Connection between the Strutinsky level density and the semiclassical level density

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We establish an analytical link between the level density obtained by means of the Strutinsky averaging method and the semiclassical level density. This link occurs only in the so-called asymptotic limit. It turns out that the Strutinsky method amounts to an approximation to the semiclassical method. This approximation contains an unavoidable remainder that constitutes an intrinsic noise in comparison to the semiclassical method. Thus, the problem of the dependency of the Strutinsky procedure on the two free smoothing parameters of the averaging is intimately connected to this noise. However, we demonstrate that the noise of the method is small in the average density of states and in the average energy, whereas it might be non-negligible in the shell correction itself. To improve this method, we give a rule that consists simply of minimizing the relative error for the average energy.

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I. INTRODUCTION

The inclusion of Strutinsky's shell correction [1–3] in the liquid-drop model [4], namely, the so-called macroscopic-microscopic method, has allowed considerable improvements in the predictions of nuclear masses [5], and in the calculations of the fission barriers as well [6,7]. Nowadays, despite progress of the more basic microscopic models (such as self-consistent models), it remains in frequent use.

This method consists essentially of combining the liquid-drop model (macroscopic model), where the binding energy varies slowly as a function of the number of nucleons N and Z, with a shell correction varying abruptly with N and Z. The latter is due to the nonuniformity of the shell structure of the energy levels. It is extracted from a single-particle Hamiltonian (microscopic model) according to an original idea of Strutinsky.

The Strutinsky method is mainly based on a particular smoothing procedure of the density of states. Although this method is very efficient, it contains two weak points:

(1) It depends on the results of two well-known inherent parameters (i.e., the width γ and the order M of the smoothing).
(2) It is difficult to treat the continuum encountered with realistic mean potentials.

The purpose of the present work is summarized in the following points:

(1) The Strutinsky method can be derived rigorously from the point of view of the least-squares approximation of the level density. The equivalence between this point of view and the well-known standard averaging appears trivial.
(2) In this work, it is proved analytically that the averaged level density obtained by the Strutinsky method is simply an approximation to the semiclassical level density. In this respect, the semiclassical level density can be considered as the "true" (i.e., exact) smooth density.
(3) It is mainly shown that, in comparison with the semiclassical method, the Strutinsky method is characterized by a remainder that contains all the dependence on the two smoothing (free) parameters and hence is the source of the "noise" of the averaging procedure.
(4) Concerning the smooth density of states and the smooth energy, it is demonstrated that the Strutinsky method is reliable. However, the shell correction itself must be treated with care because it is very sensitive to the choice of the two free averaging parameters. In this context, to improve the method, we propose the "rule of the relative remainder."
(5) It is explained why the Strutinsky method fails near the zero-energy point (top of the well) for finite mean potentials.

II. STRUTINSKY AVERAGING

A. Bases and phenomenology of Strutinsky's method

In spite of the complexity of the nuclear forces, it appears that most of the binding energy of the nuclei is well described by the so-called liquid-drop model. This simple phenomenological approach is of a classical type. This means that the quantum effects, or more precisely, the shell effects, are ignored by this model. This causes systematic discrepancies between the theoretical predictions and the experimental data

However, it is known that such effects are contained in the shell model, but the latter is unable to reproduce correctly the general trends of the binding energy. To solve this dilemma, Strutinsky has proposed combining the binding energy of the liquid-drop model with a small (but essential) correction deduced from the shell model. This can be written as

$$E\ (\text{Binding Energy}) = E\ (\text{Liquid Drop Model}) + \delta E\ (\text{Shell Correction}).$$

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The shell correction is calculated from a mathematical prescription outlined by Strutinsky. It is obtained by summing the single-particle energies of a phenomenological shell-model potential and subtracting the average (smooth) part of this quantity:

$$\delta E \text{ (Shell Correction)} = \sum_i \epsilon_i - \overline{\sum_i \epsilon_i}.$$

As already mentioned, this method is often called the macroscopic-microscopic method because it mixes two very different models. Such a duality is obviously not free from inconsistency. Nevertheless, it is possible to give a microscopic basis to this "model" within the Hartree-Fock (HF) approximation by making some simple assumptions [2,3].

This consists essentially of expanding the HF energy around its semiclassical approximation, thus obtaining the so-called Strutinsky energy theorem:

$$E(\rho) = E(\bar{\rho}) + \left(\sum_i \epsilon_i - \overline{\sum_i \epsilon_i} \right) + O_2. \tag{1}$$

Here ρ is the HF density matrix, and $\overline{\rho}$ is its semiclassical approximation, which is a smooth quantity, free of shell effects. For this reason $\overline{\rho}$ can be assimilated to the classical average part (i.e., without quantal variations) of ρ. The sums of single-particle energies $\Sigma\epsilon_i$ and $\overline{\Sigma\epsilon_i}$ are related, respectively, to ρ and $\overline{\rho}$. Finally, O_2 is a quantity of the second order in the operator $\rho - \overline{\rho}$ and is generally negligible (for details see Ref. [8]).

It is clear from Eq. (1) that this macroscopic-microscopic method described here is a "schematic" interpretation of this theorem. The quantity $E(\overline{\rho})$ can be replaced by the energy of the liquid-drop formula, and the shell correction is deduced from a phenomenological one-body Hamiltonian.

It is also to be noted that a complete microscopic approach of this theorem remains possible. For example, in Ref. [9] the authors use a method referred to as the extended Thomas Fermi plus Strutinsky integral (ETFSI) method. In the latter, the semiclassical quantity $E(\overline{\rho})$ is deduced self-consistently from a microscopic effective interaction (Skyrme III). The shell correction is then added to $E(\overline{\rho})$.

In the following, we will mainly focus on two points:

(i) the mathematical aspect of the Strutinsky smoothing and
(ii) the link between this smoothing and the semiclassical approximation, and its consequences.

B. The exact level density

Strutinsky averaging can be derived by various formal approaches [1–3,6,7,10,11]. In this work, we will derive it from the point of view of the least-squares approximation. In fact, this point was suggested earlier by Bunatian and co-authors [12]. The least-squares approximation will help us understand why Strutinsky averaging fails near the edge of realistic potentials.

For an entirely discrete spectrum the level density of states is defined by

$$g_o(\epsilon) = \sum_{n=0}^{\infty} \delta(\epsilon - \epsilon_n). \tag{2}$$

In the following, this density will be called the "exact quantum level density," or the "exact level density," because it is a true quantum quantity, as opposed to its semiclassical approximation, or as opposed to the level density obtained from $g_o(\epsilon)$ by Strutinsky averaging (see the following).

In fact, Eq. (2) concerns uniquely infinite potentials without a continuum. Finite potentials will be treated separately at the end of this paper.

C. Polynomial approximation to the exact level density

Let $g_M(\epsilon)$ be a polynomial approximation of order M to the "exact" level density. More precisely, we seek this approximation in the vicinity of a point λ (which actually represents the Fermi level) in an effective interval $[-\gamma + \lambda, \lambda + \gamma]$, by using the Gaussian weight $\exp[-(\epsilon - \lambda)^2/\gamma^2]$. For this reason, the cited polynomial must depend a priori not only on M but also on γ and λ. Therefore, it will be denoted $\overline{g}_{M,\gamma}(\epsilon, \lambda)$. For our purpose, it will be convenient to write this polynomial as a linear combination of Hermite polynomials H_k:

$$\overline{g}_{M,\gamma}(\epsilon, \lambda) = \sum_{k=0}^{M} c_k H_k \left(\frac{\epsilon - \lambda}{\gamma} \right).$$

Thus, we must look for the polynomial $g_{M,\gamma}(\epsilon, \lambda)$ that minimizes the integral

$$I(\lambda, M, \gamma) = \int_{-\infty}^{\infty} [g_o(\epsilon) - \overline{g}_{M,\gamma}(\epsilon, \lambda)]^2 e^{-\left(\frac{\epsilon-\lambda}{\gamma}\right)^2} d\epsilon. \tag{3}$$

This procedure is a local averaging in the sense of the least-squares fit. Minimizing Eq. (3) with respect to the coefficients c_k, and using the orthogonality property of the Hermite polynomials, we find

$$\begin{aligned} \overline{g}_{M,\gamma}(\epsilon, \lambda) &= \sum_{m=0}^{M} c_m(\lambda, \gamma) H_m \left(\frac{\epsilon - \lambda}{\gamma} \right), \\ c_m(\lambda, \gamma) &= \frac{1}{m! 2^m \sqrt{\pi}} \sum_{n=0}^{\infty} H_m(u_n) \frac{1}{\gamma} \exp\left[- u_n^2 \right], \\ u_n &= \frac{\epsilon_n - \lambda}{\gamma}. \end{aligned} \tag{4}$$

As we shall see in the next section, Eq. (4) is not the final definition of the averaging, which thus appears somewhat more subtle.

D. Strutinsky's averaging as a moving average

In Eq. (4) the Fermi level λ is supposed to be fixed, and the polynomial $\overline{g}_{M,\gamma}(\epsilon, \lambda)$ smoothes the exact level density only in the vicinity of λ. Thus only a part of the spectrum is "smoothed" (i.e., the part $\epsilon \simeq \lambda$). To avoid this drawback, it

is necessary to consider λ as a variable. The averaged level density is thus defined as $\overline{g}_{M,\gamma}(\epsilon,\lambda)$, making $\epsilon=\lambda$. This amounts to performing a moving average (i.e., λ is moved with ϵ, "centering" ϵ on λ).

In the following, we shall call the function $g_{M,\gamma}(\lambda,\lambda)$ the Strutinsky's level density, and we will note it simply by $\overline{g}_{M,\gamma}(\lambda)$.

Since the coefficients c_m in Eq. (4) depend on λ, the Strutinsky's quantity $\overline{g}_{M,\gamma}(\lambda)$ is, in general, not a polynomial in λ. However, it is clear that, although the Strutinsky level density is not really a polynomial, it behaves locally ($\sim\lambda\pm\gamma$), like a least deviating polynomial approximation for the exact level density $g_o(\lambda)$ given by Eq. (2).

