THE SHELL-CORRECTION METHOD

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ABSTRACT

We review the basic assumptions and definitions of Strutinsky's shell-correction method. Its derivation from Hartree-Fock and extended selfconsistent microscopical theories is presented and numerical tests based on Hartree-Fock results are summarised. A detailed discussion of the Strutinsky energy averaging procedure, its validity and its relation to other averaging methods is given. We finally mention some recent applications of the Strutinsky method, also outside nuclear physics.

1. Introduction

Strutinsky's shell-correction method[1] (SCM) grew out of the necessity to correct the wrong average behavior of the nuclear deformation energy which in the Nilsson model[2] was taken to be (proportional to) the sum of the lowest occupied single-particle energies ϵ_i of the deformed shell-model potential:

$$E_{sp}(def) = \sum_{i=1}^{A} \epsilon_i(def). \tag{1}$$

It had been realized for some time[3] that $E_{sp}(def)$ does not behave well at large deformations, in particular in attempts to calculate fission barriers. This is mainly due to the fact that Eq. (1) is not the correct expression for the binding (or deformation) energy of a self-saturated fermion system. Furthermore, the spectrum ϵ_i obtained in phenomenological shell-model potentials can approximately describe the real single-particle excitations only near the Fermi energy λ; far below or above λ the energies ϵ_i have little or no physical meaning.

This led Strutinsky[1] to *renormalize* the wrong average part of $E_{sp}(def)$ to that of the empirically known liquid drop model[5] (LDM) energy $E_{LDM}(def)$, by defining the total (deformation) energy to be

$$E_{tot}(Z,N,def) = E_{LDM}(Z,N,def) + \delta E_p(Z,def) + \delta E_n(N,def), \tag{2}$$

where the so-called *shell-correction* energy $\delta E_q(N_q, def)$ for each kind of nucleons $(q = p, n;\ N_p = Z,\ N_n = N)$ is defined to be the difference between the corresponding sum E_{sp} and its average:

$$\delta E_q(N_q, def) = \sum_{i=1}^{N_q} \epsilon_i^q(def) - \left\langle \sum_{i=1}^{N_q} \epsilon_i^q(def) \right\rangle. \tag{3}$$

The averaging $\langle\ \rangle$ in Eq. (3) is constructed in such a way that it eliminates the shell effects in E_{sp} without affecting its average part. Strutinsky designed for this a numerical averaging procedure which will be discussed in detail in Sect. 3. As a result, δE_q only depends on the single-particle levels ϵ_i^q near the Fermi energy λ.

The SCM has led to a considerable success in explaining for the first time the nature of the fission isomers[4, 1] and, more generally, in calculating nuclear masses and fission barriers[6, 7, 8] (see also Sect. 4 for more recent applications). In Eq. (2), the average energy E_{LDM} is given in terms of a set of empirical LDM[5] (or droplet model[29]) parameters whereas the shell-corrections δE_q are determined from the levels of phenomenological (deformed) shell-model potentials such as the Nilsson model[2] or other finite-range potentials[7, 8]. The SCM thus gives both empirical nuclear models their balanced role. That this method is more than an *ad hoc* renormalization, but can be solidly based upon selfconsistent Hartree-Fock or Landau theory, will be discussed in the following Sect. 2.

2. Strutinsky's Energy Theorem

We shall in this section discuss the foundation of the SCM upon selfconsistent microscopic theories using effective nucleon-nucleon interactions[1, 7, 9]. For simplicity, we treat here the nucleus as if it had only N nucleons of one kind. The extension to Z protons and N neutrons as used in Eq. (2) is straightforward.

2.1. Derivation within Hartree-Fock Theory

We start from the Hartree-Fock (HF) energy for N fermions interacting through a 2-body force $\hat{V}$:

$$E_{HF} = E_{HF}[\rho] = \mathrm{tr}\,(\mathcal{T}\rho) + \frac{1}{2}\mathrm{tr}\,(\rho\,\mathrm{tr}\,(\mathcal{V}\rho)). \tag{4}$$

Here ρ is the one-body density matrix written in terms of any single-particle basis $|\alpha\rangle$ and the occupied HF states $|i\rangle$

$$\rho_{\alpha\beta} = \sum_{i=1}^{N}\langle\alpha|i\rangle\langle i|\beta\rangle = \sum_{i}\langle\alpha|i\rangle\langle i|\beta\rangle n_i^{HF}; \tag{5}$$

n_i^{HF} are the HF occupation numbers

$$n_i^{HF} = \begin{cases} 1 & \text{for } \epsilon_i < \lambda, \\ 0 & \text{for } \epsilon_i > \lambda. \end{cases} \tag{6}$$

(Finite temperature and pairing effects will be discussed in Sect. 2.2 below.) In Eq. (4), $\mathcal{T}$ and $\mathcal{V}$ are the one-body and antisymmetrized two-body matrix elements of the kinetic energy and the two-body interaction $\hat{V}$, respectively:

$$\mathcal{T}_{\alpha\beta} = \langle\alpha|\hat{T}|\beta\rangle; \qquad \mathcal{V}_{\alpha\beta,\gamma\delta} = \langle\alpha\beta|\hat{V}|\overline{\gamma\delta}\rangle. \tag{7}$$

We now define an *average* density matrix in terms of some smoothed occupation numbers $\tilde{n}_i$ to be defined in Sect. 3.4 below:

$$\tilde{\rho}_{\alpha\beta} = \sum_{i}\langle\alpha|i\rangle\langle i|\beta\rangle\tilde{n}_i \tag{8}$$

which contains only average information without any shell effects. Next we write

$$\rho = \tilde{\rho} + \delta\rho \tag{9}$$

and Taylor expand the HF energy Eq. (4) around $\tilde{\rho}$:

$$E_{HF}[\rho] = E_{HF}[\tilde{\rho}] + \mathrm{tr}\,(\frac{\partial E_{HF}}{\partial \rho}\Big|_{\tilde{\rho}} \delta\rho) + \ldots.. \tag{10}$$

