition of the smoothing is that the smoothed level density should not reflect the shell structure of the single-particle levels. Therefore, in the smoothing procedure we have to start searching for the minimum of $\delta E(\gamma, p)$ from a (p-dependent) $\gamma_{\min}$ value for which the shell structure has already disappeared.

The most important characteristic of the single-particle spectrum is the largest gap between the occupied levels. Therefore, we must determine the largest distance between the consecutive occupied levels of the N particles (shell gap):

$$G = \max\{(e_{i+1} - e_i)\}. \tag{31}$$

This G value is a more accurate measure of the shell structure of the single-particle energies than the $\hbar\Omega_0$ in Eq. (18). To estimate a reasonable $\gamma_{\min}$ value, we have to determine the effective width of the smoothing function with a given p. The effective width corresponds to the central peak of $h_p(x)$ in the interval $x \in [-x_1^{(p)}, x_1^{(p)}]$. Because the effective range of the smoothing function decreases for increasing p, for larger p values one should use larger γ values to have the same smoothing effect. To compensate for this effect, it is

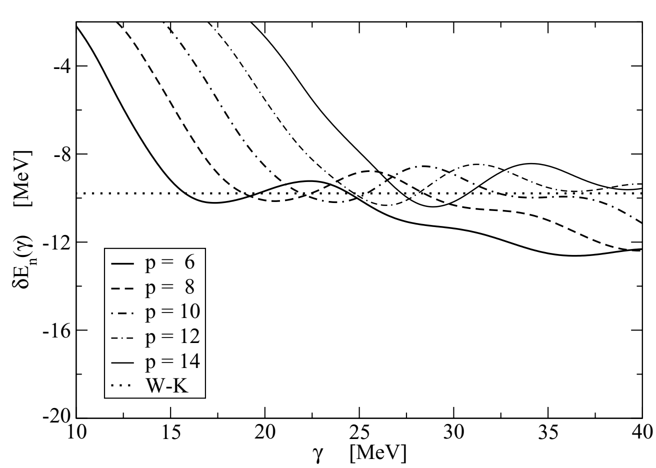

FIG. 5. Neutron shell corrections $\delta E_n(\gamma, p)$ for the nucleus ^{146}Gd as a function of the smoothing range γ calculated for $p = 6, .., 14$ by using the finite-range weight function for the smoothing functions f_p. The dotted horizontal line shows the value of the semiclassical value $\delta E_{sc} = E_{sc} - E_{sp}^n$.

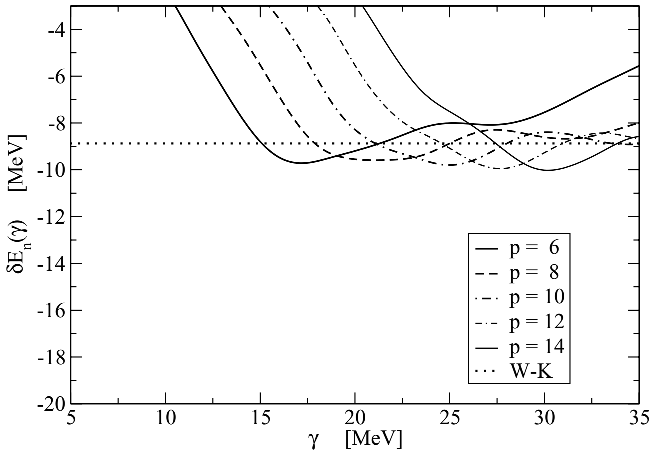

FIG. 6. Neutron shell corrections $\delta E_n(\gamma, p)$ for the nucleus ^{132}Sn as a function of the smoothing range γ calculated for a set of p values by using the finite-range smoothing function f_p. The dotted horizontal line shows the value of the semiclassical value $\delta E_{sc} = E_{sc} - E^n_{sp}$.

worthwhile to introduce a *renormalized smoothing range* as follows:

$$\Gamma_p = x_1^{(p)} \gamma_p, \tag{32}$$

in which the p dependence of the smoothing is considerably reduced.