Explicitly, we must replace ϵ with λ in Eq. (4):

$$\begin{aligned}
\overline{g}_{M,\gamma}(\lambda) &= \sum_{n=0}^{\infty} F_M(u_n), \quad u_n=\frac{\epsilon_n-\lambda}{\gamma},\\
F_M(x) &= \widetilde{P}_M(x)\frac{1}{\gamma}\exp(-x^2),\\
\widetilde{P}_M(x) &= \sum_{m=0}^{M} A_m H_m(x), \quad A_m=\frac{H_m(0)}{m!2^m\sqrt{\pi}},\\
H_m(0) &= (-1)^{m/2}m!/(m/2)! \quad \text{if } m \text{ is even},\\
H_m(0) &= 0 \text{ if } m \text{ is odd}.
\end{aligned} \tag{5}$$

In Eq. (5) the polynomial $\widetilde{P_M}$ constitutes the so-called curvature correction term.

It is easy to check that the expression (5) obtained from a least-squares fitting can be written as the usual folding procedure of the exact level density [13,14]:

$$\overline{g}_{M,\gamma}(\lambda)=\int_{-\infty}^{\infty} g_o(\epsilon)F_M\left(\frac{\epsilon-\lambda}{\gamma}\right)d\epsilon, \tag{6}$$

which demonstrates the equivalence between the two points of view [i.e., between the local least square smoothing Eq. (3) and the averaging Eq. (6)].

It should be noted that if M increases to infinity and/or γ decreases to zero, then $\overline{g}_{M,\gamma}$ tends toward $g_o(\epsilon)$. Obviously, in practice these parameters are finite.

E. Necessary condition in the smoothing procedure

The least-square smoothing Eq. (3) or its equivalent Eq. (6) gives an approximation *to the exact level density* Eq. (2). Therefore, if the averaging is too accurate (see the previous remarks) the procedure leads to a curve that is very close to Eq. (2). This curve remains characterized by strong oscillations that express shell effects. However, the aim of the Strutinsky method is precisely to remove these shell effects.

For $M=0$, the effective interval of averaging is governed by a pure Gaussian [since $\widetilde{P}_0(x)=1$ in Eq. (5)]. To eliminate the shell effects from the averaging, the parameter γ must be at least of the order of the mean spacing between the shells. (denoted here by $\overline{\hbar\omega}$) near the Fermi level:

$$\gamma \gtrsim \overline{\hbar\omega}. \tag{7}$$

In this way, we obtain a "true" smooth density. If relation (7) is not satisfied, the level density remains characterized by oscillations (quantum effects), in opposition with the character of the semiclassical density.

For $M>0$, F_M is no longer a pure Gaussian, and this case becomes more complicated. Indeed, the width of the averaging function F_M is not really γ, because in Eq. (5) the Gaussian is modulated by the polynomial $\widetilde{P}_M$.

It turns out that to maintain this width of the order of mean spacing shell we have to enlarge the parameter γ with respect to the order M. Thus, the smoothing procedure implies a "coherency" between these two parameters. Usually, the couple (γ, M) is determined by the so-called plateau condition [14] from the typical ranges: $6\lesssim M\lesssim 20$ and $\overline{\hbar\omega}\lesssim\gamma\lesssim 2\overline{\hbar\omega}$. Because of this coherency, it is easy to notice that the plateau is invariably moved toward the right-hand side (toward the largest γ), when M increases. Since in the harmonic oscillator the spacing between the shells is constant, we have in this simple case $\overline{\hbar\omega}=\hbar\omega$.

Figure 1 displays the Strutinsky level density [calculated from relation (5)] for three values of the parameter γ (with M being fixed). Since γ is too small compared to $\hbar\omega$ curve (a) is characterized by strong oscillations (shell effects), which are close to Dirac functions [see Eq. (2)]. By increasing γ (curve b) one diminishes the magnitude of these oscillations. In the third case (curve c), γ is of the order of $\hbar\omega$, the curve becomes smooth and can be regarded as the mean behavior of the exact level density [the so-called smooth component contained in the exact level density (2)].

F. Averaged particle number, averaged energy, and shell correction

The averaged particle number and the averaged energy are defined through the average density of states $\overline{g}_{M,\gamma}$ by

$$\overline{N}_{M,\gamma}(\lambda)=\int_{-\infty}^{\lambda}\overline{g}_{M,\gamma}(\epsilon)d\epsilon, \tag{8}$$

$$\overline{E}_{M,\gamma}(\lambda)=\int_{-\infty}^{\lambda}\epsilon\overline{g}_{M,\gamma}(\epsilon)d\epsilon. \tag{9}$$

The detailed expressions are given in Ref. [7].

In practice the upper bound of the integral giving the particle number is deduced from the equation

$$\overline{N}_{M,\gamma}(\lambda)=N_0, \tag{10}$$

where N_0 is the particle number of the system. The quantity λ is the Fermi level of the average density $\overline{g}_{M,\gamma}$ (i.e., the Strutinsky level density)

Finally the Strutinsky shell correction to the binding energy of the liquid drop model is defined as follows:

$$\begin{aligned}
\delta\overline{E}_{M,\gamma} &= \int_{-\infty}^{\lambda_0}\epsilon g_o(\epsilon)d\epsilon-\int_{-\infty}^{\lambda}\epsilon\overline{g}_{M,\gamma}(\epsilon)d\epsilon\\
&= \sum_{n=0}^{N_0}\epsilon_n-\overline{E}_{M,\gamma}(\lambda),
\end{aligned} \tag{11}$$

where $g_o(\epsilon)$ is the exact level density given by Eq. (2) and λ_0 is its Fermi level (the last occupied level). Sometimes, $\overline{E}_{M,\gamma}(\lambda)$ is denoted as $\overline{\sum\epsilon_n}$.

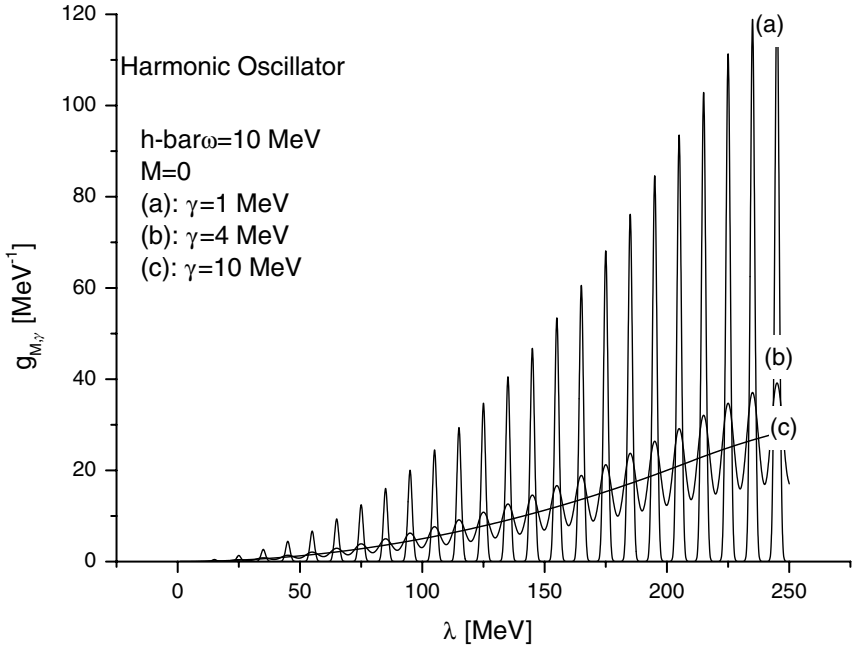

FIG. 1. Strutinsky density of states $\overline{g}_{M,\gamma}(\lambda)$ of the harmonic oscillator as a function of the Fermi level λ. Three values of the smoothing parameter γ are considered; the order of the curvature correction is $M = 0$. The shell gap is fixed arbitrarily at $\hbar\omega = 10$ MeV.

In Eq. (11), the shell correction should not contain any component of the smooth energy, which is by definition already included in the liquid-drop model. Consequently, the average density $\overline{g}_{M,\gamma}$ [or the average energy $\overline{E}_{M,\gamma}(\lambda)$] must not contain any residual shell effects.

Moreover, since $\overline{g}_{M,\gamma}$ is a least-squares approximation of g_o, one can write $g_o \approx g_{M,\gamma} + \delta g_{M,\gamma}$, with $\lambda_0 \approx \lambda$. When condition (7) is fulfilled, $g_{M,\gamma}$ becomes smooth and the exact density g_o oscillates around $g_{M,\gamma}$ making $\delta g_{M,\gamma}$ alternatively positive and negative. Consequently, from Eq. (11) one can deduce formally that

$$\delta\overline{E}_{M,\gamma}(\lambda) \approx \int_{-\infty}^{\lambda} \epsilon \delta g_{M,\gamma}(\epsilon) d\epsilon. \tag{12}$$

Thus, the oscillations of the shell correction $\delta\overline{E}_{M,\gamma}(\lambda)$ as a function of λ are due to the fluctuations of $\delta g_{M,\gamma}(\epsilon)$.

Note that, in practice, owing to the finite size of the spectrum, for the shell correction, the cutoff condition $\epsilon_{\text{last level}} - \lambda \gg \gamma$ is required (see Ref. [14]).

III. SEMICLASSICAL LEVEL DENSITY

A. Bohr's correspondence principle

Although the Strutinsky level density is mathematically well defined by Eq. (5), there is no physical basis for this smoothing. Consequently, it is necessary to build another level density free of shell effects that would be justified by physical arguments.

Shell effects are the consequence of the quantum nature of the level distribution (2). The natural way to eliminate such effects would be to go over to the classical limit. To this end, we will apply the Bohr correspondence principle, which states that the behavior of quantum systems reduces to classical physics in "the limit of large quantum numbers."

