Particle number conserving shell-correction method

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(Received 27 March 2004; published 12 October 2004)

The shell correction method is revisited. Contrary to the traditional Strutinsky method, the shell energy is evaluated by an averaging over the number of particles and not over the single-particle energies, which is more consistent with the definition of the macroscopic energy. In addition, the smooth background is subtracted before averaging the sum of single-particle energies, which significantly improves the plateau condition and allows one 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 is found in particular for highly degenerated single-particle spectra (as, e.g., in magic nuclei) while for deformed nuclei (where the degeneracy is lifted to a large extent) both estimates are close, except in the region of super or hyper-deformed states.

DOI: 10.1103/PhysRevC.70.044306 PACS number(s): 21.10.Dr, 21.10.Ma, 21.60.Cs, 21.60.Jz

I. INTRODUCTION

The macroscopic-microscopic method of evaluating the potential energy surfaces and binding energies of nuclei was proposed in the papers of Strutinsky [1] and Myers and Świątecki [2]. Despite the tremendous progress of self-consistent models to nuclear structure the macroscopic-microscopic method remains one of the most important tools. In such an approach the microscopic energy corrections are added to the macroscopic part of the nuclear binding energy described by the liquid drop model or other macroscopic methods. The microscopic part consists of shell and pairing energies. The prescription for the evaluation of the shell energy by smoothing the single-particle energy spectra was first given in Ref. [1] and then improved in Refs. [3,4]. This Strutinsky method of averaging over single-particle energies is still widely used up to now, in spite of its known problems which appear for mean-field potentials of finite depth as well as for nuclei close to the proton or neutron drip lines.

In the 1970s (see Refs. [5–10] and related papers) Strutinsky and Ivanyuk made an attempt to replace the original Strutinsky method of evaluating the smooth energy component by an averaging in the space of particle numbers ($\mathcal{N}$-space) that should be more consistent with the macroscopic part of the binding energy which is usually evaluated in a liquid-drop type approach. The parameters of such macroscopic models are usually obtained by a least-square fit to nuclear masses which corresponds to an averaging in the $\mathcal{N}$-space (e.g. in Ref. [11]). In Refs. [5,7] the smooth component of the total single-particle energy was approximated by a polynomial in $\mathcal{N}$-space with coefficients that were determined by a least-square fit. It was shown in Refs. [8,10] that the shell correction energies obtained by these two types of averaging procedures are not the same. Significant differences appear for highly degenerated single-particle spectra, as, e.g., in spherical nuclei. The method by Ivanyuk and Strutinsky of finding the smooth energy developed in Refs. [5,7,8,10] has reached sufficient accuracy to be used in practical calculations. It was, however, never widely used, probably because of its complexity.

Another way of separating out the smooth part of the sum of single-particle energies can be found in Ref. [12], where the liquid-drop type asymptotic expansion of the total single-particle energy in powers $A^{1/3}$ was used. Unfortunately this method of evaluating the average energy was not precise enough to be used in practice.

In the present paper a different method of evaluating the shell energy is proposed. The smooth component of the total single-particle energy is obtained by folding the sum of single-particle energies in the $\mathcal{N}$-space with a modified Gauss function as described in the Appendix. In addition, an average energy background as obtained by the harmonic oscillator energy sum rule (see Sec. II A below) is subtracted before performing the folding, which significantly increases the precision of the method. Our new prescription for the shell correction energy gives results close to those obtained in the Ivanyuk and Strutinsky approach of Refs. [8,10] and is extremely simple to use.

One should also mention that the shell energy evaluated with the present model conserves exactly the given number of particles, and not only on the average, as was the case in the traditional Strutinsky method.

II. THEORETICAL MODEL

In the macroscopic-microscopic method of evaluating potential energy one decomposes the nuclear binding energy into three parts

$$E(Z,A;\mathrm{def}) = E_{\mathrm{mac}}(Z,A;\mathrm{def}) + E_{\mathrm{shell}}(Z,A;\mathrm{def}) + E_{\mathrm{pair}}(Z,A;\mathrm{def}), \quad (1)$$

where Z and A are the charge and mass numbers, respectively. The macroscopic part, E_{mac}, depends on the deformation of nucleus and is usually evaluated in the liquid drop or some other more sophisticated model. The microscopic part of the energy consists of the shell and the pairing energies. The pairing energy E_{pair} is usually evaluated in the (projected or not) BCS formalism (see, e.g., [3] or [4]), while the shell energy E_{shell} is the sum of the proton and neutron contributions

$$E_{\rm shell}(Z,A;{\rm def}) = E^{p}_{\rm shell}(Z;{\rm def}) + E^{n}_{\rm shell}(A-Z;{\rm def}). \quad (2)$$

The shell correction energy of one kind of particles is equal to the difference

$$E_{\rm shell} = \sum_{i=1}^{\mathcal{N}} e_i - \widetilde{E}(N), \quad (3)$$

where $\mathcal{N}$ is the number of particle in the system and $\widetilde{E}$ is the smooth part of the total single-particle energy, where *smooth* means slowly varying with the particle number $\mathcal{N}$. In the following two different methods of evaluating of this smooth part will be presented.

A. Harmonic oscillator energy sum rule

The eigenenergies of the spherical harmonic oscillator

$$e_n = \left(n+\tfrac{3}{2}\right)\hbar\omega_0 \quad (4)$$

are strongly degenerated

$${\rm deg}_n = \tfrac{1}{2}(n+1)(n+2)\times 2. \quad (5)$$

Here $n=0,1,2,\ldots$ is the main quantum number and ω_0 is the harmonic oscillator frequency. The factor 2 in the above equation is due to the two possible orientations of the spin.