By construction, the first term in Eq. (10) contains no shell effects, i.e. it represents the average part of the HF energy which is smooth as a function of particle number(s) and deformation:

$$E_{HF}[\tilde{\rho}] = \tilde{E}_{HF}. \tag{11}$$

The second term in Eq. (10) contains all shell effects up to first order in the oscillating part of the density matrix, $\delta\rho$, which is a small quantity. Note now that the partial derivative

$$\frac{\partial E_{HF}[\rho]}{\partial \rho_{\beta\alpha}} = \langle\alpha|\hat{H}_{HF}[\rho]|\beta\rangle = (\mathcal{H}_{HF}[\rho])_{\alpha\beta} \tag{12}$$

is just the matrix element of the HF one-body operator containing the selfconsistent mean field. (This holds also for density-dependent effective interactions!) We thus can rewrite the first-order term in Eq. (10) as

$$\delta_1 E = \mathrm{tr}\,(\frac{\partial E_{HF}}{\partial \rho}\Big|_{\tilde{\rho}} \delta\rho) = \mathrm{tr}\,(\mathcal{H}_{HF}[\tilde{\rho}]\,\delta\rho) = \sum_i \hat{\epsilon}_i \delta n_i = \sum_{i=1}^{N} \hat{\epsilon}_i - \sum_i \hat{\epsilon}_i \tilde{n}_i, \tag{13}$$

where $\hat{\epsilon}_i$ are the eigenenergies of the *average HF field* $\hat{V}_{HF}[\tilde{\rho}]$ which also varies smoothly as a function of particle number(s) and deformation:

$$\hat{H}_{HF}[\tilde{\rho}]\hat{\varphi}_i = \left\{\hat{T} + \hat{V}_{HF}[\tilde{\rho}]\right\}\hat{\varphi}_i = \hat{\epsilon}_i \hat{\varphi}_i. \tag{14}$$

We thus arrive at the so-called[10] *Strutinsky energy theorem*:

$$E_{HF} = \tilde{E}_{HF} + \delta_1 E + \mathcal{O}[(\delta\rho)^2]. \tag{15}$$

It states that the HF energy of an interacting system of fermions can be written as a smooth part $\tilde{E}_{HF}$ and an oscillating part $\delta_1 E$. Most importantly, it states that the shell-correction energy $\delta_1 E$ contains *all* contributions of first order in the oscillating part $\delta\rho$ of the density matrix and can be written in the simple form on the r.h.s. of Eq. (13) in terms of the eigenvalues $\hat{\epsilon}_i$ of a smoothed average field.

In the practical shell-correction approach, the average HF energy $\tilde{E}_{HF}$ is replaced by the phenomenological LDM energy E_{LDM} and the shell-correction $\delta_1 E$ is evaluated in terms of the eigenenergies of a phenomenological shell-model potential. It remains to be checked by explicit HF calculations, to which extent these replacements can be justified and to which extent the higher-order terms $\mathcal{O}[\delta\rho]$ in Eq. (15) can be neglected. Empirically, we know that $\tilde{E}_{HF}$ is of the order of $\sim$ 1 - 2 GeV, whereas $\delta_1 E$ is only $\sim$ 10 - 15 MeV at most; there are thus good reasons to hope that Eq. (10) and thus Eq. (15) converge fast. (Corresponding numerical tests will be discussed in Sect. 2.3 below.)

Note that in the realistic case $\delta_1 E$ is a sum of neutron and proton contributions, as displayed in Eq. (2), which are obtained from the individual neutron and proton single-particle spectra. This does not mean that – at least in a selfconsistent HF calculation – these two contributions are not coupled through the dependence of the neutron mean field on the proton density and *vice versa*. Such a coupling does, however, not exist in the phenomenological approach where the shell-model potentials for neutrons and protons are fitted independently and are only correlated in a trivial way through their radii which are given in terms of the total nucleon number $A = N + Z$.

It has been repeatedly overlooked by practitioners of the SCM (and still is by some!) that there is *no double counting* of the potential energy contributions in $\delta_1 E$: due to the variational way (12) of deriving the average HF field $\tilde{V}_{HF}[\tilde{\rho}]$, the factor 1/2 in Eq. (4) is doubled and $\delta_1 E$ is just the oscillating part of the sum of occupied eigenvalues $\hat{\epsilon}_i$ of the average potential. This holds also for density-dependent effective interactions, since the so-called rearrangement contributions[10] will be taken care of automatically when the variation in Eq. (12) is correctly performed[11].

Another critique[12, 13] of the energy theorem concerned the validity of Eq. (15) as a function of deformation: the way in which it was derived above, it holds only for equilibrium deformations where E_{HF} has a (local) minimum. The SCM, however, parameterizes the deformation dependence through both the LDM energy and the shell-model potentials and is used at arbitrary deformations. The answer[9, 14, 15, 16] lies in a careful inclusion of a *constraint* in the HF equation[17] whose contributions to the first-order shell correction $\delta_1 E$ in the ideal case can be cancelled by a suitable choice of the deformation dependence of the shell-model potential and in practical cases numerically turn out to be negligible (see Fig. 2 below).

2.2. Extensions beyond Hartree-Fock

The derivation of the Strutinsky energy theorem Eq. (15) is not restricted to the pure HF case. In fact, it is a widely exploited property of the variational ground state of a correlated fermion system that to first order in small changes δn_i of the occupation numbers, the change in the ground-state energy can be written as

$$\delta E = \sum_i e_i \delta n_i , \tag{16}$$

where e_i are the single-particle, or more generally, the quasiparticle energies of the system. This is the basis of Landau theory[18] and has been used explicitly to show that the Strutinsky method can also be applied within the framework of the Landau-Migdal Fermi liquid theory[11]. Similarly, the energy theorem (15) has been extended to HF-Bogolyubov theory in order to include pairing and temperature effects selfconsistently[16, 19]. Eq. (16) can also be used to derive the famous Koopmans theorem from the density functional approach[20], and a "force theorem" has been derived in solid state theory along very similar lines[21].

We refer to an extensive presentation on the Strutinsky method and its foundation from the HF-Bogolyubov approximation at finite temperature[16], where also numerical tests are reviewed.

2.3. Numerical Tests of the Energy Theorem

At the time when Strutinsky derived Eq. (15) and formulated the shell-correction approach, no HF results with realistic effective nucleon-nucleon interactions were available to test the convergence of the expansion in Eq. (10) and the applicability of phenomenological liquid-drop and shell models. The SCM thus relied on its success in yielding nuclear masses and fission barriers in good overall agreement with experiment.

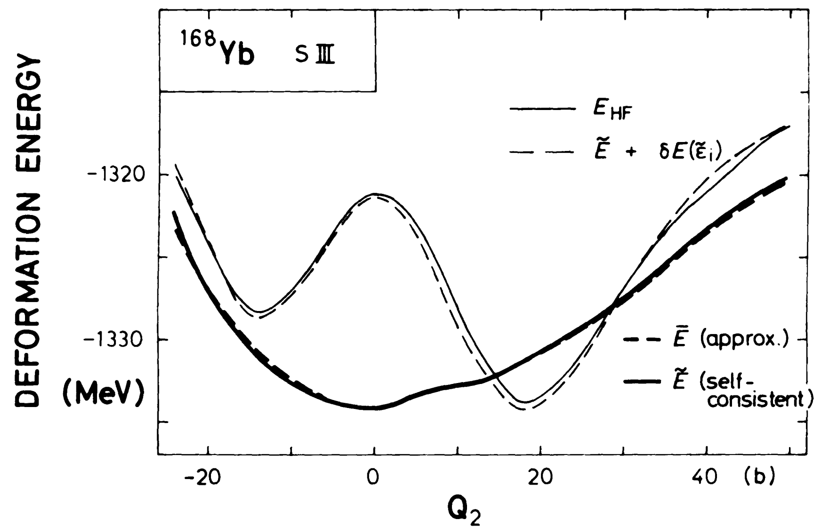

Fig. 1. HF results[26] for the deformation energy of ^{168}Yb (see text for details).