Starting from this principle, we can deduce the semiclassical level density by using the Euler-Maclaurin (EML) summation formula. In practice, this amounts to obtaining an asymptotic series that contains only three or four terms, all the others being divergent. The first term of this series coincides with the known Thomas-Fermi approximation.

The EML expansion used here is equivalent to the usual standard semiclassical methods, (e.g., the Wigner-Kirkwood expansion [15–17]), or the method of the partition function [18]. The latter is based on asymptotic series of powers of $\hbar$. Indeed, in the correspondence principle, the limit of large quantum numbers amounts to taking the classical limit $\hbar \to 0$.

B. Asymptotic limit of large quantum numbers

In practical cases, the concept of "large quantum numbers" must be précised by a more concrete definition. To illustrate this point, we start from the typical example of the three-dimensional harmonic oscillator. Such a system is very simple; its energy levels are given by

$$\epsilon_n = (n + 3/2)\hbar\omega, \quad n = 0, 1, 2, 3, \ldots, \infty.$$

The quantum number n defines a shell, and $\hbar\omega$ represents the gap between these shells. Thus, n is given by $n = (\epsilon_n - \epsilon_0)/\hbar\omega$, where $\epsilon_0 = (3/2)\hbar\omega$ is the lowest level of the spectrum.

The correspondence principle states that, for large values of $n = (\epsilon_n - \epsilon_0)/\hbar\omega$, the quantum physics reduces to classical physics, in particular, the quantum (exact) level density $g_o(\lambda)$ defined by (2) should approach the semiclassical level density denoted here by $g_{\text{sc}}(\lambda)$. This can be written as

$$\text{if } n = [(\epsilon_n - \epsilon_0)/\hbar\omega] \to \infty, \quad \text{then} \quad g_o \to g_{\text{sc}}.$$

As already noted, the shell effects are mainly determined by the small part of the spectrum $\{\epsilon_n\}$ that is located in the vicinity of the Fermi level λ. Consequently, for these levels,

we have roughly $\epsilon_n \approx \lambda$, and this limit becomes

$$\text{if } n = [(\lambda - \epsilon_0)/\hbar\omega] \to \infty, \quad \text{then} \quad g_o(\lambda) \to g_{\rm sc}(\lambda).$$

Since in general the Fermi level increases with the quantum numbers, the arguments presented for the harmonic oscillator are also valid for any other physical system. Therefore, we will consider the previous statement as general. However, we must now redefine $\hbar\omega$ as the mean shell spacing in the neighborhood of the Fermi level λ. As in relation (7), we denote it by $\overline{\hbar\omega}$:

$$\text{if } \frac{(\lambda - \epsilon_0)}{\overline{\hbar\omega}} \to \infty, \quad \text{then} \quad g_o(\lambda) \to g_{\rm sc}(\lambda). \tag{13}$$

This limit is of course unphysical. Therefore, in practice, we require the following qualitative criterion:

$$\text{if} \quad \frac{\lambda - \epsilon_0}{\overline{\hbar\omega}} \gg 1, \quad \text{then} \quad g_o(\lambda) \approx g_{\rm sc}(\lambda). \tag{14}$$

We understand by Eq. (14) that $[(\lambda - \epsilon_0)/\overline{\hbar\omega}]$ is sufficiently large compared to unity so that $g_o(\lambda)$ can be considered as close as possible to $g_{\rm sc}(\lambda)$ with "satisfactory accuracy."

Finally, the "asymptotic limit of large quantum numbers" can be defined theoretically by (13), or practically by Eq. (14).

In practical cases, $\lambda \gg \epsilon_0$; therefore the previous requirement can be replaced with $\lambda/\overline{\hbar\omega} \gg 1$. In this case, the Fermi level λ must be measured from the bottom of the well.

C. Two well-known analytical cases

The procedure just described is applied in Appendix B to two simple cases.

1. Semiclassical level density of the harmonic oscillator

The eigenenergies of the isotropic oscillator are

$$E_{n_x,n_y,n_z} = \left(n_x + n_y + n_z + \frac{3}{2}\right)\hbar\omega_0,$$
$$n_x, n_y, n_z = 0, 1, 2, \ldots, \infty.$$

The semiclassical level density of the harmonic oscillator is a simple parabola (see Appendix B):

$$g_{\rm sc}(\lambda) = \frac{1}{2}\frac{\lambda^2}{(\hbar\omega_0)^3} - \frac{1}{8}\frac{1}{\hbar\omega_0}. \tag{15}$$

This result is well known and was established very early by means of the partition function [18], or more recently by the Wigner-Kirkwood expansion [19].

2. Semiclassical level density of the infinitely deep cubic box

For the case of a cubic box with totally reflecting walls the spectrum is given by

$$\begin{aligned} E_{n_x n_y n_z} &= \left(n_x^2 + n_y^2 + n_z^2\right)E_0, \\ E_0 &= \pi^2\hbar^2/\left(2ma_0^2\right), \\ a_0 &= \text{side of thecubic box}, n_x, n_y, n_z = 1, 2, \ldots, \infty. \end{aligned} \tag{16}$$

The semiclassical level density of the infinite cubic box (see Appendix B) is also an "old" result [18,20]:

$$g_{\rm sc}(\lambda) \approx \frac{1}{E_0^{3/2}}\frac{\pi}{4}\sqrt{\lambda} - \frac{3\pi}{8}\frac{1}{E_0} + \frac{3}{8}\frac{1}{E_0^{1/2}}\frac{1}{\sqrt{\lambda}}. \tag{17}$$

D. Semiclassical shell correction

We define the semiclassical energy by relations very similar to Eqs. (8)–(11), replacing the Strutinsky level density by the one of the semiclassical density, with the corresponding Fermi level is denoted as $\lambda_{\rm sc}$:

$$N_{\rm sc}(\lambda_{\rm sc}) = \int_{-\infty}^{\lambda_{\rm sc}} g_{\rm sc}(\epsilon)d\epsilon, \tag{18}$$

$$E_{\rm sc}(\lambda_{\rm sc}) = \int_{-\infty}^{\lambda_{\rm sc}} \epsilon g_{\rm sc}(\epsilon)d\epsilon, \tag{19}$$

$$N_{\rm sc}(\lambda_{\rm sc}) = N_0, \tag{20}$$

$$\begin{aligned} \delta E_{\rm sc} &= \int_{-\infty}^{\lambda_0} \epsilon g_o(\epsilon)d\epsilon - \int_{-\infty}^{\lambda_{\rm sc}} \epsilon g_{\rm sc}(\epsilon)d\epsilon \\ &= \sum_{n=0}^{N_0} \epsilon_n - E_{\rm sc}(\lambda_{\rm sc}). \end{aligned} \tag{21}$$

Unlike $\delta\overline{E}_{M,\gamma}(\lambda)$, the quantity $\delta E_{\rm sc}$ does not depend on any free parameter.

IV. CONNECTION BETWEEN STRUTINSKY'S LEVEL DENSITY AND THE SEMICLASSICAL LEVEL DENSITY

A. Assumptions and quantitative approach of the asymptotic limit

We know from the Bohr principle given in Sec. III B that in the "asymptotic limit" (14) we must have the approximation $g_o(\lambda) \simeq g_{\rm sc}(\lambda)$. Since Strutinsky averaging (6) gives an approximation to the exact level density $g_o(\lambda)$, normally in this limit it should also give an approximation to the semiclassical level density $g_{\rm sc}(\lambda)$. The role of the curvature correction term would be to improve the approximation.

We start from the averaging (6), substituting $g_{\rm sc}(\lambda)$ for $g_o(\lambda)$ in the "asymptotic limit" (14). In Strutinsky averaging the parameter γ must be of the order of the mean shell spacing $\overline{\hbar\omega}$ near the Fermi level [see Eq. (7)]. Consequently, in Eq. (14) we should replace $\overline{\hbar\omega}$ with γ:

$$\begin{aligned} \overline{g}_{M,\gamma}(\lambda) \approx \int_{-\infty}^{\infty} g_{\rm sc}(\epsilon)\widetilde{P}_M\left(\frac{\epsilon - \lambda}{\gamma}\right)\frac{1}{\gamma} \\ \times \exp\left[-\left(\frac{\epsilon - \lambda}{\gamma}\right)^2\right]d\epsilon, \end{aligned} \tag{22}$$

with

$$\frac{\lambda - \epsilon_0}{\gamma} \gg 1 \text{ and } \gamma \gtrsim \overline{\hbar\omega}. \tag{23}$$

Setting $X = (\epsilon - \lambda)/\gamma$, we obtain

$$\overline{g}_{M,\gamma}(\lambda) \approx \int_{-\infty}^{\infty} g_{\rm sc}(\lambda + \gamma X)\widetilde{P_M}(X)\exp(-X^2)dX, \quad M \text{ even}.$$

Now, one replaces the semiclassical density $g_{\rm sc}(\lambda + \gamma X)$ by its $(M+2)$ first terms of the Taylor expansion around λ [M must be even in $\widetilde{P}_M(X)$]. The last term gives an estimation of the remainder:

$$\overline{g}_{M,\gamma}(\lambda) \approx \int_{-\infty}^{\infty} \left[g_{\rm sc}(\lambda) + \sum_{k=1}^{M+1} \frac{(\gamma X)^k}{k!} \frac{d^k g_{\rm sc}(\lambda)}{d\lambda^k} + \frac{(\gamma X)^{M+2}}{(M+2)!} \frac{d^{M+2} g_{\rm sc}(\lambda)}{d\lambda^{M+2}} \right] \widetilde{P}_M(X) \exp\left(-X^2\right) dX.$$

It is easy to show that $\widetilde{P}_M(X)\exp(-X^2)$ behaves like a delta function with respect to any polynomial of order $k \leqslant M$. Consequently the first term gives back $g_{\rm sc}(\lambda)$, and the second has no contribution (notice that X^{M+1} is odd). The remaining integral,

$$I(M) = \int_{-\infty}^{\infty} X^{M+2} \widetilde{P}_M(X) \exp\left(-X^2\right) dX,$$

is obtained from Appendix A.