According to Ref. [13] the degeneracy of the main harmonic oscillator shell can be approximated by

$${\rm deg}_n \approx \left(n+\frac{3}{2}\right)^2 = \left(\frac{e_n}{\hbar\omega_0}\right)^2. \quad (6)$$

The total number of particles $\mathcal{N}$ occupying all shells up to $n=N$ is

$$\mathcal{N}(N) = \sum_{n=0}^{N} {\rm deg}_n = \frac{1}{3}(N+1)(N+2)(N+3). \quad (7)$$

It is easy to show [13] that for large N values the following approximation holds:

$$\mathcal{N}(N) \approx \frac{1}{3}\left(N+\frac{3}{2}\right)^3 = \frac{1}{3}\left(\frac{e_N}{\hbar\omega_0}\right)^3. \quad (8)$$

The last equation can serve as the average relation between the single-particle energy e and the number of particles which occupy the levels with energy smaller or equal to e,

$$\mathcal{N}(e) = \frac{1}{3}\left(\frac{e}{\hbar\omega_0}\right)^3, \quad (9)$$

or

$$e(\mathcal{N}) = (3\mathcal{N})^{1/3}\hbar\omega_0. \quad (10)$$

Equation (9) leads to the known expression for the average density of the harmonic oscillator single-particle levels

$$g = \frac{\partial\mathcal{N}}{\partial e} = \frac{e^2}{(\hbar\omega_0)^3} = \frac{(3\mathcal{N})^{2/3}}{\hbar\omega_0}. \quad (11)$$

The sum E of single-particle energies of all occupied levels is

$$E = \sum_{n=0}^{N} e_n {\rm deg}_n = \hbar\omega_0 \sum_{n=0}^{N}\left(n+\frac{3}{2}\right)(n+1)(n+2) \quad (12)$$

and can be approximated by the integral

$$\overline{E} = \int_0^{\mathcal{N}} e(\mathcal{N}')d\mathcal{N}'. \quad (13)$$

Inserting here Eq. (10) one obtains the following energy sum rule:

$$\overline{E} \equiv \overline{\left(\sum_{i=1}^{\mathcal{N}} e_i\right)} = \frac{1}{4}(3\mathcal{N})^{4/3}\hbar\omega_0. \quad (14)$$

The sum of energies of nucleons which occupy the harmonic oscillator levels is thus proportional to the $4/3$ *power of the total number of particles in the system.*

A more accurate estimate than the above one was made in Ref. [13]:

$$\overline{E} = \left[\tfrac{1}{4}(3\mathcal{N})^{4/3} + \tfrac{1}{8}(3\mathcal{N})^{2/3}\right]\hbar\omega_0. \quad (15)$$

The term proportional to $\mathcal{N}^{2/3}$ is important in the light systems but in the heavier nuclei it can be neglected as much smaller than the leading $\mathcal{N}^{4/3}$ term.

In the top l.h.s. part of Fig. 1 the sum E of single-particle energies (solid line) and its approximation $\overline{E}$ (dashed line) by Eq. (14) are shown as function of the number of particles $\mathcal{N}$. The deviation ΔE between both lines is hardly visible on this scale, so we present it separately in the top r.h.s. part of Fig. 1. The coefficient in front of the term $\mathcal{N}^{4/3}$ was obtained by a least square fit and turns out to be very close to the value of the approximate expression (14) which is exact in the limit $N\to\infty$. A strong shell structure corresponding to the harmonic oscillator magic numbers: $\mathcal{N}_n$=2, 8, 20, 40, 70, 112, 168, 240, 330, 440,… is observed. Using Eq. (9) one can obtain the approximate distance between the harmonic oscillator major shells as function of the particle number

$$\mathcal{N}_{n+1}^{1/3} - \mathcal{N}_n^{1/3} = \frac{1}{3^{1/3}}\frac{e_{n+1}-e_n}{\hbar\omega_0} = 3^{-1/3}. \quad (16)$$

The deviation ΔE of the energy sum from its approximate behavior as function of $N^{1/3}$ is presented in the bottom l.h.s. part of Fig. 1. It is seen that the distance between closed shells is nearly constant and roughly equal to $\Delta(\mathcal{N}^{1/3}) \approx 0.7$ which is the estimate, Eq. (16). It is worth noticing that the same data plotted as function of the single-particle energies e shows a structure (bottom r.h.s. of Fig. 1) which seems hard to interpret at first sight. Obviously the shell structure of the harmonic oscillator is more visible when one plots ΔE as function of $\mathcal{N}^{1/3}$.

The relation (14) was obtained assuming that the single-particle energies are measured with respect to energy zero. Assuming that the minimum of the harmonic oscillator potential corresponds to V_0 (i.e., $e_i \to e_i + V_0$) one can get the more general relation

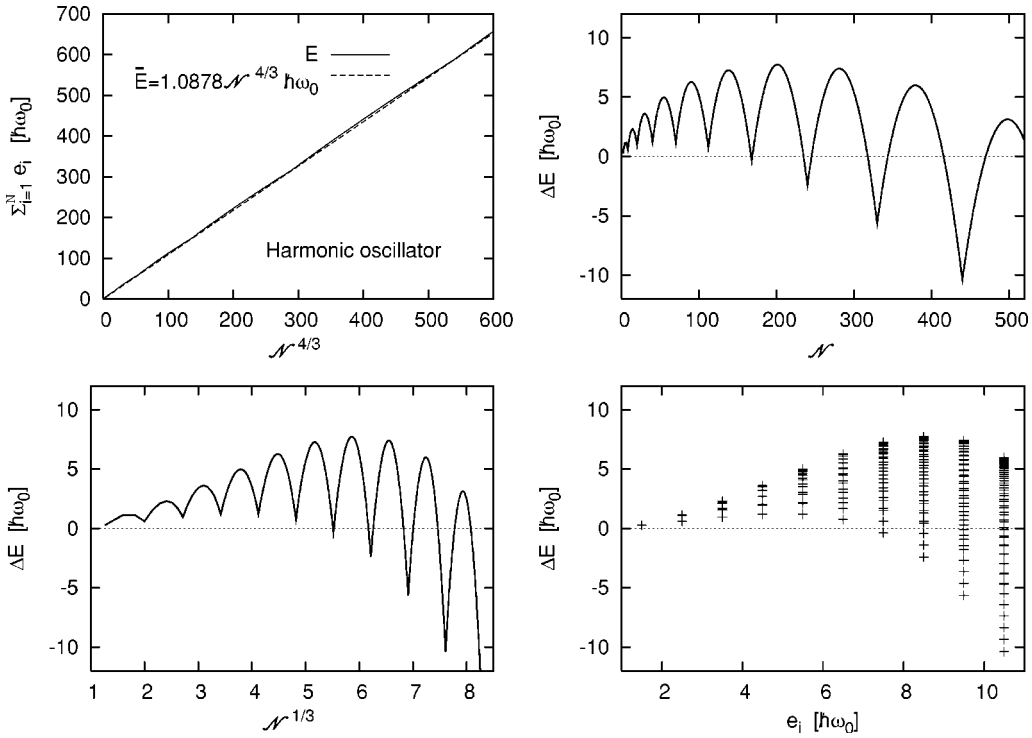

FIG. 1. Sum of the single-particle energies (E, solid line) and its approximation $\overline{E}$, dashed line) by Eq. (14) (top l.h.s. plot) as well as their difference ($\Delta E = E - \overline{E}$) in function of the number of particles $\mathcal{N}$ (top r.h.s. plot) $\mathcal{N}^{1/3}$ (bottom l.h.s. plot) and the single particle energies (e_i) (bottom r.h.s. plot).

$$\overline{E} = \overline{\left(\sum_{i=1}^{\mathcal{N}} e_i\right)} = a\mathcal{N}^{4/3} + V_0\mathcal{N}. \tag{17}$$

We have verified (numerically) that the above harmonic oscillator energy sum rule is universal and not only fulfilled by the spectra of the modified harmonic oscillator (Nilsson potential) or other finite depth model mean-field potentials (e.g., Saxon-Woods) but also by the single-particle spectra obtained self-consistently for the Hamiltonians associated with the Gogny or Skyrme effective forces.