With the successful development of Skyrme's effective nuclear interactions [22, 23], HF calculations for heavy deformed nuclei became possible in the early seventies[17, 24] (see also the presentation of J.-F. Berger for HF calculations with Gogny's finite-range force[25]). This allowed to perform extensive numerical tests [26, 27] of the convergence in Eq. (10) and to compare the phenomenological LDM and shell-model results to selfconsistent HF results of ground-state masses and deformation energies.

We refer to a detailed presentation[16] of these tests using various types of Skyrme interactions and give here only some typical illustrations and a summary of the most important results. The main idea is to compute first the fully microscopical HF energy Eq. (4), then to use the numerically Strutinsky-averaged density matrix (8) to obtain the averaged energy (11) and the averaged HF potential appearing in Eq. (14) from which the first-order shell-correction (13) is extracted, and finally to investigate the difference

$$\delta_2 E = E_{HF} - \tilde{E}_{HF} - \delta_1 E \tag{17}$$

which gives the sum of all higher-order terms in the expansion (10).

Figure 1 shows the deformation energy of ^{168}Yb as a function of the total mass quadrupole moment Q_2, obtained with the Skyrme III interaction[28] and a quadratic constraint[17] in the HF equation. The thin solid line is the HF energy E_{HF} (4), the heavy lines are obtained by including the average density matrix $\tilde{\rho}$ (8) either perturbatively in the last HF iteration (dashed line) or iteratively to obtain a *selfconsistent* average HF energy $\tilde{E}_{HF}$ (solid line). The thin dashed line gives the "Strutinsky approximation" to the HF energy, i.e. the sum of $\tilde{E}_{HF}$ and $\delta_1 E$.

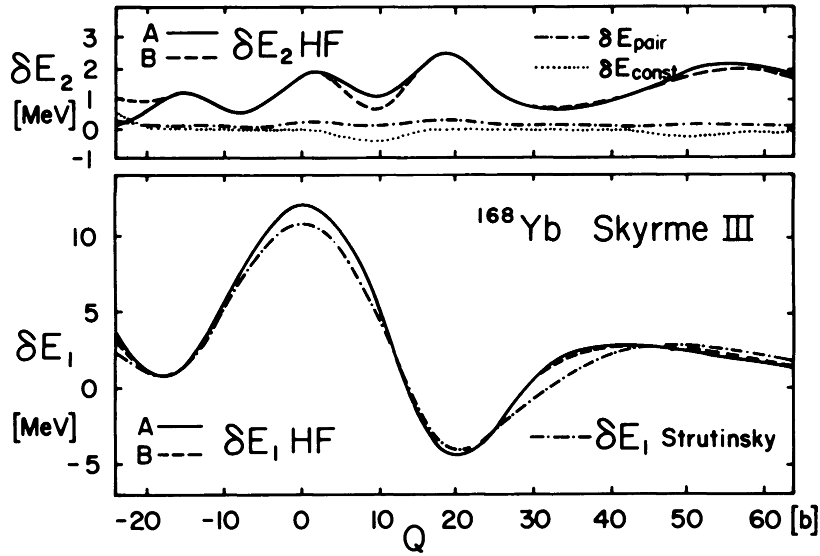

Fig. 2. First-order and sum of higher-order shell-corrections extracted from the HF results[26] shown in Fig. 1.

In the lower part of Figure 2, the shell correction $\delta_1 E$ extracted from the HF results is compared to that from a Woods-Saxon type shell-model potential. In the upper part, the quantity $\delta_2 E$ in Eq. (17) is shown along with the specific (and very small) contributions from pairing correlations and the constraint energy. (See

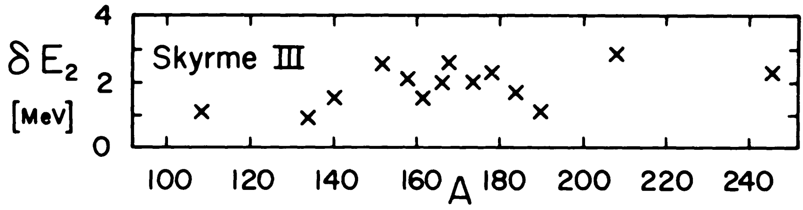

Fig. 3. Sum of higher-order shell-corrections extracted from HF results[26] for a series of nuclear ground states.

ref.[26] for details.) Figure 3 shows the same quantity $\delta_2 E$ for the ground states of a series of nuclei.

The results of these and similar tests can be summarized as follows:

(i) The sum of all second and higher-order corrections defined by Eq. (17) is small; apart from an average value of ~ 2 MeV (which in practice will be renormalized into the average LDM energy, it fluctuates by less than $\pm \sim 1$ MeV for nuclei with $A \gtrsim 50$.

(ii) $\delta_2 E$ is smallest when the averaging (through the smooth occupation numbers $\tilde{n}_i$) is performed iteratively, thus implying a selfconsistency between the average energy $\tilde{E}$ (usually represented by the LDM) and the average potential $\tilde{V}$ (usually represented by the shell-model potential).

(iii) $\tilde{E}_{HF}$ behaves exactly like a LDM energy: it is smooth as a function of both deformation and nucleon numbers and has its minimum at the spherical shape.

(iv) The first-order shell-correction energy $\delta_1 E$ extracted from the HF results is close (usually within less than ~ 1 MeV at all deformations) to the δE obtained in the deformed phenomenological shell-model potentials.

(v) For small nuclei with $A \lesssim 50$, the quantity $\delta_2 E$ can be considerably larger than for heavier systems. It depends rather critically on the inclusion of pairing correlations.

To illustrate the last point, we show in Figure 4 the quantities $\delta_1 E$ and $\delta_2 E$ obtained as above for the nucleus ^{40}Ca. Depending on the strength of the average pairing gap $\tilde{\Delta}$ (see Ref.[7] for its definition and use), the magnitude of these quantities can vary by a factor of two or more and give a much slower convergence of Eq. (10) than that found for heavier nuclei.