Finally,

$$\overline{g}_{M,\gamma}(\lambda) \approx g_{\rm sc}(\lambda)\{1 + R_{M,\gamma}(\lambda)\},$$

$$R_{M,\gamma}(\lambda) = \gamma^{M+2} \frac{C_{M+2}}{(M+2)!} \frac{1}{g_{\rm sc}(\lambda)} \frac{d^{M+2} g_{\rm sc}(\lambda)}{d\lambda^{M+2}},$$

$$C_{M+2} = (-1)^{M/2} \frac{1 \cdot 3 \cdot 5 \cdots (M+1)}{2^{(M+2)/2}},$$

$$M \text{ even, with } \lambda - \epsilon_0 \gg \gamma \gtrsim \overline{\hbar\omega}. \qquad (24)$$

Equation (24) is fundamental and gives the straightforward link between the semiclassical level density $g_{\rm sc}(\lambda)$ and the Strutinsky level density $\overline{g}_{M,\gamma}(\lambda)$ in the asymptotic limit $\lambda - \epsilon_0 \gg \gamma$, with the necessary condition of the smoothing procedure $\gamma \gtrsim \overline{\hbar\omega}$.

It should be noted that it is $\overline{g}_{M,\gamma}(\lambda)$ that is deduced from $g_{\rm sc}(\lambda)$ and not the opposite. Moreover, $g_{\rm sc}(\lambda)$ does not depend on any free parameter. Therefore $g_{\rm sc}(\lambda)$ must be considered as the "true" smooth level density [the so-called smooth component of the quantum density (2)], and λ is its Fermi level.

The quantity $R_{M,\gamma}(\lambda)$ is the remainder of the averaging. From Eq. (24), it can easily be identified with the relative error:

$$|R_{M,\gamma}(\lambda)| \approx \left| \frac{g_{\rm sc}(\lambda) - \overline{g}_{M,\gamma}(\lambda)}{g_{\rm sc}(\lambda)} \right|$$

and represents the noise (for the density of states) of the Strutinsky method. In actual calculations, it is implicit, and thus unknown. It is contained intrinsically in $\overline{g}_{M,\gamma}(\lambda)$.

It is easy to check from Eq. (24) that the coefficient $C_{M+2}/(M+2)!$ in the remainder decreases theoretically to zero as M increases to infinity (with λ, γ being fixed), provided that $g_{\rm sc}(\lambda)$ is sufficiently regular. This in principle improves the average. Nevertheless, we have seen in Sec. II E that large values of M involve a necessary slight increase of γ in the smoothing procedure, which in turn increases somewhat the remainder, as can easily be seen from Eq. (24). Thus, it is not possible to further reduce the remainder. In practical cases, the "optimal choice" $M \sim 16$–30 leads to very good precision (i.e., $|R_{M,\gamma}(\lambda)| < 0.01$).

From Eq. (24) it is clear that the dependency on the two parameters (M, γ) becomes weaker and weaker as the remainder decreases to zero. The only special case where the remainder vanishes rigorously is where $g_{\rm sc}(\lambda)$ is a pure polynomial of degree less than or equal to M. This happens in the harmonic oscillator case. For this reason, the Strutinsky method must not be "judged" in this example when $M \geqq 2$.

Fundamentally, the Strutinsky level density appears in Eq. (24) only as an approximation (and thus is not strictly equivalent as is often claimed) to the semiclassical level density. Consequently, the smooth Strutinsky energy of Eq. (9) and the Strutinsky shell correction of Eq. (11) must also be considered as approximations to the respective semiclassical quantities given by Eqs. (19) and (21).

In fact, we shall see in the next section that the remainder tends also to zero with λ like $(\gamma/\lambda)^{M+2}$, and thus it becomes negligible only in the "asymptotic limit" $(\gamma/\lambda) \ll 1$.

B. The relative error for the Strutinsky level density in two special cases

It is instructive to apply our result (24) for the cases seen previously, that is, the harmonic oscillator (15) and the cubic box (17), with the previous assumptions $\lambda - \epsilon_0 \gg \gamma \gtrsim \overline{\hbar\omega}$. For these calculations we choose $M = 0$ and $M = 2$ (M must be even).

For the harmonic oscillator case, using $g_{\rm sc}(\lambda)$ from Eq. (15), we find for $M = 0$

$$\overline{g}_{M=0,\gamma}(\lambda) \approx g_{\rm sc}(\lambda)\left[1 + \frac{1}{2}\frac{\gamma^2}{\lambda^2}\right], \quad \text{with} \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \qquad (25)$$

(where, of course, the mean spacing between the shells is constant, and we have simply $\overline{\hbar\omega} = \hbar\omega$), and for $M = 2$

$$\overline{g}_{M=2,\gamma}(\lambda) \approx g_{\rm sc}(\lambda)\,[1 + 0], \quad \text{with} \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega}. \qquad (26)$$

Since the semiclassical level density is a parabola, the derivative that appears in the remainder $R_{M,\gamma}$ in Eq. (24) cancels for $M \geqslant 2$; therefore one obtains the exact result (the remainder is 0). However, one should not be too impressed by this case (see Sec. IV A).

For the infinite cubic box, using $g_{\rm sc}(\lambda)$ from Eq. (17) we get for $M = 0$ and $M = 2$

$$\overline{g}_{M=0,\gamma}(\lambda) \approx g_{\rm sc}(\lambda)\left[1 - \frac{1}{16}\frac{\gamma^2}{\lambda^2}\right], \quad \text{with} \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega}, \qquad (27)$$

$$\overline{g}_{M=2,\gamma}(\lambda) \approx g_{\rm sc}(\lambda)\left[1 + \frac{15}{512}\frac{\gamma^4}{\lambda^4}\right], \quad \text{with} \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega}. \qquad (28)$$

Here also, for both cases, we obtain very similar relations.

Thus, in these four cases, the Strutinsky level density approaches the semiclassical level density, and the relative error (remainder) tends to zero only in the asymptotic limit $\gamma/\lambda \ll 1$. Moreover, it is clear that, in this limit, the Strutinsky densities become practically independent of the smoothing parameters (γ, M).

In realistic cases, the Fermi level λ is fixed for a given nucleus. It turns out that for medium and heavy nuclei, the quantity λ lies several units of $\overline{\hbar\omega}$ above the bottom of the well; since $\overline{\hbar\omega} \approx \gamma$, the quotient γ/λ is thus small and the remainder is practically negligible. Consequently, for these cases, the Strutinsky density of states is very close to the semiclassical level density.

The relative error of the Strutinsky density for the cubic box is illustrated in Fig. 2. In Fig. 2 (top) we compare the "numerical" Strutinsky level density (curve a) calculated by means of Eq. (5) to the semiclassical density (curve b) given by Eq. (17). Apart from the region near zero (very small λ), and in spite of the "low" order $M = 0$ of the curvature correction, it is clear that the two densities are practically indistinguishable. The theoretical link between both densities is given by Eq. (27).

In Fig. 2 (bottom), we can see that the "numerical" relative error $(g_{sc} - \overline{g}_{M=0,\gamma})/g_{sc}$ of the Strutinsky density [denoted by (b − a)/b] with respect to the semiclassical density (regarded as the true smooth density) is very small, especially in the asymptotic limit ($\gamma/\lambda \ll 1$). In the latter, this error becomes close to the theoretical value $\gamma^2/16\lambda^2$ given by Eq. (27).

C. The relative error for the Strutinsky energy in the two previous cases

The average energy $\overline{E}_{M,\gamma}(\lambda)$ can be deduced by combining Eq. (9) and Eq. (24) with the assumptions of the asymptotic limit and the necessary condition of smoothing made in Eq. (24):

$$\overline{E}_{M,\gamma}(\lambda) \approx E_{sc}(\lambda)[1 + \rho_{M,\gamma}(\lambda)], \tag{29}$$

$$\rho_{M,\gamma}(\lambda) = \frac{S_{M,\gamma}(\lambda)}{E_{sc}(\lambda)}, \tag{30}$$

$$S_{M,\gamma}(\lambda) = \frac{\gamma^{M+2} C_{M+2}}{(M+2)!} \int_{-\infty}^{\lambda} \epsilon \frac{d^{M+2} g_{sc}(\epsilon)}{d\epsilon^{M+2}} d\epsilon, \tag{31}$$

$$\text{with } \lambda - \epsilon_0 \gg \gamma \gtrsim \overline{\hbar\omega}, \tag{32}$$

where $\rho_{M,\gamma}(\lambda)$ and $S_{M,\gamma}(\lambda)$ are, respectively, the relative and the absolute errors on the smooth (Strutinsky) energy $\overline{E}_{M,\gamma}(\lambda)$.

We know from Eq. (24) that $\overline{E}_{M,\gamma}(\lambda)$ must be considered as an approximation to $E_{sc}(\lambda)$. Besides, unlike $\overline{E}_{M,\gamma}(\lambda)$, the quantity $E_{sc}(\lambda)$ does not depend on any unphysical parameter. As before, the remainder $\rho_{M,\gamma}(\lambda)$ of the Strutinsky energy must be related to the relative error:

$$\left|\rho_{M,\gamma}(\lambda)\right| \approx \left| \frac{E_{sc}(\lambda) - \overline{E}_{M,\gamma}(\lambda)}{E_{sc}(\lambda)} \right|. \tag{33}$$

Once again, to illustrate some features of the Strutinsky method we apply this result for the harmonic oscillator and for the cubic box with $M = 0$ and $M = 2$.