A typical deviation of the sum of the single-particle energies (with respect to the bottom of the effective mean-field potential) from the estimate (17) is of the order of a few promilles for heavier nuclei. In Fig. 2 the sum of the single-particle energies (l.h.s. column) and its deviation (ΔE) (r.h.s. column) from the average trend, Eq. (17), is plotted as function of $Z^{4/3}$ for protons (top row) and $\mathcal{N}^{4/3}$ for neutrons (bottom row). The single particle energies of spherical ^{208}Pb were obtained self-consistently using the Hartree-Fock approximation to the Gogny Hamiltonian with the D1S force [14]. The parameters a and V_0 of Eq. (17) given in Fig. 2 are obtained by a least square fit. The arrows point to the Fermi-level positions and the dotted vertical lines mark the end of the bound state spectrum. A very pronounced shell structure of the proton and neutron spectra is visible in the r.h.s. plots.

B. Average of the sum of single-particle energies

Let us define a discrete sample of data, S_n, as the difference between the sum of the lowest available single-particle energies of the n fermion system and the corresponding background energy, $\overline{E}(n)$, obtained using the harmonic oscillator sum rule, Eq. (17),

$$S_n \equiv \sum_{i=1}^{n} e_i - \overline{E}(n) = \sum_{i=1}^{n} e_i - an^{4/3} - V_0 n. \tag{18}$$

The parameters a and V_0 are determined by minimizing the square deviation between the single-particle energy sum and $\overline{E}$,

$$\sum_{n=1}^{\mathcal{N}_{max}} S_n^2 = \min, \tag{19}$$

where $\mathcal{N}_{max}$ can be chosen as the maximal number of nucleons which can be put on the given single-particle energy spectrum.

Using the Gauss-Hermite folding procedure described in detail in the Appendix one can evaluate the average value of S_n corresponding to $\mathcal{N}$ nucleons,

$$\widetilde{S}_{\mathcal{N}} = \frac{1}{\gamma\sqrt{\pi}} \sum_{n=2,4}^{\mathcal{N}_{max}} \frac{2}{3n^{2/3}} S_n \exp\left\{-\left(\frac{\mathcal{N}^{1/3} - n^{1/3}}{\gamma}\right)^2\right\} \times f_6\left(\frac{\mathcal{N}^{1/3} - n^{1/3}}{\gamma}\right), \tag{20}$$

where f_6 is the sixth order polynomial given by Eq. (A26). The folding is performed not directly in the particle number n but in its cubic root since the distance between the major

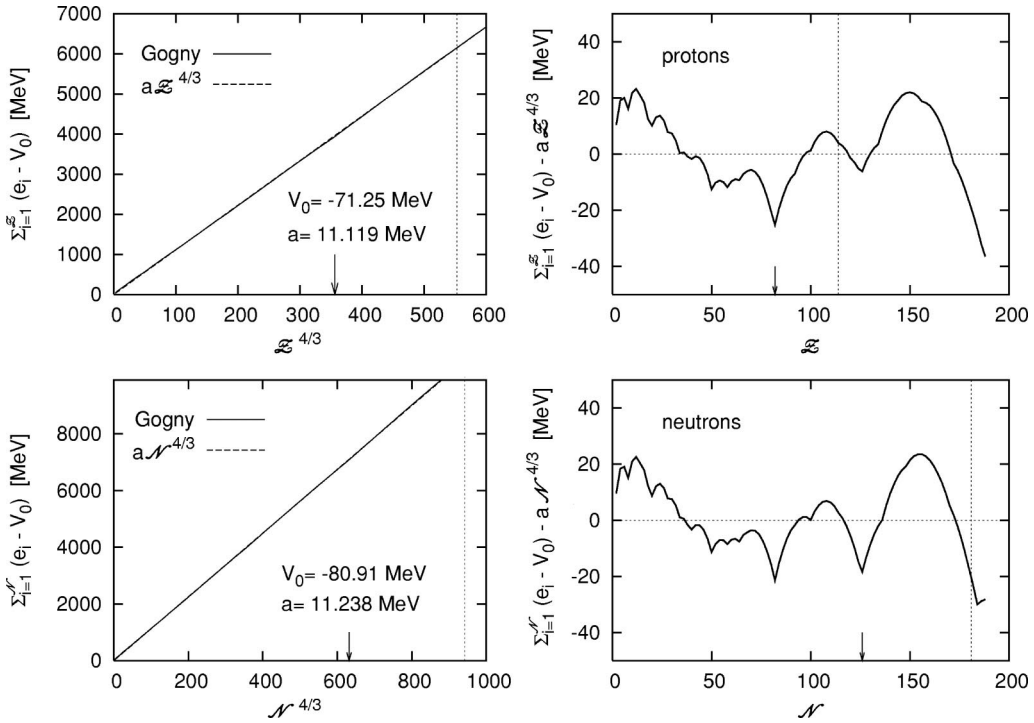

FIG. 2. Sum of the single-particle energies (E, solid line) obtained self-consistently with the Gogny D1S force for ^{208}Pb and its approximation ($\overline{E}$, dashed line) by Eq. (17) as well as the deviation from this average trend (r.h.s. plots) as function of the number of protons (top) or neutrons (bottom). Arrows indicate the position of the Fermi energy and the vertical lines mark the end of the bound spectrum.

harmonic oscillator shells is constant in $n^{1/3}$ and approximately equal 0.7 as we have shown above. The factor $3n^{2/3}$ in the denominator of Eq. (20) is the direct consequence of the transformation $n \rightarrow n^{1/3}$, while the factor 2 in the numerator is due to the spin degeneracy of the single-particle levels.