The above results check the validity of the Strutinsky method under *ideal conditions*, i.e. when starting from consistent average (LDM type) energies and mean field (shell-model type) potentials derived from the same effective nuclear interaction. In practice, the two models are fitted independently to different experimental data and no such consistency can be guaranteed. This may lead to larger discrepancies and uncertainties than what could be concluded from the above. A well-studied example is the so-called "Pb anomaly"[7, 30] (see Refs.[31, 32, 33] for

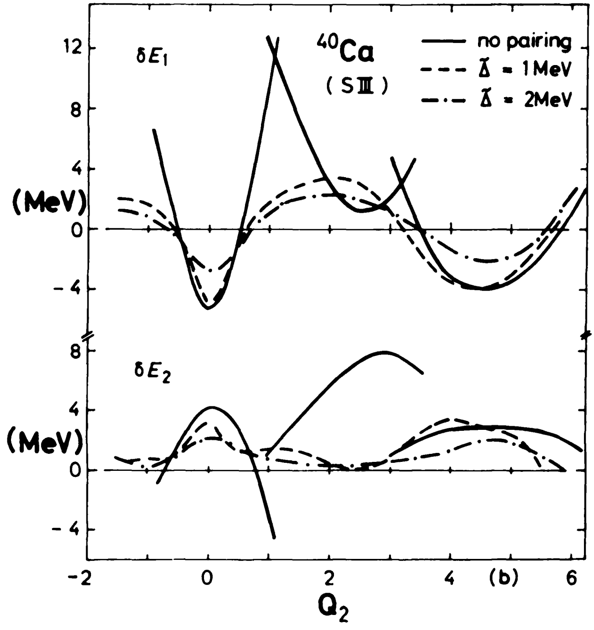

Fig. 4. Same as Fig. 2 for ^{40}Ca using two strengths of the paring gap[27].

its detailed discussion). In general, no reliable results should be expected for nuclei with $A < 40 - 50$.

3. Strutinsky's Energy Averaging Method

The aim of Strutinsky's energy averaging method[1] is to extract the fluctuating part of the sum (1) of occupied single-particle energies in a unique way. In the present section we shall discuss this technique in detail.

In the seventies, a series of alternatives to the Strutinsky energy averaging method has been proposed of which the extended Thomas-Fermi (ETF) model[34], the asymptotic $N \to \infty$ expansion[35, 36], a numerical N-averaging[37, 32], and a "temperature method"[38] were the most promising ones. All of them have some inherent uncertainties of $\lesssim$ 1 MeV in determining the average s.p. energy sum for heavy nuclei and of up to $\sim$ 2 MeV for light nuclei, thus of the same order as the plateau uncertainties of the energy averaging to be discussed in Sect. 3.3 below. We shall in Sect. 3.5 discuss briefly the ETF model, which has been the most successful of these alternatives, and refer to Ref.[31] for an evaluation of the other methods.

3.1. Smoothing Functions and Curvature Corrections

We consider one kind of N particles in a given potential with energy spectrum $\{\epsilon_i\}$. Sums over i are understood to include all degeneracies of the spectrum.

Let us first introduce the exact quantum-mechanical level density

$$g(E) = \sum_i \delta(E - \epsilon_i). \tag{18}$$

The single-particle energy sum E_{sp} can be given by the integral

$$E_{sp} = \sum_{i=1}^{N} \epsilon_i = \int_{-\infty}^{\lambda} E\, g(E)\, dE, \tag{19}$$

where the Fermi energy λ is fixed by the particle number:

$$N = \int_{-\infty}^{\lambda} g(E)\, dE. \tag{20}$$

The basic idea is to assume that $g(E)$ can be written as a sum of a smooth part $g_0(E)$ and an oscillating part $\delta g(E)$:

$$g(E) = g_0(E) + \delta g(E). \tag{21}$$

It has, in fact, be shown by Gutzwiller[39] in the so-called "periodic orbit theory" that this is always possible: $\delta g(E)$ can be expressed in terms of a sum over all classical periodic trajectories of a particle in the given potential (see also Refs.[40, 41, 42]), whereas the average level density $g_0(E)$ may be obtained from the (extended) Thomas-Fermi model (see Sect. 3.5 below). Except for a few model potentials, the two parts in Eq. (21) cannot be determined analytically. Therefore one must resort to numerical methods to determine them approximately.

Strutinsky's method[1] for extracting $g_0(E)$ as accurately as possible by means of a numerical energy averaging of the spectrum $\{\epsilon_i\}$ may be presented in the following way[43]. We start defining an *averaging function* $f(x)$ which is assumed to be analytical, positive, normalized to unity, and, to simplify matters, symmetric in x with a maximum at $x = 0$ (see Figure 5). In a first step, we then define an averaged level density $\tilde{g}_0(E, \gamma)$ by folding $g(E)$ Eq. (18) with f over a range γ:

$$\tilde{g}_0(E,\gamma) = \frac{1}{\gamma}\int_{-\infty}^{+\infty} g(E')\, f\left(\frac{E-E'}{\gamma}\right) dE' = \frac{1}{\gamma}\sum_i f\left(\frac{E-\epsilon_i}{\gamma}\right). \tag{22}$$

This achieves the following result: If the oscillating part $\delta g(E)$ of the level density is dominated by a fundamental period $\hbar\omega$ and its harmonics (like in a spherically symmetric harmonic oscillator potential, see Sect. 3.2 below), the function $\tilde{g}_0$ Eq. (22) will be smooth as soon as $\gamma \gtrsim \hbar\omega$. It will, however, depend on γ except if $g_0(E)$ is a linear function of energy (this is so due to the symmetry and the normalization of f). Furthermore, if $g_0(E)$ is a *polynomial* of degree n in energy, then $\tilde{g}_0$ will also be a polynomial of degree n (with γ-dependent coefficients for $n \geq 2$). In order to get rid of this γ dependence, Strutinsky introduced a *curvature correction*[1]. (This name was chosen because $g_0(E)$ in general is not linear, i.e. it has a nonzero curvature.) To show how this correction works, we first rewrite the folding integral in Eq. (22)

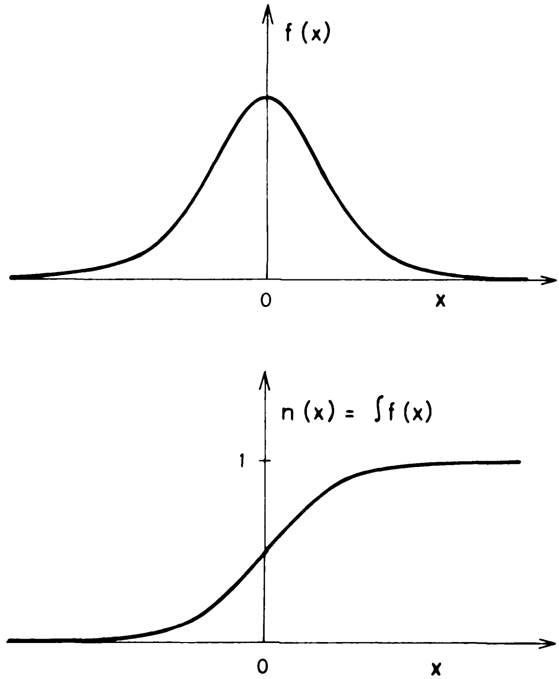

Fig. 5. Upper part: Schematic plot of a smoothing function $f(x)$. Lower part: First integral $n(x)$ of the smoothing function.