For the harmonic oscillator,

$$\overline{E}_{M=0,\gamma}(\lambda) \approx E_{sc}(\lambda)\left[1 + \frac{\gamma^2}{\lambda^2}\right], \quad \text{with} \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega}, \tag{34}$$

$$\overline{E}_{M=2,\gamma}(\lambda) \approx E_{sc}(\lambda)\,[1 + 0]\,, \quad \text{with} \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega}, \tag{35}$$

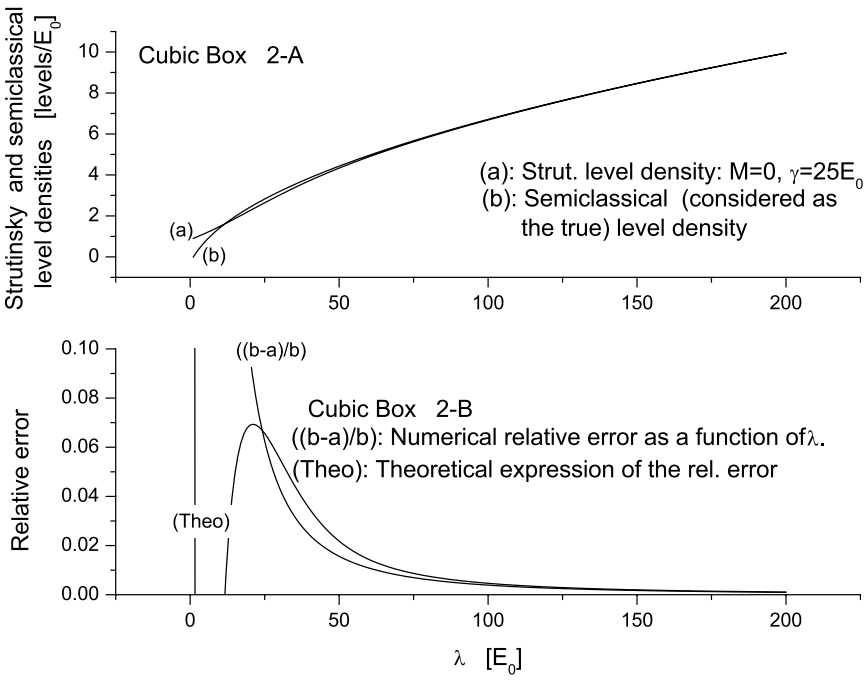

FIG. 2. (Top) Strutinsky density of states $\overline{g}_{M,\gamma}(\lambda)$ (curve a) and semiclassical density of states $g_{sc}(\lambda)$ (curve b) of the cubic box as a functions of the Fermi level λ. The Strutinsky level density is calculated with the order $M = 0$, and the smoothing parameter $\gamma = 25E_0$ (for the definition of E_0 see Sec. III C). The two level densities are practically indistinguishable. (Bottom) Relative error of the Strutinsky density of states defined by (b − a)/b compared to the theoretical value (see text).

where $E_{\rm sc}(\lambda)$ of the harmonic oscillator is given in Appendix B.

In the same way, we obtain for the cubic box

$$\overline{E}_{M=0,\gamma}(\lambda) \approx E_{\rm sc}(\lambda)\left[1-\frac{5}{16}\frac{\gamma^2}{\lambda^2}\right], \quad \text{with} \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega}, \tag{36}$$

$$\overline{E}_{M=2,\gamma}(\lambda) \approx E_{\rm sc}(\lambda)\left[1-\frac{25}{512}\frac{\gamma^4}{\lambda^4}\right], \quad \text{with} \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega}, \tag{37}$$

where $E_{\rm sc}(\lambda)$ of the cubic box is also given in Appendix B.

Thus, in the asymptotic limit $(\gamma/\lambda) \ll 1$ (i.e., for medium and heavy nuclei), as for the density of states (24), the relative error is small, and we have also $\overline{E}_{M,\gamma}(\lambda) \approx E_{\rm sc}(\lambda)$. Thus, for the smooth energy, the Strutinsky method is a good approximation of the semiclassical method. A straightforward consequence is that the smooth (Strutinsky) energy $\overline{E}_{M,\gamma}$ becomes practically independent of the smoothing parameters (M, γ) in this limit.

We give in Fig. 3 an illustration of the relative error for the Strutinsky energy for the cubic box. In the top panel, we reach the same conclusions as in Fig. 2 (top), that is, $\overline{E}_{M=0,\gamma}(\lambda)$ and $E_{\rm sc}(\lambda)$ are indistinguishable. In Fig. 3 (bottom), we see that the relative error on the Strutinsky energy (with respect to the semiclassical energy) tends toward zero in the asymptotic limit $(\gamma/\lambda) \ll 1$ and approaches the theoretical value $5\gamma^2/16\lambda^2$ given by Eq. (36).

D. A new understanding of the plateau condition on the average (Strutinsky) energy

As seen before, the relative error plays a major role in the Strutinsky energy. From Eq. (33), it is clear that, if $|\rho_{M,\gamma}(\lambda)| \ll 1$, the relative variations of the Strutinsky energy $\overline{E}_{M,\gamma}(\lambda)$ *are small compared to* $\overline{E}_{M,\gamma}(\lambda)$ itself [or to $E_{\rm sc}(\lambda)$]. For instance, if one plots $\overline{E}_{M,\gamma}(\lambda)$ as a function of the parameter γ (with M and λ being constant) a "plateau" appears in the graph. This means that $\overline{E}_{M,\gamma}(\lambda)$ is "practically constant at the scale of its own value" (at least in the interval $\lambda \gg \gamma \gtrsim \overline{\hbar\omega}$); that is,

$$\left(\frac{\Delta\overline{E}_{M,\gamma}(\lambda)}{\overline{E}_{M,\gamma}(\lambda)}\right)_{\lambda\gg\gamma\gtrsim\overline{\hbar\omega}} \ll 1 \tag{38}$$

[which is close to Eq. (33)]. This does not necessarily mean that the derivative of $\overline{E}_{M,\gamma}(\lambda)$ cancels as in the traditional plateau condition [14]. The same remark holds for the Strutinsky density.

We must point out that the relative error is proportional to the quantity $(\gamma/\lambda)^{M+2}$, so that the plateau is improved at large values of M.

Figure 4 shows an illustration of the plateau [defined by Eq. (38)] for the energy in the cubic box case. In the top panel the Strutinsky energy $\overline{E}_{M,\gamma}$ of the cubic box is plotted as a function of γ for four values of the order M. The particle number is fixed arbitrarily at $N_0 = 200$ with a Fermi level $\lambda = 64.255E_0$. It is clear that the fluctuations $\Delta\overline{E}_{M,\gamma}$ are small compared to $\overline{E}_{M,\gamma}$. At this scale a clear plateau is noticed.

The bottom panel of Fig. 4, at a reduced scale, shows the important variations of the plateau, especially on the right-hand side of the figure. If we continue to zoom on in the curve, several minima and maxima appear (i.e., $\partial\overline{E}_{M,\gamma}/\partial\gamma = 0$). Some of them have nothing to do with a plateau. For example, in the vicinity of $\gamma \approx 154E_0$ a minimum occurs for the order $M = 16$ that does not really belong to any plateau. Thus our "macroscopic" definition of the plateau seems more "adapted" than the old version based on the "stationarity" of $\overline{E}_{M,\gamma}$ with respect to γ. In fact, it contains implicitly the concept of the relative error, which plays a central role in the numerical applications in the method. Indeed, the minimization of the relative error (see following) avoids the ambiguity of the (old)

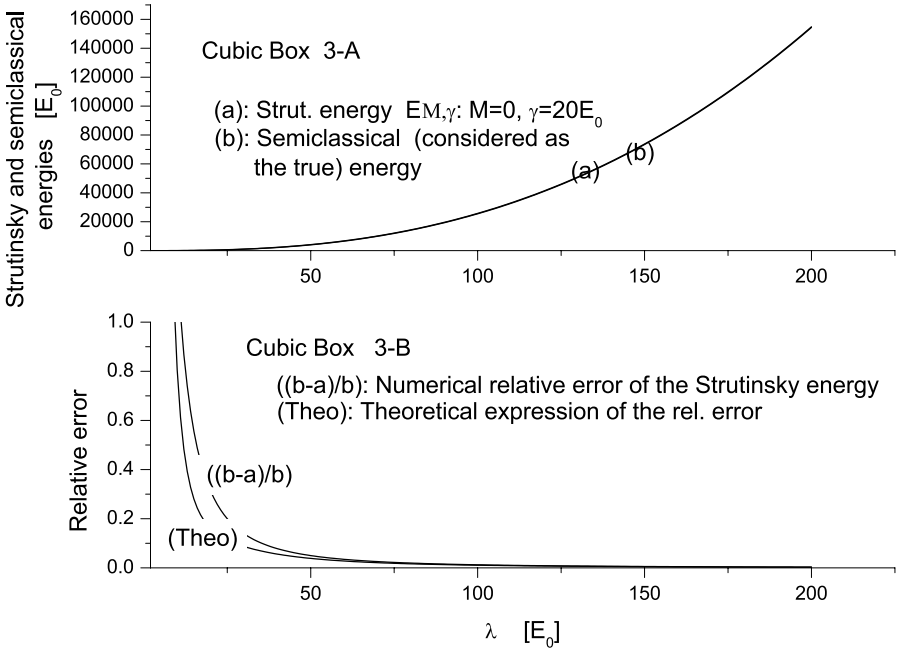

FIG. 3. (Top) Strutinsky smooth energy $\overline{E}_{M,\gamma}(\lambda)$ (curve a) and semiclassical energy $E_{\rm sc}(\lambda)$ (curve b) of the cubic box as a functions of the Fermi level λ. The two free parameters are given in the graph. As in Fig. 2 (top), the two smooth energies are indistinguishable. (Bottom) Relative error of the Strutinsky smooth energy compared to the theoretical value (see also text).