The smoothed energy of an even or odd N system is then

$$\widetilde{E}(\mathcal{N}) = \widetilde{S}_{\mathcal{N}} + a\mathcal{N}^{4/3} + V_0\mathcal{N}, \tag{21}$$

where we have restored the background energy $\overline{E}(\mathcal{N})$, Eq. (17), which has been subtracted from the single-particle energy sum in Eq. (18). Subtracting $\overline{E}(n)$ in (18) increases significantly the accuracy of evaluating the smoothed part $\widetilde{E}$ of the energy since the deviations S_n is two to three orders of magnitude smaller than the value of $\overline{E}(\mathcal{N})$. The smoothed energy obtained in this way is 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.

In Fig. 3 the sum of the single-particle energies (solid line) is compared with the new particle-number smoothed energy (dashed line) and the old Strutinsky energy (dotted line). The single particle spectrum is the one evaluated for the spherical Saxon-Woods mean-field potential for the ^{208}Pb nucleus with the parameters taken from Ref. [15]. The background energy $\overline{E}$ is subtracted from all three energies pre-

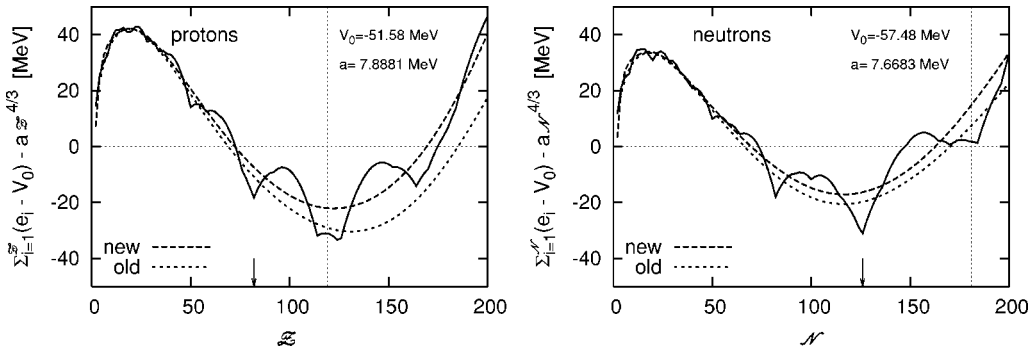

FIG. 3. Sum of the single-particle energies E (solid lines) obtained for the Saxon-Woods potential of ^{208}Pb and its smooth part obtained with Eq. (21) (fat dashed lines) as well as within the traditional Strutinsky method (thin dotted lines). From all the curves is subtracted the background energy evaluated as in Eq. (17). The data for protons and for neutrons are presented in the left and right parts, respectively. Arrows indicate the positions of the Fermi energies and the vertical dotted lines indicate the end of the bound spectra.

sented separately for protons (l.h.s. plot) and neutrons (r.h.s. plot). One notices that the Strutinsky energy is always smaller than the present estimate of the smoothed energy [16]. The difference between both estimates grows with the number of particles and for ^{208}Pb (arrows in Fig. 3) is of the order of a few MeV. This result is similar to the one obtained with the Ivanyuk and Strutinsky method [8,10], where the smoothed part of the sum of single-particle energies was approximated by a local polynomial in the $\mathcal{N}$-space.

C. Strutinsky smoothed energy

It is worthwhile to recall here the original Strutinsky method of evaluating of the smooth energy [1,3,4] in order to better understand the difference between both approaches. Strutinsky's way of evaluating the smooth energy consists of two steps. First one finds the smoothed single-particle level density $\tilde{g}(e)$ and determines the corresponding average position λ of the Fermi level, assuming the average particle number conservation. Then in the next step one evaluates the smoothed energy by integrating the product of the single-particle energy and smooth level density. It means that in this method the number of particles is conserved only on the average and the Strutinsky smoothed energy does not correspond exactly to the averaged sum of the occupied single-particle energies.

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

$$g(e) = \sum_i \delta(e - e_i), \tag{22}$$

with a smoothing function $j_n(e,e')$ of the nth order which is given by Eq. (A11). The smooth single-particle level density $\tilde{g}(e)$ is then given by

$$\tilde{g}(e) = \sum_i j_n\left(\frac{e - e_i}{\gamma_S}\right). \tag{23}$$

Taking the sixth-order (so-called "*curvature correction*") polynomial into account (see Eq. (A26)) the smoothing function has the following form:

$$j_6(u) = \frac{1}{\gamma_S\sqrt{\pi}} e^{-u^2}\left(\frac{35}{16} - \frac{35}{8}u^2 + \frac{7}{4}u^4 - \frac{1}{6}u^6\right). \tag{24}$$

The smearing parameter γ_S in Eqs. (23) and (24) is the width of the Gauss folding function and should be of the order of the energy distance between major shells (i.e., $\hbar\omega_0$) in order to wash out the shell structure.

According to Strutinsky [1] the average of the sum of the energies of the occupied single particle levels (E_{Str}) is given by the integral

$$E_{\mathrm{Str}} = \int_{-\infty}^{\lambda} 2e\tilde{g}(e)de, \tag{25}$$

where λ is the position of the Fermi energy in the system with the washed out shell structure and is fixed by the particle number condition

$$\mathcal{N} = \int_{-\infty}^{\lambda} 2\tilde{g}(e)de. \tag{26}$$

Here the average number of particles $\mathcal{N}=Z$ for protons or $\mathcal{N}=N$ for neutrons. The factor 2 in the above two equations is due to the spin degeneracy of the single particle levels. One solves Eq. (26) for λ by iterations.

The Strutinsky energy E_{Str} (25) is not equal to the average of the sum of single-particles energies $\tilde{E}$, Eq. (21), but corresponds to the energy of a system which conserves the number of particles only on the average (and not exactly as in Eq. (21)). A comparison of the resulting smoothed energies obtained in both methods will be presented below.

III. COMPARISON OF BOTH ESTIMATES OF THE SMOOTHED ENERGY

A significant difference between the new estimate of the smooth energy $\tilde{E}$ given by Eq. (21) and the Strutinsky energy, E_{Str}, Eq. (25), is demonstrated in Fig. 3. It can be easily explained as follows:

The sum of single-particle energies can be roughly approximated by Eq. (14) as shown in Sec. II A,

$$\overline{\left(\sum_{i=1}^{\mathcal{N}} e_i\right)} = a\mathcal{N}^{4/3} + b\mathcal{N}, \tag{27}$$

where the parameter a is proportional to the distance $\hbar\omega_0$ between major shells and b to the effective depth of the mean-field potential. Let us assume, just as a matter of discussing our method, that this average trend represents the true energy sum and that we are dealing with the degenerate spectrum. Also let $\mathcal{N}_k$ be the number of particles which can be placed on the single-particle levels which are below the kth degenerate level. Note that the numbers $\mathcal{N}_k$ (with $k=1,2,\ldots$) are simply the magic numbers in case of spherical nuclei.