as the result of an operator $\widehat{G}_0$, which can be expanded into an infinite sum of derivative operators, acting on $g(E)$:

$$\tilde{g}_0(E,\gamma) = \left(\sum_{\mu=0}^{\infty} \frac{c_{2\mu}}{(2\mu)!} \gamma^{2\mu} \frac{d^{2\mu}}{dE^{2\mu}} \right) g(E) = \widehat{G}_0[g(E)], \tag{23}$$

where $c_{2\mu}$ are moments of the smoothing function f:

$$c_m = \int_{-\infty}^{+\infty} x^m f(x) dx. \tag{24}$$

(Only the even moments appear in (23) due to the assumed symmetry of f). We then define the inverse operator $\widehat{G}_0^{-1}$ and expand it correspondingly:

$$\widehat{G}_0^{-1} = \sum_{\mu=0}^{\infty} a_{2\mu} \gamma^{2\mu} \frac{d^{2\mu}}{dE^{2\mu}}. \tag{25}$$

The coefficients $a_{2\mu}$ can always be gained recursively from the $c_{2\mu}$ using $\widehat{G}_0^{-1} \times \widehat{G}_0 \equiv 1$. Next we define the "curvature-correction operator" $\widehat{C}_M$ by truncating the sum in

Eq. (25) at $\mu = M$:

$$\widehat{C}_M = \sum_{\mu=0}^{M} a_{2\mu}\gamma^{2\mu}\frac{d^{2\mu}}{dE^{2\mu}}. \tag{26}$$

We now arrive at the *Strutinsky averaging* operator $\widehat{S}_M$

$$\widehat{S}_M = \widehat{C}_M \times \widehat{G}_0 = \frac{1}{\gamma}\sum_{\mu=0}^{M} a_{2\mu}\gamma^{2\mu}\frac{d^{2\mu}}{dE^{2\mu}}\int_{-\infty}^{+\infty} f\left(\frac{E-E'}{\gamma}\right) dE' \times \tag{27}$$

which by construction leaves any polynomial $P_n(E)$ of degree $n \leq 2M+1$ unchanged, independently of $\gamma > 0$

$$\widehat{S}_M[P_{2M+1}(E)] \equiv P_{2M+1}(E) \qquad \forall\, \gamma > 0, \tag{28}$$

since all missing terms with $\mu > M$ of the truncated inverse operator $\widehat{G}_0^{-1}$ are identically zero.

We thus define the *Strutinsky-averaged level density* for a given level spectrum $\{\epsilon_i\}$ by

$$\tilde{g}_M(E) = \widehat{S}_M[g(E)] = \frac{1}{\gamma}\sum_i\sum_{\mu=0}^{M} a_{2\mu}\gamma^{2\mu}\frac{d^{2\mu}}{dE^{2\mu}} f\left(\frac{E-\epsilon_i}{\gamma}\right). \tag{29}$$

For clarity we repeat the two main features of $\tilde{g}_M(E)$:

(i) If the averaging width γ is chosen to be larger than the main distance $\hbar\omega$ of the shells in the spectrum $\{\epsilon_i\}$, the oscillating part $\delta g(E)$ of the exact level density is suppressed and $\tilde{g}_M(E)$ is a smooth function of energy.

(ii) If the average part $g_0(E)$ of the exact level density is a polynomial of degree $2M+1$ (or less), it is identically reproduced in $\tilde{g}_M(E)$ for any $\gamma > 0$.

One usually refers to $2M$ as to the order of the curvature corrections. As shown numerically[43], the results for $\tilde{g}_M(E)$ do not depend on the particular form of the averaging function $f(x)$, as long as it fulfils the above requirements. The standard choice is a Gaussian

$$f(x) = \frac{1}{\sqrt{\pi}}\exp(-x^2) \quad \text{with} \quad \widehat{G}_0 = \exp\left(\frac{\gamma}{2}\frac{d}{dE}\right)^2, \quad a_{2\mu} = \frac{(-1)^\mu}{2^{2\mu}\mu!}. \tag{30}$$

The curvature-corrected average level density $\tilde{g}_M(E)$ Eq. (29) can then be written as a sum of Gaussians multiplied by a linear combination of Hermite polynomials; this is the usual way to present the Strutinsky energy averaging[1, 6, 7]. Another example for the averaging function is

$$f(x) = \frac{1}{2[\cosh(x)]^2}, \quad \widehat{G}_0 = \frac{\frac{\pi}{2}\hat{d}}{\sin(\frac{\pi}{2}\hat{d})}\ (\hat{d} = \gamma\frac{d}{dE}), \quad a_{2\mu} = \left(\frac{\pi}{2}\right)^{2\mu}\frac{(-1)^\mu}{(2\mu+1)!}. \tag{31}$$

[Note that the integral of $f(x)$ in Eq. (31) is a Fermi function and thus leads to the Fermi occupation numbers of a grand canonical ensemble (cf. Sect. 3.4)]. Further examples of averaging functions and their curvature-correction coefficients $a_{2\mu}$ may be found in Ref.[43].

From $\widetilde{g}_M(E)$ we now define the average part of the single-particle energy sum E_{sp}:

$$\widetilde{E}_{sp} = \left\langle \sum_{i=1}^{N} \epsilon_i \right\rangle = \int_{-\infty}^{\widetilde{\lambda}} E\, \widetilde{g}_M(E)\, dE, \tag{32}$$

where the average Fermi energy $\widetilde{\lambda}$ is given by the particle number integral:

$$N = \int_{-\infty}^{\widetilde{\lambda}} \widetilde{g}_M(E)\, dE. \tag{33}$$

3.2. An Analytical Example

For a spherically symmetric 3-dimensional harmonic oscillator potential, the exact level density can be written as[44]

$$g(E) = \frac{1}{(\hbar\omega)^3}\left[E^2 - \frac{1}{4}(\hbar\omega)^2\right]\left\{1 + 2\sum_{n=1}^{\infty}(-1)^n \cos\left(n\frac{2\pi E}{\hbar\omega}\right)\right\}\Theta(E). \tag{34}$$

We thus know the analytical form of its average part:

$$g_0(E) = \frac{1}{(\hbar\omega)^3}\left[E^2 - \frac{1}{4}(\hbar\omega)^2\right]. \qquad (E \geq 0) \tag{35}$$