To smooth the fluctuations due to the major shells this Γ_p range should be larger than the shell gap $\Gamma_p > G$. To achieve this we introduce the factor $F > 1$ and calculate a minimal value for the renormalized range $\Gamma_{p,\min} = FG$. (We observed that the optimal value for the factor F is $F = 1.5$–2 for light and $F = 2.5$–3.5 for heavier nuclei.) Having fixed this minimum we search for the first minimum of $\delta E(\gamma, p)$ for

$$\gamma \geqslant \gamma_{p,\min} = \frac{FG}{x_1^{(p)}}. \tag{33}$$

This criteria serves as a guide to select the proper minimum of the plateau curve $\delta E(\gamma_p, p)$. For most nuclei the plateau curves have multiple minima at $\gamma_{p,1} < \gamma_{p,2} <, \ldots, < \gamma_{p,l}$. The number of minima l generally increases when p increases. We observed that for $p = 2$ we have at most two minima, that is, $l = 1$ or $l = 2$, and one of them satisfies the following condition:

$$\Gamma_{2,l} = x_1^{(2)} \gamma_{2,l} \sim FG. \tag{34}$$

For higher p values the proper minimum should be close to this value because we reduced the p dependence considerably by using the renormalized smoothing range. Therefore, we have to select the kth minimum, for which $\Gamma_{p,k} = x_1^{(p)} \gamma_{p,k} \approx \Gamma_{2,l}$. If we select the smoothing range according to this criteria, then the variation of the corresponding $\delta E(\gamma_{p,k}, p)$ values will be small.

VI. DETAILS OF THE NUMERICAL CALCULATIONS

We used a Saxon-Woods (SW) potential with a spin-orbit term. For protons it was complemented by a Coulomb potential of a uniformly charged sphere with a diffuse edge (having this this form is necessary to be able to calculate the semiclassical results for comparison.) The parameters of the potentials were that of the so-called *universal potential* given in Ref. [28]. The depth of the central potential for neutrons ($\tau = \nu$) $t_3 = 1/2$ or for protons ($\tau = \pi$) $t_3 = -1/2$ is given by

$$V_\tau(Z, N) = -V \left[1 - 2\kappa t_3 \frac{N - Z}{A} \right], \tag{35}$$

where $\kappa = 0.86$ and $V = 49.6$ MeV. The depth of the spin-orbit potential is

$$V_{so} = -\frac{\lambda_{so} V_\tau}{4} \left(\frac{\hbar}{2\mu c} \right)^2, \tag{36}$$

with the reduced mass μ of the nucleon and $\lambda_{so} = 35(36)$ for neutrons (protons). The diffuseness was $a = a_{so} = a_C = 0.7$ fm, the same for all potential terms. The radius parameters were $r_0 = 1.347$ fm and $r_0 = r_C = 1.275$ fm for neutrons and protons, respectively, while for the spin-orbit term $r_{so} = 1.31(1.32)$ fm for neutrons (protons). These potential parameters might not be optimal for the individual nuclei but give a good general N and Z dependence all over the nuclear chart, at least for our purpose of testing our method.

The single-particle energies e_i of the single-particle Hamiltonian were calculated by diagonalizing the matrix of the Hamiltonian in the h.o. basis having 20 principal h.o. quanta and maximal orbital angular momentum 9. (An increase of the

TABLE II. Neutron shell corrections δE_n and their variations σ calculated using the finite-range weight function (FR) and the generalized Strutinski procedure G in comparison with the semiclassical shell correction $\delta E_{sc} = E_{sc} - E^n_{sp}$ calculated for several nuclei. Their deviations from the semiclassical results $\Delta_{FR} = |\delta E_{sc} - \delta E_n(\text{FR})|$ and $\Delta_G = |\delta E_{sc} - \delta E_n(G)|$ are also shown. All energies are in MeV units.