The Strutinsky prescription for the smoothed energy corresponding to

$$\mathcal{N} = \tfrac{1}{2}(\mathcal{N}_{k+1} + \mathcal{N}_k) \tag{28}$$

particles (i.e., half filled shell) can be written as

$$E_{\mathrm{Str}} = a\mathcal{N}^{4/3} + b\mathcal{N}, \tag{29}$$

while the average over the interval $[\mathcal{N}_k,\mathcal{N}_{k+1}]$ of the energy, Eq. (27), is given by the integral

$$\widetilde{E} = \frac{1}{\Delta}\int_{\mathcal{N}-\Delta/2}^{\mathcal{N}+\Delta/2} (an^{4/3} + bn)dn, \tag{30}$$

where $\Delta = \mathcal{N}_{k+1} - \mathcal{N}_k$ is the degeneracy of the corresponding single-particle level. In the approximation (27) the difference between the average of the single-particle energy sum and the Strutinsky energy is

$$\Delta E = \widetilde{E} - E_{\mathrm{Str}} \approx \frac{1}{54}a\frac{\Delta^2}{\mathcal{N}^{2/3}}, \tag{31}$$

where $a \approx 3^{4/3}/4\hbar\omega_0$. This approximate expression indicates that the difference between the new and the old Strutinsky

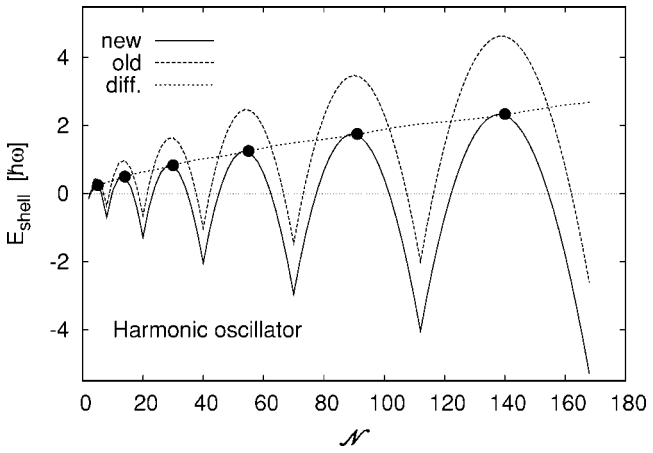

FIG. 4. Strutinsky shell energies for a spherically symmetric harmonic oscillator potential obtained with the new (Eq. (21), solid line) and the old (Eq. (25), dashed line) method (see the text) as well as the difference between them (dotted line) as function of number of particles $\mathcal{N}$. The estimates for the differences ΔE, given by Eq. (31), are marked as the closed circles.

energy is negligible (of the order of 0.01 MeV for heavier nuclei) when the degeneracy is $\Delta=2$ which is the case for deformed nuclei, while it grows significantly (up to a couple of MeV) when the degeneracy is important, as, e.g., in spherical nuclei.

In Fig. 4 we show the shell energy E_{shell} for the spherical harmonic oscillator single-particle levels in function of the nucleon number ($\mathcal{N}$). The solid line corresponds to the new approach described in Sec. II B while the dashed one to the old Strutinsky method (see Sec. II C). The difference between both estimates and its approximation with Eq. (31) are shown by the dotted line and the closed circles, respectively.

The proton and neutron shell energies E_{shell} for the nuclei ^{208}Pb and ^{232}Th obtained with a deformed Saxon-Woods potential are plotted in Fig. 5 as function of the elongation parameter c of Ref. [4]. The solid line corresponds to the new approach described in Sec. II B while the dashed one to the old Strutinsky method (see Sec. II C). The difference between both estimates is shown by the dotted line. The parameters of the Saxon-Woods potential are taken from Ref. [15]. It is seen that the difference between the shell energies evaluated with the new particle number conserving method and the traditional Strutinsky approach becomes negligible with growing nuclear deformation, i.e., when the degeneracy of single particle levels is lifted, a result which is in line with the prediction of the approximate expression (31).

In both (new and old) Strutinsky shell correction methods it is very important to choose the appropriate value of the smearing parameter (γ or γ_S). This is usually done by fixing its value such that the obtained shell energy is, over a certain range of that parameter independent of its specific value, a constraint known as the "*plateau condition*" of the Strutinsky method. Typical examples of such plateaus are shown in Fig. 6, where the shell energies for ^{208}Pb at a deformation of $c=1.2$ obtained with the appropriately chosen Saxon-Woods potential [15] are drawn. It is seen in Fig. 6 that our new approach leads to a much more pronounced plateau as compared to the old method. Note the different values of the smoothing parameter ($\gamma\approx 0.78$ for both kinds of particles versus $\gamma_S\approx 1.20\hbar\omega_0$ for protons and $\gamma_S\approx 1.05\hbar\omega_0$ for neutrons).