This is a quadratic polynomial, and therefore the Strutinsky averaging with $M = 1$ should reproduce exactly this average part. Inserting Eq. (34) into Eq. (19), one obtains for the smooth part of E_{sp}:

$$E_{sp}^{(0)} = \hbar\omega\left[\frac{1}{4}\left(\frac{\widetilde{\lambda}}{\hbar\omega}\right)^4 - \frac{1}{8}\left(\frac{\widetilde{\lambda}}{\hbar\omega}\right)^2 - \frac{7}{320}\right], \tag{36}$$

where $\widetilde{\lambda}$ is given by the positive root of

$$N = \frac{1}{3}\left(\frac{\widetilde{\lambda}}{\hbar\omega}\right)^3 - \frac{1}{4}\left(\frac{\widetilde{\lambda}}{\hbar\omega}\right). \tag{37}$$

[Note that some contributions to Eq. (36) also come from the lower limit ($E = 0$) of the integral over the oscillating terms in Eq. (34). The expressions (36,37), which easily can be extended to a triaxially deformed harmonic oscillator, are identical to those obtained in the extended Thomas-Fermi model; see Sect. 3.5 below.] Since $E_{sp}^{(0)}$ is a fourth-order polynomial in the Fermi energy, one has to use a fourth-order curvature-correction ($M = 2$) in the Strutinsky averaging to obtain a γ-independent average energy $\widetilde{E}_{sp}$ (32).

As an illustration, we show in Figure 6 the results obtained for the shell-correction energy δE by Strutinsky averaging using the standard Gaussian averaging function (30) for various values of M. For any value $M \geq 2$ one obtains, indeed, a unique value of δE (and thus of $\widetilde{E}_{sp}$) which is constant as soon as $\gamma \gtrsim \hbar\omega$. The upper end of the "plateau" in Fig. 6 is merely due to the finite number of levels used in the

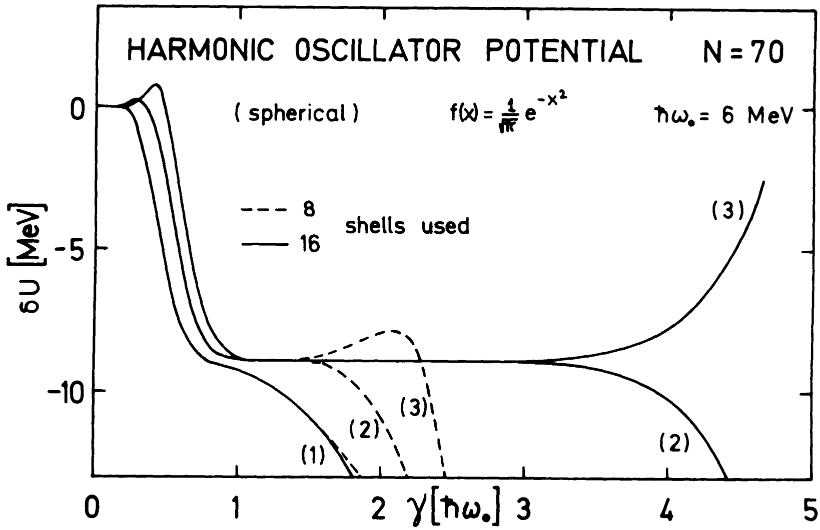

Fig. 6. Shell-correction energy δE versus averaging width γ for 70 fermions in a spherical harmonic oscillator, for various values of M and for two truncations of the energy spectrum[43].

summation. Very similar curves with identical plateau values of δE were obtained in Ref.[43] also with the averaging function in Eq. (31); in fact, it was shown there analytically that the plateau value of $\tilde{E}_{sp}(\gamma)$ equals $E_{sp}^{(0)}$ Eq. (36) independently of $f(x)$.

The harmonic oscillator represents an ideal case for the Strutinsky averaging. The Nilsson model, for which the method was first applied, also is near to ideal because it is not much different from an oscillator model. In general, however, the average part $g_0(E)$ of the level density is not a polynomial. As a consequence no ideal plateaux like in Fig. 6 can be found. This is particularly so in situations where the local level density is high and δE has a maximum, as e.g. near fission barriers of heavy nuclei[45]. In such cases, a more careful investigation of the plateau in $\tilde{E}_{sp}(\gamma)$ and its dependence on the correction order $2M$ is necessary.

3.3. The Plateau Condition

When $g_0(E)$ is not a polynomial, $\tilde{E}_{sp}$ can, in general not be made independent of γ. Some alternatives to the original Strutinsky energy averaging, assuming expansions in non-integer powers of energy, have been investigated[32, 37] but not been able to solve the problem of this γ dependence.

It is, however, still possible to employ the standard averaging method in order to find ***a local plateau*** in $\tilde{E}_{sp}(\gamma)$. As we have demonstrated above, this method consists essentially in a polynomial expansion of the average level density. This always works locally, i.e. in a limited energy interval around the Fermi energy

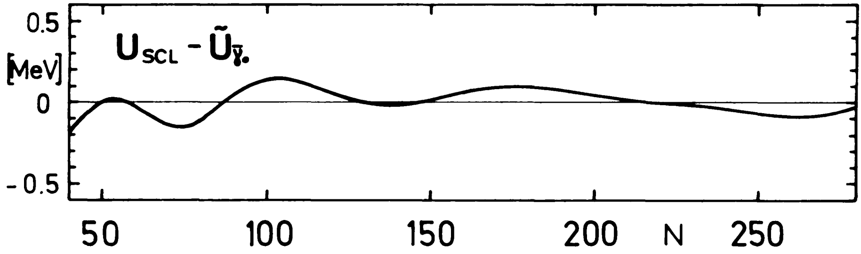

Fig. 7. Difference between semiclassical and Strutinsky-averaged s.p. energy sum in a cubic Hill-Wheeler box[43].

(except at possible – but usually uninteresting – singular points of $g_0(E)$). Hereby the curvature-correction order $2M$ must be varied to find the best degree of the local polynomial approximation to $g_0(E)$. One therefore has to fulfil at least locally the ***plateau condition***[7, 43] with respect to both γ and M:

$$\frac{\partial \tilde{E}_{sp}(M_0)}{\partial \gamma}\bigg|_{\gamma_0} = 0; \qquad \frac{\Delta \tilde{E}_{sp}(\gamma_0)}{\Delta M}\bigg|_{M_0} = 0. \tag{38}$$

[The plateau condition has also been discussed in connection with the stationarity of a selfconsistently Strutinsky-averaged HF energy[16].] Typically, solutions of (38) can be found with values of the order

$$\gamma_0 \sim (1 - 1.6)\, \hbar\Omega; \qquad M_0 \sim 3 - 8, \tag{39}$$

where $\hbar\Omega$ is the main-shell spacing in the spectrum $\{\epsilon_i\}$.

The uncertainties in finding unique plateau values of $\tilde{E}_{sp}$ or the shell-correction δE are usually less than ± 1 MeV for nuclei with N or $Z \gtrsim$ 40 - 50. For smaller particle numbers, uncertainties up to $\sim$ 2 MeV or more may be found, in particular in finite-depth potentials as discussed below. (See Ref.[31] for a more detailed summary.)