Nucleus	δE_n(FR)	σ	$\delta E_n(G)$	σ	δE_{sc}	Δ_{FR}	Δ_G
^{68}Ni	0.16	0.12	0.50	0.07	0.81	0.65	0.31
^{78}Ni	−3.59	0.07	−2.78	0.16	−4.21	0.62	1.43
^{90}Zr	−7.42	0.06	−7.35	0.17	−6.82	0.60	0.53
^{122}Zr	−5.92	0.11	−4.52	0.15	−6.33	0.41	1.81
^{124}Zr	−4.12	0.12	−3.25	0.13	−4.35	0.23	1.10
^{100}Sn	−8.16	0.20	−6.95	0.23	−7.50	0.66	0.55
^{132}Sn	−9.85	0.14	−8.58	0.10	−8.87	0.98	0.29
^{146}Gd	−10.26	0.07	−10.33	0.20	−9.79	0.47	0.54

TABLE III. Proton shell corrections δE_p and their variations σ calculated using the finite-range weight function (FR) and the generalized Strutinski procedure G in comparison with the semiclassical shell correction $\delta E_{\rm sc} = E_{\rm sc} - E^n_{\rm sp}$ calculated for several nuclei. Their deviations from the semiclassical results $\Delta_{\rm FR} = |\delta E_{\rm sc} - \delta E_p({\rm FR})|$ and $\Delta_G = |\delta E_{\rm sc} - \delta E_p(G)|$ are also shown. All energies are in MeV units.

Nucleus	δE_p(FR)	σ	$\delta E_p(G)$	σ	$\delta E_{\rm sc}$	$\Delta_{\rm FR}$	Δ_G
^{90}Zr	1.59	0.19	1.88	0.20	1.44	0.15	0.44
^{100}Sn	−7.47	0.064	−7.42	0.14	−7.01	0.46	0.41
^{132}Sn	−7.39	0.068	−6.04	0.12	−6.64	0.75	0.60
^{146}Gd	4.89	0.10	5.28	0.24	4.52	0.37	0.76
^{180}Pb	−8.94	0.15	−7.78	0.04	−8.62	0.32	0.84
^{208}Pb	−7.57	0.07	−6.73	0.03	−7.29	0.28	0.56

size of the basis did not change the results.) The same basis was used for diagonalizing the free Hamiltonian (without nuclear potential terms) to get the positive energies $e_i^{(0)}$ needed to include the effect of the continuum in the Green's function method described in Ref. [16] in detail. From the difference of the smoothed level densities of the spectra of the true and the free Hamiltonians, the effect of the artificial nucleon gas cancels out and we get the same smoothed continuum level density as we could get by smoothing the continuum level density derived from the derivative of the scattering phase shifts [16].

In Fig. 5 we show the plateau curves for the ^{146}Gd nucleus with the finite-range smoothing and the result of the Wigner-Kirkwood calculation as a reference. The range of the p values used in the present work was taken to be the same as in Ref. [15] to make comparison with those results possible. Using the new method with the finite-range smoothing we are able to use the local plateau condition to choose the γ_p values where the $\delta E(\gamma, p)$ curves have minima for all the plateau curves shown. The shell correction values at the minima of the curves agree very well (within 500 keV) with the horizontal line representing the result of the semiclassical calculation. Because the σ variation of the $\delta E(\gamma_p, p)$ values in Eq. (24) is small the shell correction value calculated from the mean in Eq. (23) is well defined.

In Fig. 6 we show an example of the double-magic ^{132}Sn nucleus where the σ variation is smaller than 200 keV and the deviation from the semiclassical value Δ is less than 1 MeV. This is the largest deviation from the cases listed in Table II. One can observe in both Figs. 5 and 6 that the γ_p values, where the minima of the $\delta E(\gamma_p, p)$ appear, are increasing with increasing p values. This can be compensated to some extent if we use the renormalized smoothing range Γ_p defined in Eq. (32).