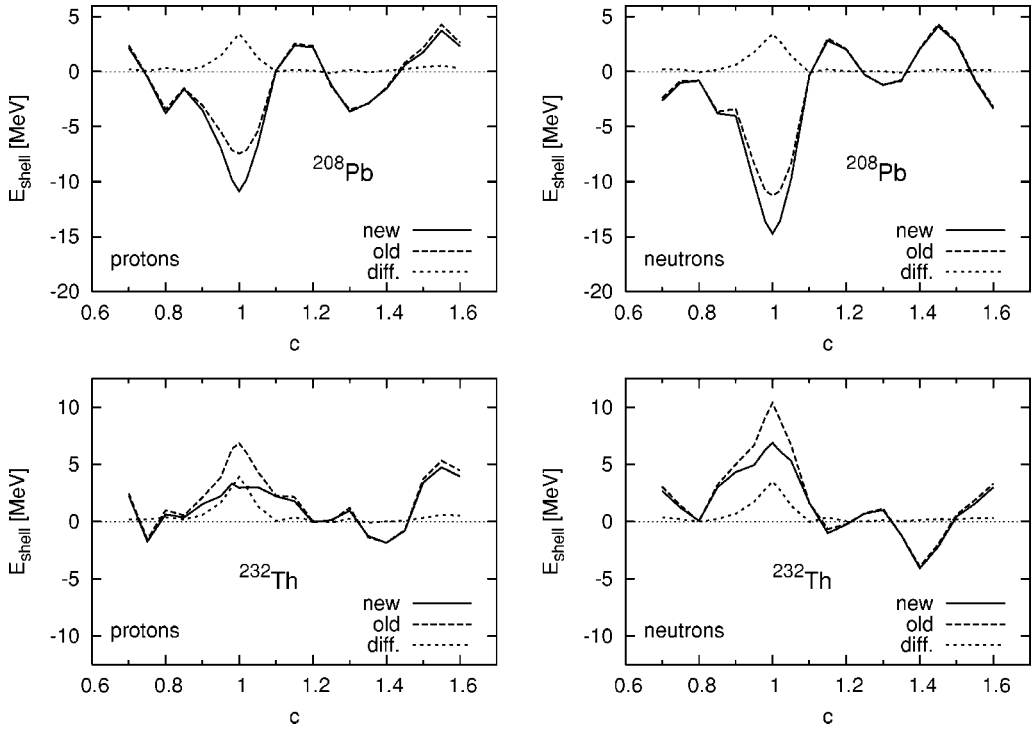

FIG. 5. Protron (left) and neutrons (right) Strutinsky shell energies for the Saxon-Woods single-particle levels of ^{208}Pb (top) ^{232}Th (bottom) obtained with the new (Eq. (21), solid line) and the old (Eq. (25), dashed-line) methods as well as their difference (dotted line) as functions of the elongation parameter c [4].

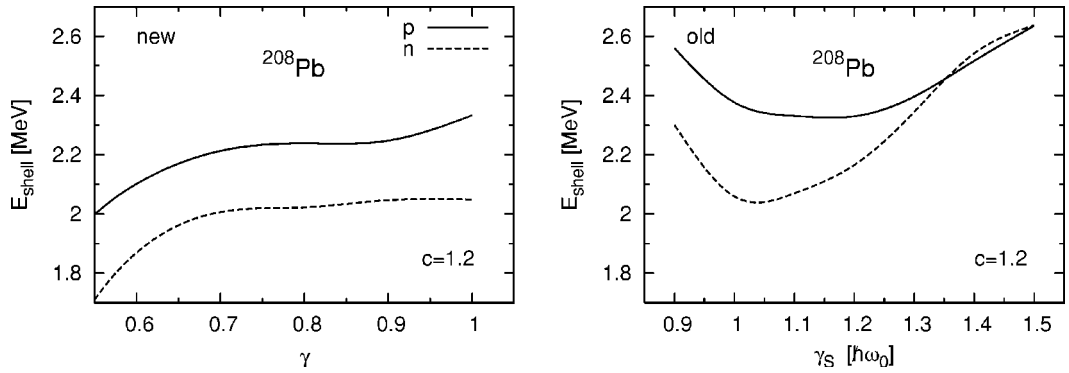

FIG. 6. Dependence of proton (solid line) and neutron (dashed line) Strutinsky shell energies as function of the smearing parameter γ (or γ_S) obtained with the new (Eq. (21), left) and the old (Eq. (25), right) estimates for the smooth energy for a nucleus ^{208}Pb described by an appropriate Saxon-Woods potential at a deformation of $c=1.2$.

Looking at Fig. 5 one could have the impression that a significant difference between the shell energies obtained by the averaging in the particle-number or single-particle energy spaces appears around spherical shapes and vanishes with growing deformation. On the other hand, Eq. (31) predicts that a significant difference between both types of averaging procedures should appear whenever a large degeneracy of the single-particle levels is present. A good example of the spectrum which becomes strongly degenerate at some deformation points is the eigenenergies of the anisotropic harmonic oscillator. The degeneracy clearly appears at those ellipsoidal deformation (ε, [3]) points where the ratio of the axes is equal to the ratio of small integers as can be seen in the left part of Fig. 7, where such a spectrum is plotted. The harmonic oscillator single-particle levels presented there were used to evaluate the shell energy of a system composed of $\mathcal{N}=100$ particles. The difference between the new and the old estimates ($\widetilde{E}$ and E_{Str}) is plotted as function of the quadrupole deformation parameter ε [3]. A large difference between both approaches appears where the degeneracy of levels grows. A similar effect was already observed in Ref. [8]. This result clearly shows that using the new approach one can expect some modifications in the potential energy surface not only around spherical shapes but also at deformations which correspond to the super- or hyper-deformed isomers.

IV. SUMMARY AND CONCLUSIONS

A new method of evaluating the smooth part of the total single-particle energy is proposed. The folding of the sums of single-particle energies is performed in the particle-number space rather than in the one of single-particle energies as done in the old Strutinsky method. The averaging in the $\mathcal{N}$-space is consistent with the definition of the macroscopic energy component which represents the average behavior in Z and A of the nuclear binding energy.

One has also to notice that the integral over $\mathcal{N}$ of the shell energy evaluated with the new prescription is close to zero for sufficiently large number of particles, while this is not the case for the traditional Strutinsky shell correction which grows systematically with $\mathcal{N}$. This indicates that the original Strutinsky prescription generates shell energy which does not fluctuate around zero when the number of particles is increased which modifies systematically the macroscopic part of the energy. In addition this modification depends on the shape of nucleus, so that this deficiency of the traditional approach cannot be corrected by an adjustment of the parameters of the macroscopic energy.

The global particle-number dependence of the energy given by the harmonic oscillator sum-rule (14) is subtracted from the sum of the single-particle energies when its average in the $\mathcal{N}$-space is evaluated. The effect of this renormaliza-