As an illustration we take the Hill-Wheeler box[46], i.e. an infinite rectangular box potential with side lengths a, b and c subject to the volume conservation condition $abc = L^3$. Its semiclassical average level density is known (see also Ref.[47]):

$$g_0(E) = \frac{\pi}{4}\frac{1}{E_0}\left[\sqrt{E/E_0} - \frac{\pi}{8}(S/2L^2) + \frac{1}{8}(C/L)\sqrt{E_0/E}\right]. \tag{40}$$

Hereby $E_0 = (\pi^2\hbar^2)/(2mL^2)$ is the natural energy unit, $S = 2(ab + ac + bc)$ is the surface and $C = a+b+c$ the "mean curvature" of the box. Since this $g_0(E)$ is not a polynomial in E, the local plateau conditions Eq. (38) must be solved at each energy. In Figure 7 we show the results[43] for the *difference* between the semiclassical average s.p. energy obtained from Eq. (40) by integration and the plateau values of $\tilde{E}_{sp}$ in the case of the cubic box. The difference is seen to be less than ± 0.2 MeV for all particle numbers $N > 40$, demonstrating that the local polynomial approximation to (40) works very well.

A basic problem is met with the finite-depth potentials frequently used in nuclear physics. Here the spectrum has a continuum for $E > 0$, and the problem is how to treat this continuum. In particular when the Fermi energy comes close to the continuum, i.e. if the separation energy of a nucleon is comparable to or less than the main shell spacing $\hbar\Omega$ (and thus γ), the Strutinsky-averaged results depend rather crucially on the lowest continuum states. In practice, one diagonalizes the potential in a finite harmonic oscillator basis[7, 8]. This leads – for not too large basis sizes – to a set of discrete states with $E > 0$ which approximate the lowest resonances. Including them in the averaging, the plateau conditions (38) can usually be fulfilled reasonably well for not too small nuclei. This has been carefully studied for a realistic spherical Woods-Saxon potential in Ref.[36]. As a rather extreme example where one has to go relatively high correction orders $2M$ to obtain convergence of (38), we show in Figure 8 the neutron shell-correction δE for $N = 170$.

A more rigorous inclusion of the resonances in the continuum by a calculation of the corresponding phase shifts[48] has shown that, indeed, very good plateaux can be found if resonances up to sufficiently high energies $E > 0$ are included.

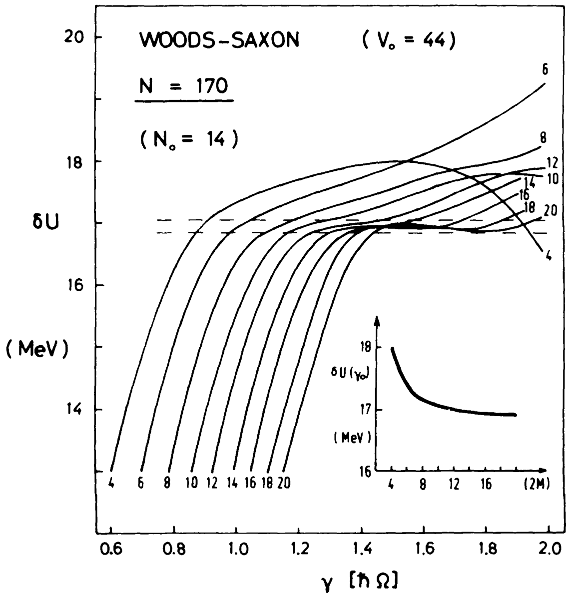

Fig. 8. Shell-correction energy δE versus γ for 170 neutrons in a spherical Woods-Saxon potential for various values of $2M$. The two dashed horizontal lines give the estimated error bars for the optimal plateau value. (Note that the semiclassical ETF energy discussed in Sect. 3.5 lies within these error bars.) The insert shows the plateau values versus curvature-correction order[36].

3.4. Averaged Occupation Numbers

Since Eq. (29) for the Strutinsky-averaged level density can be written in the form

$$\tilde{g}_M(E) = \sum_i \tilde{g}_i(E), \tag{41}$$

it is straightforward to define *averaged occupation numbers*[7, 43] by

$$\tilde{n}_i = \int_{-\infty}^{\tilde{\lambda}} \tilde{g}_i(E)\, dE \tag{42}$$

such that

$$N = \sum_i \tilde{n}_i. \tag{43}$$

[See Figure 5 for a schematic plot of the integral of $f(x)$ appearing in the explicit evaluation of Eq. (42).] It may be shown by algebraic manipulations[43] that, independently of the averaging function $f(x)$, the quantity $\tilde{E}_{sp}$ in Eq. (32) fulfils the following differential equation:

$$\tilde{E}_{sp} = \sum_i \epsilon_i \tilde{n}_i + \gamma \frac{d\tilde{E}_{sp}}{d\gamma}. \tag{44}$$

If the plateau condition (38) can be fulfilled, one can therefore write the shell-correction energy δE in a particularly attractive form:

$$\delta E = \sum_i \epsilon_i (n_i^{HF} - \tilde{n}_i) = \sum_i \epsilon_i \delta n_i. \tag{45}$$

The form (45) of the shell correction shows that it only depend on the s.p. levels near the Fermi energy: far above or below it, the averaged occupation numbers tend towards the HF ones and thus δn_i tends to zero. This is illustrated in Figure 9 for a realistic case of $Z = 94$ protons in a Woods-Saxon potential.

The occupation numbers $\tilde{n}_i$ (42) can also be used to define Strutinsky-averaged nucleon densities[7]

$$\tilde{\rho}(r) = \sum_i |\varphi_i(r)|^2\, \tilde{n}_i \tag{46}$$

or the density matrices $\tilde{\rho}_{\alpha\beta}$ (8) used in Sect. 2.1.