The $\delta E(\gamma_p, p)$ plateau curves are very similar for most nuclei we calculated if we select the values of the first γ_p minima of the different p curves beyond $\gamma_{p,\rm min}$ in Eq. (33). We identify the shell correction with the mean values of the $\delta E(\gamma_p, p)$ in Eq. (23) and its σ variation with the uncertainty of the shell correction.

In Table II we show the shell corrections for neutrons and for a set of medium and heavy nuclei resulting from the new smoothing procedure $\delta E_n(FR)$ and those of the generalized Strutinski procedure $\delta E_n(G)$. Their σ variations are in the third and fifth columns. In the last two columns we compare their values to those of the semiclassical procedure given in Ref. [13]. The differences from $\delta E_{\rm sc}$ are below 1 MeV for the new procedure, which is a bit better agreement than when using the generalized Strutinski procedure. The averages of the differences are 0.6 and 0.8 MeV for these two procedures, respectively.

In Table III we show similar results for protons, where the averages of the differences from the semiclassical results are 0.4 and 0.6 MeV for the new procedure and for the generalized Strutinski procedure, respectively. So the new procedure can be applied for protons as well.

TABLE IV. Shell correction δE_n, the variation σ in Eq. (24), and the semiclassical shell correction $\delta E_{\rm sc} = E_{\rm sc} - E^n_{\rm sp}$ calculated for several nuclei. The deviations $\Delta = |E_{\rm sc} - \tilde{E}|$ are also shown. All energies are in MeV units.

Nucleus	δE_n	σ	$\delta E_{\rm sc}$	Δ
^{16}O	−1.63	0.04	−1.57	0.06
^{18}O	2.67	0.04	3.01	0.34
^{20}O	3.25	0.24	3.11	0.14
^{22}O	0.12	0.53	0.09	0.03
^{24}O	−1.68	0.49	−1.69	0.01
^{20}Ne	3.07	0.56	3.01	0.06
^{40}Ca	−1.77	0.35	−0.66	0.97
^{48}Ca	−2.91	0.24	−2.59	0.32

TABLE V. Shell correction δE_p, the variation σ in Eq. (24), and the semiclassical shell correction $\delta E_{\rm sc} = E_{\rm sc} - E^p_{\rm sp}$ calculated for several nuclei. All energies are in MeV units.

Nucleus	δE_p	σ	$\delta E_{\rm sc}$	Δ
^{16}O	−1.65	0.03	−1.44	0.21
^{18}O	−1.65	0.10	−1.66	0.01
^{20}O	−2.09	0.19	−1.90	0.19
^{22}O	−2.30	0.15	−2.14	0.16
^{24}O	−3.10	0.66	−2.36	0.74
^{40}Ca	−1.62	0.12	−0.91	0.71
^{48}Ca	−1.70	0.19	−1.44	0.26
^{48}Ni	−0.80	0.36	−1.23	0.43
^{56}Ni	−3.67	0.29	−3.45	0.22