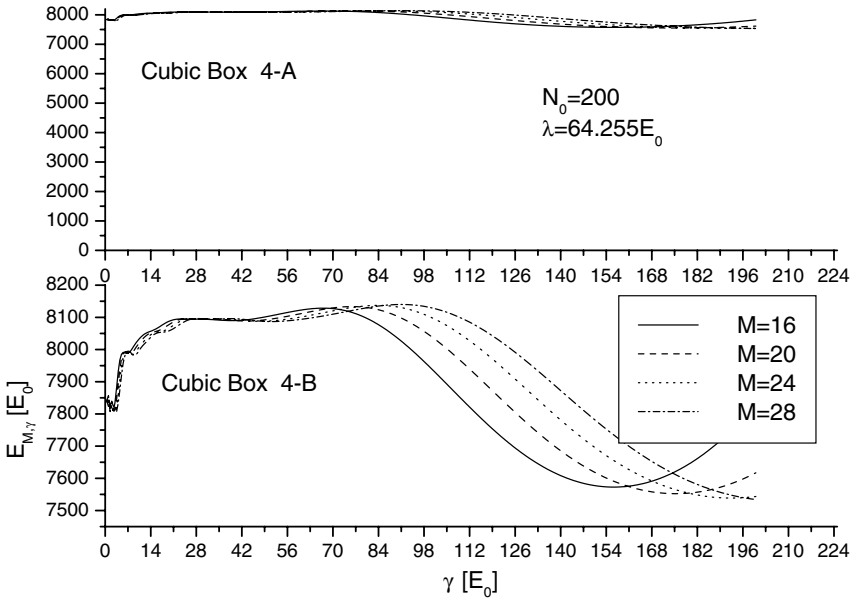

FIG. 4. (Top) The new understanding of the plateau condition is that the relative variations of the Strutinsky energy $\overline{E}_{M,\gamma}(\lambda)$ are so small compared to $\overline{E}_{M,\gamma}(\lambda)$. This means that, at the scale of the plateau's value, the fluctuations are negligible. (Bottom) Same as Fig. 4 (top), but at a reduced scale. Here, the fluctuations of the plateau are obvious.

plateau condition, because a stationary point is not necessarily a plateau, whereas the minimization of the relative error leads indisputably to the true value (at the very least to the optimal value) of the smooth energy and hence of the shell correction (see the following).

E. Strutinsky shell correction

1. *Critical point of the Strutinsky method*

First, one must recall that the Strutinsky shell correction and the semiclassical shell correction are, respectively, defined through Eqs. (11) and (21), that is,

$$\delta\overline{E}_{M,\gamma} = \sum_{\text{occupied}} \epsilon_n - \overline{E}_{M,\gamma}(\lambda),$$

$$\delta E_{\text{sc}} = \sum_{\text{occupied}} \epsilon_n - E_{\text{sc}}(\lambda).$$

Subtracting the second equation from the first, and using Eq. (29), one obtains a straightforward relation between these two quantities.:

$$\delta\overline{E}_{M,\gamma}(\lambda) \approx \delta E_{\text{sc}}(\lambda) - S_{M,\gamma}(\lambda) \tag{39}$$

Since $\overline{E}_{M,\gamma}(\lambda)$ is considered as an approximation to $E_{\text{sc}}(\lambda)$ (see previous section), the Strutinsky shell correction $\delta\overline{E}_{M,\gamma}(\lambda)$ must also be regarded as an approximation to the semiclassical shell correction $\delta E_{\text{sc}}(\lambda)$. In this respect, $S_{M,\gamma}(\lambda)$ represents the same absolute error in both formulas (29) and (39). However, the essential point is that this error does not have the same importance in these two results.

Indeed, the two shell corrections $\delta E_{M,\gamma}(\lambda)$, and $\delta E_{\text{sc}}(\lambda)$ are obtained as the difference between two close large numbers (i.e., the sum of single-particle energies and their averages); therefore they are significantly smaller compared to these quantities (i.e., $\overline{E}_{M,\gamma}$ or E_{sc}). For example, Ref. [21] gives for the case of ^{154}Sn (neutrons) the typical "realistic" values $\sum \epsilon_i = -1122.5$ MeV, $\overline{E}_{M,\gamma} = -1132.0$ MeV (where the order M is not précised in that work), and hence the shell correction $\delta\overline{E}_{M,\gamma} = 9.5$ MeV is thus much smaller than $\overline{E}_{M,\gamma}$. Consequently, the same absolute error $S_{M,\gamma}(\lambda)$, which is relatively small in Eq. (29), might become non-negligible in Eq. (39) for the Strutinsky shell correction.

In addition, in a number of cases the shell correction might also become so small that the relative error (*in the shell correction*) no longer makes sense. Thus, for the shell correction, the relative error does not play the same leading role as for the Strutinsky energy (or the Strutinsky density), so that the (Strutinsky) shell correction might become strongly dependent to the choice of the parameter γ. This means that the error could exceed the shell correction itself if this error is not optimized (i.e., minimized).

2. *Optimization of the method with the rule of the relative remainder*

The shell correction is defined as the difference between two quantities, $\sum \epsilon_i$ and $\overline{E}_{M,\gamma}(\lambda)$. Only the latter depends on the parameter γ (and also M) through the remainder $\rho_{M,\gamma}(\lambda)$ from Eq. (29). By minimizing this remainder (i.e., the relative error) with respect to γ, we make $\overline{E}_{M,\gamma}(\lambda)$ as close as possible to E_{sc}; therefore we make $\delta\overline{E}_{M,\gamma}(\lambda)$ as close as possible to $\delta E_{\text{sc}}(\lambda)$ (i.e., the true shell correction). Thus, the minimization of the relative error made on $\overline{E}_{M,\gamma}(\lambda)$, should lead to the independence (or at least to a weak dependence) of $\delta\overline{E}_{M,\gamma}(\lambda)$ on the parameters (γ, M). Hence we can affirm that it is the minimization of this relative error that is the source of the plateau, not the opposite. This should be the most appropriate way for finding the true (or the best) value of the shell correction. Figure 5 displays a practical illustration of this minimization (the so-called 'rule of relative remainder).

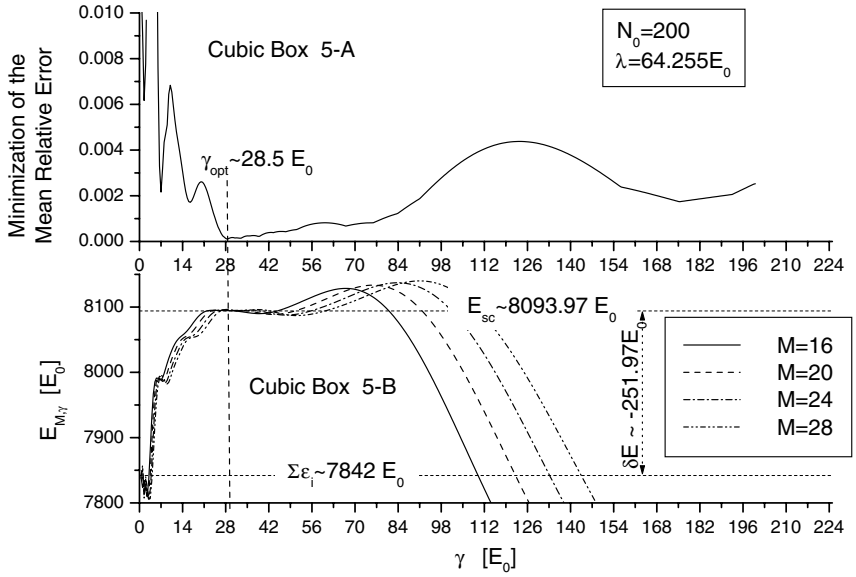

FIG. 5. (Top) Minimization of the mean relative error (see text). The minimum occurs approximately at $\gamma \approx 28.5E_0$. (Bottom) Comparison between the semiclassical energy and the different values of the Strutinsky smooth energy used in Fig. 5 (top). Note that the optimization [see Fig. 5 (top)] is made on the smooth energy and not on the shell correction itself as in the old method of the plateau.

We show in Fig. 5 (top) how to find the optimal value for the parameter γ in the cubic box case. We again consider in Fig. 5 (top) the case given in Fig. 4 (top).

The steps are the following:

(i) First we calculate the Strutinsky energy at the Fermi level $\overline{E}_{M,\gamma}(\lambda)$ as a function of the parameter γ (λ being fixed), for some close values of the order M.

(ii) We must minimize the remainder of Eq. (33) as follows:

$$\left|\frac{\partial}{\partial\gamma}\rho_{M,\gamma}(\lambda)\right| = \left|\frac{\partial}{\partial\gamma}\frac{E_{\rm sc}(\lambda)-\overline{E}_{M,\gamma}(\lambda)}{E_{\rm sc}(\lambda)}\right| \approx 0$$
$$= \left|\frac{\frac{\partial\overline{E}_{M,\gamma}(\lambda)}{\partial\gamma}}{E_{\rm sc}(\lambda)}\right| \approx \left|\frac{\frac{\partial\overline{E}_{M,\gamma}(\lambda)}{\partial\gamma}}{\overline{E}_{M,\gamma}(\lambda)}\right|.$$

(iii) Then, this quantity is plotted as a function of γ for each value of M. We then should look for the minimum of this function (relative error).

However for a fixed M, this function has an oscillatory behavior (around zero), which leads to several local minima. Nevertheless, because these curves do not cancel simultaneously, it is possible to remove these unpleasant oscillations by considering the mean relative error over some (relative close) values of M.

The mean relative error (over $M = 16, 20, 24, 28$) on the Strutinsky energy is plotted against γ. The minimum (optimal) value is found to be about $\gamma_{\rm opt} \approx 28.6E_0$ and corresponds effectively to the best value [see Fig. 5 (bottom)]. Note a good agreement between the true value (semiclassical) given by the upper straight line $\overline{E}_{\rm sc} \approx 8093.97E_0$ and the Strutinsky values [Fig. 5 (bottom)]. In fact, for the optimized γ, the calculated values are $\overline{E}_{16,\gamma_{\rm opt}} \approx 8094.52E_0$, $\overline{E}_{20,\gamma_{\rm opt}} \approx 8094.64E_0$, $\overline{E}_{24,\gamma_{\rm opt}} \approx 8095.21E_0$, and $\overline{E}_{28,\gamma_{\rm opt}} \approx 8096.31E_0$, for $M = 16$, 20, 24, and 28, respectively.

The sum of single-particle energies is $\sum_{\text{occ. states}} \epsilon_i \approx 7842E_0$.