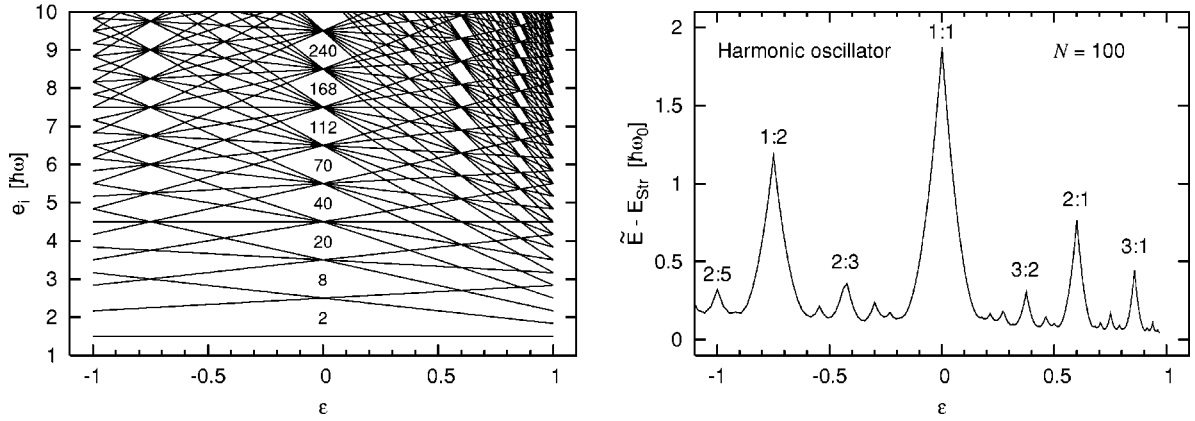

FIG. 7. The eigenfunction of the deformed harmonic oscillator potential (l.h.s. plot) and the difference between the new ($\widetilde{E}$, Eq. (21)) and the old (E_{Str}, Eq. (25)) estimates of the smooth energy as function of the axial quadrupole deformation ε [3].

tion (18)–(21) on the value of the shell energies is almost neligible for the β-stable nuclei but it becomes more important in case of nuclei close to the proton or neutron drip-line. It is due to the fact that the renormalized sum of the single-particle energies (S_n, Eq. (18)) is of the order of a few tens of MeV only, not thousands of MeV as it was in the traditional Strutinsky method. It means that the energy cut-off of the single-particle spectrum produces much smaller inaccuracy in evaluating of the shell-energy. The same is true when one discusses the effect of the continuum, which gives hope that the new $\mathcal{N}$-averaging method will give reliable shell energies in a broad range of isotopes and isotones. In forthcoming papers we are going to compare the estimates obtained with the present method with the results given by the semiclassical Wigner-Kirkwood expansion [17] or by the method based on the Green's function [18] especially developed for nuclei close to the drip-lines.

The new estimate differs significantly from the Strutinsky smoothed energy when a large degeneracy of the single-particle levels is present as this is the case in spherical and nearly-spherical nuclei or in some shape isomers. In such nuclei the shell energy is shifted down by a few MeV with respect the old predictions while its amplitude is almost unchanged as function of the particle number. This means that the macroscopic-microscopic method with the new estimate of the shell energy will, *when leaving the parameters of the macroscopic and microscopic parts untouched*, predict the magic and quasi-magic nuclei as well as some shape isomers more bound than this were predicted by the calculations done with the old Strutinsky method. Also the deformation energies of non-magic nuclei will be smaller and one could obtain different equilibrium shapes (i.e., ground state quadrupole moments). The fission barrier for spherical nuclei will also be significantly increased and, as a consequence, the spontaneous fission of such nuclei (e.g., some super-heavy isotopes) will be less probable. In addition the Q-value for an α-decay will be modified when it occurs between deformed and spherical isotopes (or vice versa). This means that the consequences of the naive use of the new method could be dramatic. One must also not forget that taking into account the particle-phonon coupling can significantly decrease the magnitude of the shell energy for spherical nuclei and its dependence on deformation as was shown in Ref. [16]. This effect, of the order 5 MeV for double-magic nuclei, was omitted in the majority macroscopic-microscopic calculations with the traditional Strutinsky shell correction.

I would therefore like to end with the following warning:

Do not use the new prescription for the shell energy (Eqs. (18)–(21)) in practical calculations without an appropriate readjusting of the parameters of the mean-field potentials (e.g., Saxon-Woods, Nilsson, Yukawa-folded), macroscopic models (e.g. liquid drop, finite range droplet or Thomas-Fermi), and the pairing force.

ACKNOWLEDGMENTS

The author wishes to express his thanks for the warm hospitality extended to him by the Institute for Subatomic Research (IReS) and the Louis Pasteur University of Strasbourg where part of this work was done. Discussions with Professor Jerzy Dudek who was *Spiritus Movens* of this research and Professor Johann Bartel from IReS as well as Professor Fedor Ivanyuk of the Institute of Nuclear Physics in Kiev and Professor Klaus Dietrich from TU-Munich were also very helpful.

APPENDIX: FOLDING OF DISCRETE DATA

1. General formulas

Our aim is to approximate a sample of N ordered points $\{x_i, y_i\}$ by a continuous smooth function $\tilde{y}(x)$. We would like to solve this problem using the Gauss-Hermite folding method which was an idea originally proposed by V.M. Strutinsky [1] and later on generalized in Ref. [3]. Having the width of the folding function comparable with the average distance between points x_i one can obtain the folded function which is very close to the data points but increasing this width one can also wash out the fine structure stored in the data. Usually the Strutinsky method was used to realize the second scope. The parameter of the folding procedure will be determined by the requirement that the integral of the folded function should be the same as the integral evaluated with the sample of $\{x_i, y_i\}$ pairs using the trapezium rule.

Let $j_n(x,x')$ be a symmetric function of its arguments (i.e., $j_n(x,x')=j_n(x',x)$) having the following properties:

$$\int_{-\infty}^{+\infty} j_n(x,x')dx = 1 \tag{A1}$$

for each $x' \in (-\infty, +\infty)$ and

$$P_k(x) = \int_{-\infty}^{+\infty} P_k(x') j_n(x,x')dx', \tag{A2}$$

where $k \leqslant n$ are even natural numbers and $P_k(x)$ is an arbitrary polynomial of order k. In the following, the function $j_n(x,x')$ will be called the folding function of the nth order. The last equation, frequently called the *Strutinsky condition*, ensures that the folding does not change the average behavior of the function $Y(x)$ which is represented by the ensemble of $\{x_i, y_i\}$ points. An example of such a folding function can be a combination of the Gauss function and the Hermite polynomials of the argument proportional to $|x-x'|$, frequently used in the Strutinsky shell correction method [1,3]. More detailed description of such a folding function will be given in the next section.