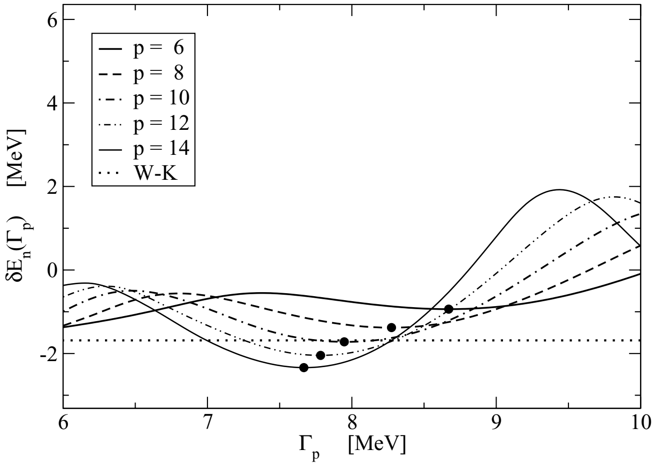

FIG. 7. Neutron shell correction $\delta E_n(\Gamma_p)$ for the nucleus ^{24}O as a function of the renormalized smoothing range Γ_p calculated for a set of p values by using the finite-range smoothing function f_p. The dotted horizontal line shows the semiclassical value $\delta E_{\rm sc} = E_{\rm sc} - E^n_{\rm sp}$.

These differences are not large, neither for neutrons nor for protons. The result of the new procedure is generally closer to the semiclassical result if we approach the drip lines. See, for example, the ^{78}Ni, ^{122}Zr, and ^{124}Zr nuclei for neutrons and the ^{180}Pb nucleus for protons. Therefore, we believe that the finite-range smoothing allows us to approach the drip line closer than we can approach it by using the infinite-range Gaussian weight function.

The basic advantage of the new method is, however, that the determination of the proper shell correction value is better defined. The values resulting from the new procedure are free from most of the uncertainties of the generalized Strutinski smoothing procedure. For example, they do not depend on the position of the interval where the linearity of the smoothed level density is required.

The most important advantage of the new procedure is that it can be applied for light nuclei where, as we have discussed in Sec. IV, the generalized Strutinski procedure cannot be applied.

The results of the new method for light nuclei are shown in Table IV for neutrons and in Table V for protons. One can see that the agreement with the semiclassical values is as good it was for heavier nuclei. We received especially good agreement for oxygen isotopes, even at the neutron drip line.

In Fig. 7 we show the neutron plateau curves for the new double-magic nucleus ^{24}O as functions of the renormalized smoothing range parameter Γ_p, for $p = 6, 8, \ldots, 14$. The semiclassical result is the dotted horizontal line. The minima of each curve are denoted by solid circles on the corresponding curves. One can see that the $\delta E_n(\Gamma_p, p)$ values denoted by circles are between -0.9 and -2.3 MeV and their Γ_p values are quite similar at $\Gamma_p \sim 8$ MeV. The variation of the $\delta E_n(\Gamma_p, p)$ values is $\sigma \sim 0.5$ MeV and their mean value coincides with the semiclassical value. This is certainly an accident but one can see that the Δ value is small for the other O isotopes too. Observe also that the positions of the minima of the different p curves in this figure scatter much less in Γ ($\sim$15%) than the locations of the minima in Fig. 6 where the smoothing range γ was used ($\sim$90%) or in Fig. 5 where the smoothing range γ was used ($\sim$70%).

Therefore, we believe that the finite-range smoothing allows us to approach the drip line closer than we can approach it by using the infinite-range Gaussian weight function.

VII. CONCLUSION

The new method uses a finite-range smoothing function that makes it possible to localize the effect of a single-particle state with energy e_i to a finite energy range: $[e_i - \gamma, e_i + \gamma]$. This localization makes it possible to extend the region of applicability of the emthod to closer to the end regions of the spectrum. This helps in calculating shell corrections for slightly bound nuclei lying closer to drip lines and also for lighter nuclei, where the shell gap is large; therefore, larger values of γ values are needed to smooth the shell structure out. The new method works equally well for calculating neutron and proton shell corrections.

We introduced a renormalized smoothing range in which the p dependence of the smoothing range was reduced considerably. Using this renormalized range the selection of the proper minima of the plateau curves was easier.

Therefore, we recommend the use of the new procedure with finite-range smoothing first of all for light nuclei, where the generalized Strutinski method cannot be applied. We also recommend its use in regions close to drip lines where the finite-range smoothing seems to work somewhat better than the generalized Strutinski method.

ACKNOWLEDGMENTS

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