The true shell correction $\delta\overline{E}_{\rm sc} \approx -251.97E_0$ and the corresponding Strutinsky shell corrections are thus $\delta\overline{E}_{16,\gamma_{\rm opt}} \approx 252.52E_0$, $\delta\overline{E}_{20,\gamma_{\rm opt}} \approx 252.64E_0$, $\delta\overline{E}_{24,\gamma_{\rm opt}} \approx 253.21E_0$, and $\delta\overline{E}_{28,\gamma_{\rm opt}} \approx 254.31E_0$, which are in good agreement with the true (exact) value. Without optimization the results of the Strutinsky shell correction will certainly be random.

F. Case of realistic wells

1. Strutinsky level density

First, we must note that the spectrum of the finite potential is composed of discrete negative levels plus a continuum. For this potential, the definition of the exact level density (2) must be modified by adding an appropriate continuous expression $g_c(\epsilon)$:

$$g_o(\epsilon) = \sum_n \delta(\epsilon - \epsilon_n) + g_c(\epsilon). \tag{40}$$

For spherical potentials, the continuum is defined by the scattering phase shift, whereas for the deformed case it can be solved by the more complicated S-matrix method (see Ref. [22]).

Next, one recalls that the result (24) (which is the basis of the present work) comes from Eq. (6) The latter is valid for any smooth potential regardless of whether it is infinite or not. Indeed, it is to be noted that the interval of averaging in Eq. (6) goes from $-\infty$ up to $+\infty$, so the preceding demonstration remains valid for a finite well. One simply has to add the continuum of Eq. (40) to the discrete spectrum in this integral. As for infinite potentials, it is clear that the Strutinsky's level density should also be an approximation to the semiclassical level density for finite wells.

In practice, a rigorous treatment of the continuum is not an easy task. The standard recipe consists of using the discrete positive energies to "simulate" this continuum [7]. These energies are usually obtained by diagonalizing the Hamiltonian

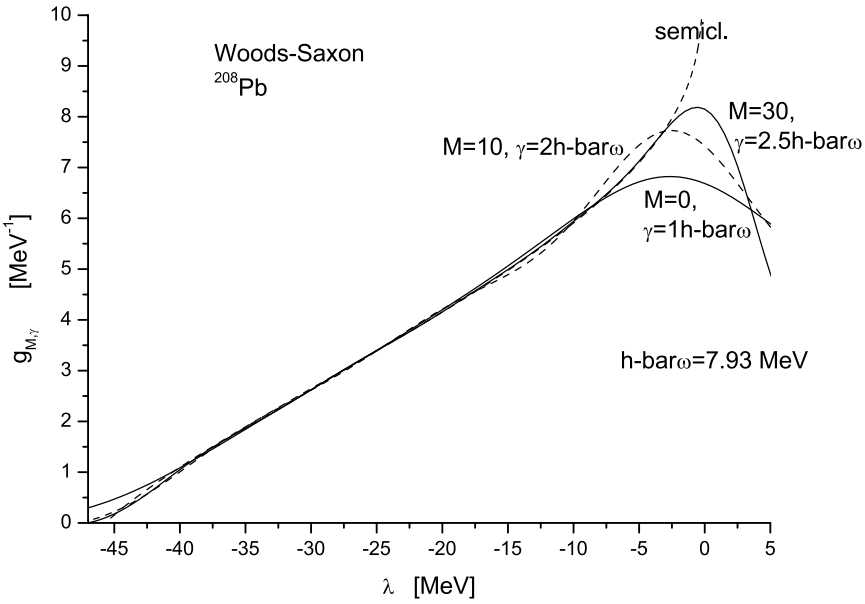

FIG. 6. Semiclassical and Strutinsky level densities for a finite well (here the Woods-Saxon potential). The main differences occur at the top of the well, near the singularity of the semiclassical density.

matrix in a truncated harmonic oscillator basis. In fact, this delicate problem seems now to be solved by the so-called Green's function oscillator expansion (GFOE) method [21,25], which improves upon the standard method.

2. *Semiclassical level density*

It is well known that the level density of the finite potential becomes singular at the top of the well [22,23]. For this reason, it is not possible to find a local polynomial approximation to the semiclassical level density in the vicinity of this singularity. In other words, the least-squares averaging (3) does not hold in this case, precisely because $g_{sc}(\lambda) \to \infty^{-}$, as $\lambda \to 0$ (i.e., at zero energy). This explains why the two methods do not lead to the same results, especially for weakly bound nuclei. Far from the zero-energy point there is no problem.

3. *Comparison between the two level densities*

It would be interesting to determine the limit where the Strutinsky level density deviates significantly from the semiclassical density. To this end, we will be comparing numerically the Strutinsky level density to the semiclassical (Wigner-Kirkwood) level density by employing the result of Ref. [24]:

$$g_{sc}(\lambda) = \frac{dN_{sc}(\lambda)}{d\lambda_{sc}}, \tag{41}$$

with

$$N_{sc} = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2}\int_0^{r_{sc}} d^3r\left[(\lambda_{sc}-U)^{3/2} + \left(\frac{2m}{\hbar^2}\right)^{-1}\Omega\right],$$
$$\Omega = \left[\frac{3}{4}\kappa^2\left(\vec{\nabla} f_{so}\right)^2(\lambda_{sc}-U)^{1/2} - \frac{1}{16}\nabla^2 U(\lambda_{sc}-U)^{-1/2}\right]. \tag{42}$$

This formula contains the "classical" Thomas-Fermi term plus an $\hbar^2$ Wigner-Kirkwood correction. In this formula $U(\vec{r})$ is the central mean potential and also contains the Coulomb interaction for the protons, and $f_{so}(\vec{r})$ is the spin-orbit interaction. The classical turning points r_{sc} are defined by $U(\vec{r}_{sc}) = \lambda_{sc}$, where λ_{sc} is the Fermi level.

The numerical integration giving N_{sc} is made with the help of an "improved" Gauss-Legendre quadrature formula. The eigenvalues used in the Strutinsky level density are calculated by the code published in Ref. [26].

In the two methods we employ strictly the same Hamiltonian and the same set of parameters; that is, we use the Woods-Saxon potential with spin-orbit term and the Coulomb potential for the protons. For this test we work with ^{208}Pb (neutrons) with a spherical nuclear shape. The parameters are $V_0 = -47.083$ MeV and $a_v = 0.66$ fm, $R_V = 7.36$ fm, $\varkappa = 12.0$ Mev fm^2, $a_{so} = 0.55$ fm, and $R_{so} = 6.698$ fm. Their definition is given in Ref. [26].

In Fig. 6, we have drawn the semiclassical level density (denoted by semicl.) and the Strutinsky density as function of the Fermi level for three cases (with the numerical values of the smoothing parameters given in the figure).

(i) We can check in the three cases that the Strutinsky level density is practically equal to the semiclassical density in the "intermediate" region (between the top and the bottom of the well) irrespective of the order M of the smoothing procedure. Indeed, we have shown in Sec. IV B that in the asymptotic limit (i.e., for medium and heavy nuclei) the Strutinsky density of states (not the Strutinsky shell correction!) should be rather insensitive to the two free parameters of the method. However, although with $M = 0$ one obtains a good relative error on the density of states, one improves this error more at sufficient large values of M.

(ii) As expected, for the reason previously invoked, Fig. 6 shows that the Strutinsky densities differ from the

semiclassical result essentially at the top of the well. In the "intermediate region" there is no difference. Near the singularity, it is more advantageous to choose high values for the order M. With $M = 30$, the Strutinsky calculation seem to work reasonably well up to about -2.5 MeV; beyond this limit the precision is lost.

(iii) However, we should not forget that it is the semiclassical density that is the "true" quantity. Because of the importance of the difference between the two methods near the zero-energy point, the semiclassical method must in principle be preferred for the weakly bound nuclei.

V. CONCLUSION

Although this paper explains a number of aspects and subtleties of the Strutinsky method, we will insist on some essential points:

(i) The Strutinsky level density appears in the fundamental relation (24) only as an approximation (and is not strictly equivalent as is often claimed) to the semiclassical level density. Consequently, the shell correction calculated by Strutinsky's method should also be considered as an approximation to the semiclassical shell correction.

(ii) Semiclassical quantities such as the level density, the energy, and the shell correction must be considered as the "true" quantities compared to those obtained with the Strutinsky method. Moreover, they do not depend on any free parameter. Unlike the semiclassical method, the Strutinsky method contains an intrinsic noise (remainder). The ambiguity of the method comes from the dependence on the two free parameters through this remainder.

(iii) It turns out that the remainder is proportional to $(\gamma/\lambda)^{M+2}$ and is defined in this paper as the relative error. In the asymptotic limit $(\gamma/\lambda) \ll 1$ (i.e., for medium and heavy nuclei), the relative error is small, especially for higher M. Therefore, it is found that the Strutinsky method gives good results for the average level density and the average energy. In these cases the dependency on the free parameters is weak. In contrast, in the shell correction the relative error is no longer small. The shell correction might become strongly (γ, M) dependent. The choice of these two free parameters must be treated with care. In this context, to minimize the relative error, we propose the "rule of the relative remainder."

(iv) For realistic potentials, the semiclassical level density admits a singularity at the top of the well. Since the Strutinsky method is a least-squares approximation to the semiclassical level density (demonstrated in this paper), the averaging fails near this singularity. In this case, the two densities are different, and it is not surprising to note a strong dependence on the parameters (γ, M) in this region, even if the continuum is treated properly. Consequently, for the weakly bound nuclei (drip line) it is better to use the semiclassical method.

Our personal conclusion is that the semiclassical method with a good numerical treatment should, in theory, be quite superior to the Strutinsky method. The latter can be considered only as a good palliative method.

APPENDIX A: CALCULATION OF THE INTEGRAL $I(M)$

In this Appendix we calculate the value of

$$I(M) = \int_{-\infty}^{\infty} x^{M+2} \widetilde{P_M}(x) \exp(-x^2) dx$$

(see Sec. IV A).