With each discrete point (x_i, y_i) one can associate the function $\tilde{y}_i(x)$ defined by

$$\tilde{y}_i(x) = \int_{-\infty}^{+\infty} y_i \delta(x' - x_i) j_n(x,x')dx', \tag{A3}$$

where $\delta(x)$ is the Dirac δ-function. A straightforward calculation gives

$$\tilde{y}_i(x) = y_i j_n(x,x_i). \tag{A4}$$

Using Eq. (A1) it is easy to verify that the integral of the function $\tilde{y}_i(x)$ is

$$\int_{-\infty}^{+\infty} \tilde{y}_i(x)dx = y_i. \tag{A5}$$

Let us construct the function $\tilde{y}(x)$ by summing up, with weight w_i all functions $\tilde{y}_i(x)$,

$$\tilde{y}(x) = \sum_{i=1}^{N} w_i \tilde{y}_i(x). \tag{A6}$$

The function $\tilde{y}(x)$ is an approximation of $y(x)$ if the weights w_i are determined from the assumption that the integrals of the unfolded and folded function are (nearly) equal:

$$\sum_{i=1}^{N} y(x_i)\Delta x_i = \int_{-\infty}^{+\infty} \tilde{y}(x)dx = \sum_{i=1}^{N} w_i y_i, \tag{A7}$$

where Δx_i is set to

$$\Delta x_i = \tfrac{1}{2}(x_{i+1} - x_{i-1}). \tag{A8}$$

Equation (A7) implies that a reasonable choice of the weight is

$$w_i = \Delta x_i. \tag{A9}$$

Thus the folded function $\tilde{y}(x)$ is given by

$$\tilde{y}(x) = \sum_{i=1}^{N} y_i \Delta x_i j_n(x, x_i). \tag{A10}$$

2. Gauss-Hermite folding function

Let the folding function $j_n(x,x')$ be defined with the help of the Gauss function as

$$j_n(x,x') = \frac{1}{\gamma\sqrt{\pi}} \exp\left[-\left(\frac{x-x'}{\gamma} \right)^2 \right] f_n\left(\frac{x-x'}{\gamma} \right), \tag{A11}$$

where γ is a parameter and $f_n((x-x')/\gamma)$ is the so-called corrective polynomial of nth order, determined by the Strutinsky condition (A2). In the following we would like to evaluate the coefficients of the corrective polynomial using some properties of the Hermite polynomials which are orthogonal with the weight equal to the Gauss function.

Let us introduce a variable $u=(x-x')/\gamma$ defined in the interval $(-\infty, +\infty)$. The smearing function $j_n(x,x')$ and the polynomial $P_n(x)$ in (A2) can now be written as

$$j_n(x,x') = \frac{e^{-u^2}}{\gamma\sqrt{\pi}} f_n(u), \tag{A12}$$

$$P_n(x') = P_n(x - \gamma u) \equiv P'_n(u), \tag{A13}$$

and

$$P_n(x) = P_n(x + \gamma 0) \equiv P'_n(0). \tag{A14}$$

The so far arbitrary polynomial $P'_n(u)$ can be written down as a series of the Hermite polynomials of order i,

$$P'_n(u) = \sum_{i=1}^{n} a_i H_i(u). \tag{A15}$$

Now the condition (A2) can be written as

$$P'_n(0) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} P'_n(u) \mathrm{e}^{-u^2} f_n(u)du \tag{A16}$$

and inserting relation (A15) into (A16) one obtains

$$\sum_{i=1}^{\mathrm{p}} a_i \left\{ \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-u^2} H_i(u) f_n(u)du - H_i(0) \right\} = 0. \tag{A17}$$

On the other hand, the last equation should be fullfiled for arbitrary values of $a_i \neq 0$, which leads to the following set of equations:

$$\frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-u^2} H_i(u) f_n(u)du = H_i(0), \tag{A18}$$

where $i=0,2,\ldots,n$. From the other side the corrective function $f_n(u)$ can also be decomposed in terms of the Hermite polynomials

$$f_n(u) = \sum_{k=1}^{n} C_k H_k(u). \tag{A19}$$

Inserting the above relation into Eq. (A18) gives

$$H_i(0) = \sum_{k=1}^{r} C_k \frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} \mathrm{e}^{-u^2} H_i(u) H_k(u)du. \tag{A20}$$

Then using the orthogonality properties of the Hermite polynomials

$$\frac{1}{\sqrt{\pi}} \int_{-\infty}^{+\infty} e^{-u^2} H_i(u) H_k(u)du = 2^i i!\, \delta_{ik}, \tag{A21}$$

one obtains the coefficients of the corrective polynomial (A19),

$$C_i = \frac{1}{2^i i!} H_i(0). \tag{A22}$$

The values of the Hermite polynomials at zero are

$$H_i(0) = \begin{cases} 1 & \text{for } i = 0 \\ 2^n(-1)^n(2n-1)!! & \text{for } i = 2n \\ 0 & \text{for } i = 2n+1, \end{cases} \tag{A23}$$

so that

$$C_i = \begin{cases} 1 & \text{for } i = 0 \\ (-1)^n \dfrac{(2n-1)!!}{2^n(2n)!} & \text{for } i = 2n > 0 \\ 0 & \text{for } i = 2n+1. \end{cases} \tag{A24}$$

The first few coefficients C_i and the corresponding Hermite polynomials are:

$$\begin{aligned} C_0 &= 1, \quad H_0(u) = 1, \\ C_2 &= -\tfrac{1}{4}, \quad H_2(u) = 4u^2 - 2, \\ C_4 &= +\tfrac{1}{32}, \quad H_4(u) = 16u^4 - 48u^2 + 12, \\ C_6 &= -\frac{1}{384}, \quad H_6(u) = 64u^6 - 480u^4 + 720u^2 - 120, \end{aligned} \tag{A25}$$

and the resulting corrective polynomials have the following form:

$$\begin{aligned} f_0(u) &= 1, \\ f_2(u) &= \tfrac{3}{2} - u^2, \\ f_4(u) &= \tfrac{15}{8} - \tfrac{5}{2}u^2 + \tfrac{1}{2}u^4, \\ f_6(u) &= \tfrac{35}{16} - \tfrac{35}{8}u^2 + \tfrac{7}{4}u^4 - \tfrac{1}{6}u^6. \end{aligned} \tag{A26}$$

Finally the function $\tilde{y}(x)$ approximated using the Gauss-Hermite folding reads:

$$\tilde{y}(x) = \frac{1}{\gamma\sqrt{\pi}} \sum_{i=1}^{N} y_i \Delta x_i \exp\left[-\left(\frac{x - x_i}{\gamma} \right)^2 \right] f_n\left(\frac{x - x_i}{\gamma} \right). \tag{A27}$$

In principle the smearing parameter γ is arbitrary and it can be different at each point x_i. But it should be related to the distance Δx_i between subsequent points if one would like to approximate the function stored in the mesh of $\{x_i, y_i\}$ points. Similarly one has to choose γ of the order of the period-length of the fine structure (e.g., shell effects) in case where one would like to wash out this structure from the function $y(x)$.

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