First, one must note that $\widetilde{P_M}(x)$ of Eq. (5) can be expressed as

$$\widetilde{P_M}(x) = \frac{H_M(0)}{2^{M+1} M! \sqrt{\pi}} \frac{H_{M+1}(x)}{x}.$$

Indeed, with the help of the Christoffel-Darboux formula (Chap. 22 of Ref. [27])

$$\sum_{k=0}^{n} \frac{H_k(x) H_k(y)}{2^k k!} = \frac{H_{n+1}(x) H_n(y) - H_{n+1}(y) H_n(x)}{2^{n+1} n! (x - y)}$$

one finds for our case

$$\begin{aligned} \widetilde{P}_M(x) &= \sum_{m=0}^{M} \frac{H_m(0)}{m! 2^m \sqrt{\pi}} H_m(x) \\ &= \frac{H_{M+1}(x) H_M(0) - H_{M+1}(0) H_M(x)}{2^{M+1} M! \sqrt{\pi} (x - 0)}. \end{aligned}$$

Since M is even, $H_{M+1}(0) = 0$, which gives the cited expression.

To calculate the integral $I(M)$, we have to replace $\widetilde{P_M}(x)$ by the preceding result. We obtain

$$I(M) = \frac{H_M(0)}{2^{M+1} M! \sqrt{\pi}} \int_{-\infty}^{\infty} x^{M+1} H_{M+1}(x) \exp(-x^2) dx.$$

Now we use the following property [27]:

$$\int_{-\infty}^{\infty} t^k H_k(st) \exp(-t^2) dt = \sqrt{\pi} k! P_k(s),$$

where $P_k(s)$ is a Legendre polynomial. For our purpose, we choose $s = 1$, with $P_k(1) = 1$. Setting $k = M + 1$ in the previous result, one finds

$$\int_{-\infty}^{\infty} x^{M+1} H_{M+1}(x) \exp(-x^2) dx = \sqrt{\pi} (M + 1)!,$$

so that

$$I(M) = \frac{H_M(0)}{2^{M+1} M! \sqrt{\pi}} \sqrt{\pi} (M + 1)! = \frac{H_M(0)}{2^{M+1}} (M + 1),$$

where $H_M(0)$ is given in Sec. II D. Finally, the result can be cast into the following form:

$$I(M) = \left(\frac{(-1)^{M/2}}{2^{(M+2)/2}} 1 \cdot 3 \cdot 5 \cdots (M + 1) \right).$$

APPENDIX B: TWO APPLICATIONS OF THE EULER MACLAURIN FORMULA

In the present work, to obtain some analytical results we employ the Euler-MacLaurin formula [27]

$$\sum_{k=1}^{n-1} F(k) = \int_0^n F(k)dk - \frac{1}{2}[F(0) - F(n)] + \frac{1}{12}[F'(n) - F'(0)] - \frac{1}{720}[F'''(n) - F'''(0)] + \cdots.$$

Of course this formula can be used to calculate discrete finite sums. But here our interest lies in this formula's application to determining the asymptotic behavior ($n \to \infty$) of the discrete sum. In explicit terms, if we take a few terms (integral plus a few derivatives) in this formula, we obtain a quantity that is equivalent to the discrete sum. This means that the error (difference between the discrete sum and its equivalent from the EML formula) tends to zero as n increases to infinity.

In general, the higher orders of this formula are divergent and must be simply ignored. For this reason, an asymptotic expansion does not exceed three or four terms.

We apply this formula for two cases:

(i) The harmonic oscillator: Here we take just the integral in the EML formula, thus neglecting the divergent terms (Dirac delta functions) in the result

$$\sum_{n=0}^{\infty} D(n)\delta\left[\epsilon - (n+3/2)\hbar\omega\right] \approx \frac{1}{\hbar\omega}\int_0^{\infty} D(n)\delta\left[\frac{\epsilon}{\hbar\omega} - (n+3/2)\right]dn = g_{\rm sc}(\epsilon),$$

where $D(n) = (n+1)(n+2)/2$ is the degeneracy of the level n, and we find

$$g_{\rm sc}(\epsilon) \approx \frac{1}{2\hbar\omega}\left[\left(\frac{\epsilon}{\hbar\omega}\right)^2 - \frac{1}{4}\right].$$

Now, it is easy to deduce the semiclassical energy

$$\overline{E}_{\rm sc}(\lambda) \approx \int_0^{\lambda} \epsilon\,\overline{g}_{\rm sc}(\epsilon)d\epsilon = \frac{\lambda^4}{8\,(\hbar\omega)^3} - \frac{\lambda^2}{16\hbar\omega}.$$

(ii) The cubic box: Here the degeneracy is unknown, and we have to evaluate a threefold integral. We work with a "basic" EML formula, that is, without derivatives:

$$\sum_{k=1}^{\infty} F(k) \approx \int_0^{\infty} F(k)dk - \frac{1}{2}F(0).$$

Starting from that, we apply this formula in the case of the threefold sum. Because all axes are equivalent, we obtain

$$\sum_{n_x=0}^{\infty}\sum_{n_y=0}^{\infty}\sum_{n_z=0}^{\infty} F(n_x,n_y,n_z) = \int_0^{+\infty}\int_0^{+\infty}\int_0^{+\infty} F(n_x,n_y,n_z) \times dn_x dn_y dn_z - (3/2) \times \int_0^{+\infty}\int_0^{+\infty} F(n_x,n_y,0)dn_x dn_y + (3/4)\int_0^{+\infty} F(n_x,0,0)dn_x - (1/8)F(0,0,0) = I_3 + I_2 + I_1 + I_0,$$

respectively, where $F(n_x,n_y,n_z) = \delta[\epsilon - (n_x^2 + n_x^2 + n_x^2)E_0]$.

Using spherical coordinates we find

$$I_3 = \frac{\pi}{4}\frac{\sqrt{\epsilon}}{E_0^{3/2}}, \quad I_2 = -\frac{3\pi}{8E_0},$$

$$I_1 = \frac{3}{8E_0^{1/2}\sqrt{\epsilon}}, \quad I_0 = -\frac{1}{8}\delta(\epsilon).$$

Here also we omit I_0 (the delta function) and so

$$g_{\rm sc}(\epsilon) = \frac{\pi}{4}\frac{\sqrt{\epsilon}}{E_0^{3/2}} - \frac{3\pi}{8E_0} + \frac{3}{8E_0^{1/2}\sqrt{\epsilon}}.$$

Therefore

$$\overline{E}_{\rm sc}(\lambda) \approx \int_0^{\lambda} \epsilon\,\overline{g}_{\rm sc}(\epsilon)d\epsilon = \frac{\pi}{10}\frac{1}{E_0^{3/2}}\lambda^{5/2} - \frac{3\pi}{16E_0}\lambda^2 + \frac{1}{4E_0^{1/2}}\lambda^{3/2}.$$

[1] V. M. Strutinsky, Yad. Fiz. **3**, 614 (1966) [Sov. J. Nucl. Phys. **3**, 449 (1966)].
[2] V. M. Strutinsky, Nucl. Phys. **A95**, 420 (1967).
[3] V. M. Strutinsky, Nucl. Phys. **A122**, 1 (1968).
[4] W. D. Myers and W. J. Swiatecki, Nucl. Phys. **A81**, 1 (1966).
[5] P. Moller, J. R. Nix, W. D. Myers, and W. S. Swiatecki, At. Data Nucl. Data Tables **59**, 185 (1995).
[6] M. Brack, L. Damgaard, A. S. Jensen, H. C. Pauli, V. M. Strutinsky, and C. Y. Wong, Rev. Mod. Phys., **44**, 320 (1972).
[7] M. Bolsterli, E. O. Fiset, J. R. Nix, and J. L. Norton, Phys. Rev. C **5**, 1050 (1972).
[8] P. Quentin and H. Flocard, Annu. Rev. Nucl. Part. Sci. **28**, 523 (1978).
[9] Y. Aboussir, J. M. Pearson, A. K. Dutta, and F. Tondeur, At. Data Nucl. Data Tables **61**, 127 (1995).
[10] K. Pomorski, Phys. Rev. C **70**, 044306 (2004).
[11] A. Diaz-Torres, Phys. Lett. **B594**, 69 (2004).
[12] G. G. Bunatian, V. M. Kolomietz, and V. M. Strutinsky, Nucl. Phys. **A188**, 225 (1972).
[13] B. K. Jennings, Nucl. Phys. **A207**, 538 (1973).
[14] M. Brack and H. C. Pauli, Nucl. Phys. **A207**, 401 (1973).
[15] E. P. Wigner, Phys. Rev. **40**, 749 (1932).
[16] E. P. Wigner, Phys. Rev. **46**, 1002 (1934).
[17] J. G. Kirkwood, Phys. Rev. **44**, 31 (1933).
[18] R. K. Badhuri and C. K. Ross, Phys. Rev. Lett. **27**, 606 (1971).

[19] J. Caro, E. Ruiz Arriola, and L. L. Sacedo, J. Phys. G **22**, 981 (1996).
[20] D. L. Hill and J. A. Wheller, Phys. Rev. **89**, 1102 (1953).
[21] T. Vertse, A. T. Kruppa, and W. Nazarewicz, Phys. Rev. C **61**, 064317 (2000).
[22] T. Vertse, A. T. Kruppa, R. J. Liotta, W. Nazarewicz, N. Sandulescu, and T. R. Werner, Phys. Rev. C **57**, 3089 (1998).
[23] B. K. Jennings and R. K. Bhaduri, Nucl. Phys. **A237**, 149 (1975).
[24] B. K. Jennings, R. K. Bhaduri, and M. Brack, Nucl. Phys. **A253**, 29 (1975).
[25] S. Shlomo, V. M. Kolomietz, and H. Dejbakhsh, Phys. Rev. C **55**, 1972 (1997).
[26] B. Mohammed-Azizi and D. E. Medjadi, Comput. Phys. Commun. **156**, 241 (2004).
[27] M. Abramotiz and I. A. Stegun, *Handbook of Mathematical Functions* (Dover, New York, 1970).