Eq. (44) suggests an interesting analogy[31] of the Strutinsky averaging to the temperature averaging appropriate to a canonical ensemble of (non-interacting) fermions. For the latter, the free energy F is well-known to fulfil the differential equation

$$F = \sum_i \epsilon_i n_i(T) + T\frac{dF}{dT}, \tag{47}$$

where T is the temperature in energy units ($k \equiv 1$), $n_i(T)$ are the Fermi occupation numbers

$$n_i(T) = \frac{1}{1 + \exp\left(\frac{\epsilon_i - \mu}{T}\right)}, \tag{48}$$

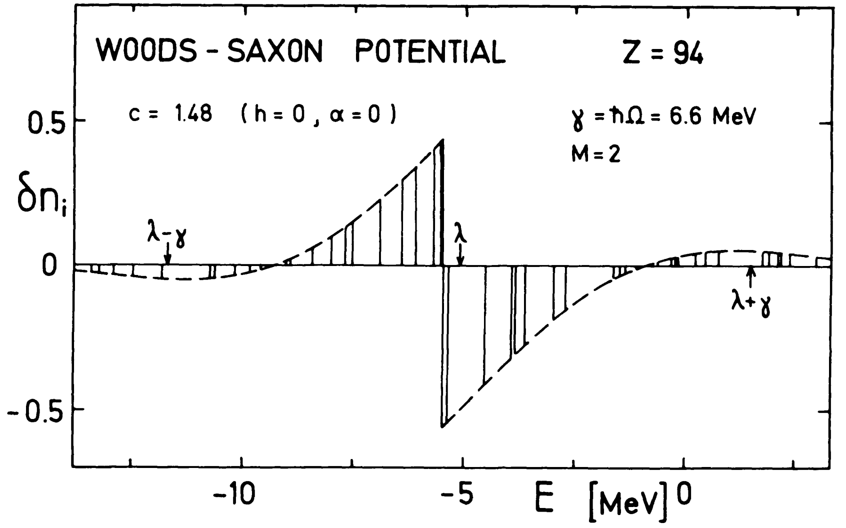

Fig. 9. Occupation number difference $\delta n_i = n_i^{HF} - \tilde{n}_i$ versus energy for a Woods-Saxon potential corresponding to the $Z = 94$ protons of the Pu fission isomer[7]. The vertical lines indicate the positions of the proton s.p. levels ϵ_i.

μ is the chemical potential and the derivative in Eq. (47) gives the negative entropy S:

$$\frac{dF}{dT} = -S. \tag{49}$$

We thus have the following one-to-one correspondence:

$$\begin{aligned} \tilde{E}_{sp} &\longleftrightarrow F \\ \gamma &\longleftrightarrow T \\ \frac{d\tilde{E}_{sp}}{d\gamma} &\longleftrightarrow -S. \end{aligned} \tag{50}$$

This shows that the Strutinsky averaging is very similar to that brought about by a finite temperature – however, with one important difference: it leaves the system unexcited since, due to the curvature corrections (with $M > 0$), the "effective entropy" $-d\tilde{E}_{sp}/d\gamma$ can be kept to zero by the plateau condition (38).

The close relation of Strutinsky and temperature averaging has been exploited in the so-called "temperature method"[38] for extracting the smooth part of the s.p. energy sum (1) in an alternative way.

3.5. Relation to the Extended Thomas-Fermi Model

Bhaduri and coworkers[34] proposed to use the extended Thomas-Fermi (ETF) model as a semiclassical alternative to Strutinsky averaging. In fact, the close relation between the two methods had been pointed out early[1, 7, 49]. The main idea[34] is to start from the semiclassical expansion of the partition function – which is the Laplace transform of the level density $g(E)$ Eq. (18) – in powers of Planck's constant $\hbar$, using e.g. the Wigner-Kirkwood method[50]. By inverse Laplace transform term by term one arrives at a semiconverging asymptotic expansion of $g(E)$ whose finite part is identical to $g_0(E)$ in Eq. (21). By integration analogously to Eq. (19) one obtains the semiclassical part of E_{sp} in the form of an asymptotic expansion

$$E_{ETF} = E_{TF} + E_2 + E_4 + \ldots.. \qquad (51)$$

The first term is the pure Thomas-Fermi result and the terms E_m come from the semiclassical corrections proportional to $\hbar^m$. The series (51) converges very fast; usually the term E_4 is only of order 1 - 2 MeV.

For a three-dimensional (spherical or deformed) harmonic oscillator potential, E_{ETF} has been shown analytically[43, 44] to be identical to the Strutinsky-averaged energy $\tilde{E}_{sp}$ given by Eq. (32). For realistic Woods-Saxon potentials including spin-orbit interaction, the two energies have been compared carefully[51] and found to be equal within less than ~ 1 MeV for not too small particle numbers, i.e. within the overall accuracy of either method. (See also Sec. 3.3 and Fig. 7 for the case of a cubic box potential.)

The ETF model may also be used in semiclassical density variational calculations[52, 53] to obtain selfconsistent average nuclear properties from a given effective nucleon-nucleon interaction. The resulting binding and deformation energies have been shown[52] to be very close to the Strutinsky-averaged HF energies (11).

In a series of papers[54], the variational ETF model has been combined with the Strutinsky method to develop a microscopically based mass formula which has been successfully applied also to large deformations and nuclei far from β stability.

4. Some Recent Applications

Strutinsky's shell-correction method – by some authors also termed the "macroscopic-microscopic" method – has been extremely successful in calculations of nuclear masses and deformation energies, in particular fission barriers. We refer to the presentation of R. Wyss[55] for some detailed examples and comparisons of the results, also in applications to high-spin physics. The status of fission barrier calculations with the SCM and the HF(B) method in early 1979 was summarized in Ref.[31]. Very recently, a critical assessment of nuclear mass models employing the SCM was given by Möller and Nix[56], covering also the newest results[57] of the ETFSI model by Pearson and coworkers[54].

We shall conclude this little review by mentioning two applications of Strutinsky's ideas in other domains of physics.

Metal clusters have recently obtained much attention – not least because of their striking similarity to nuclei. (See some recent review articles[58, 59] for the detailed literature.) Pronounced shell effects can be observed in mass yields and ionization potentials and suggest that the valence electrons can be described to a good approximation in a mean-field approximation. Since metal clusters can be made neutral, there is no limitation to their size, in contrast to nuclei. Accordingly, one has been able to observe "magic numbers" corresponding to filled major shells up to $N \sim 3000$. Most spectacularly, the so-called "super-shell" structure has been observed[60], which already was obtained theoretically by Balian and Bloch[40] in the level density of a spherical box. For metal clusters, microscopical calculations with a phenomenological Woods-Saxon potential[61] or with the self-consistent jellium model[62] give, indeed, a beating pattern in the level density and the shell-correction energy of metal clusters which is in good agreement with the experimental observations. The Strutinsky energy theorem has been used as a technical means for simplifying the rather time consuming selfconsistent microscopical calculations at finite temperatures[63]. A direct use of the SCM, renormalizing the wrong surface energy of the jellium model to its experimental value, has been made in calculations for deformation energies of large clusters[64]. As an example of the results, we show in Figure 10 the shell-correction energy δE for Na clusters with up to $N = 850$ atoms, evaluated at their axially symmetric ground states. The deepest minima correspond to spherical clusters with atomic numbers 58, 92, 138, 186, 254, 338, etc., whereas the smaller minima marked by arrows correspond to oblate or prolate ground-state shapes. Most of the spherical and many of the deformed magic numbers have been experimentally seen within the statistical error bars of the extracted fluctuating part of the mass yields.

Finally we mention that the Strutinsky energy averaging has been found very useful[65] for extracting the oscillating part $\delta g(E)$ of the quantum-mechanical density

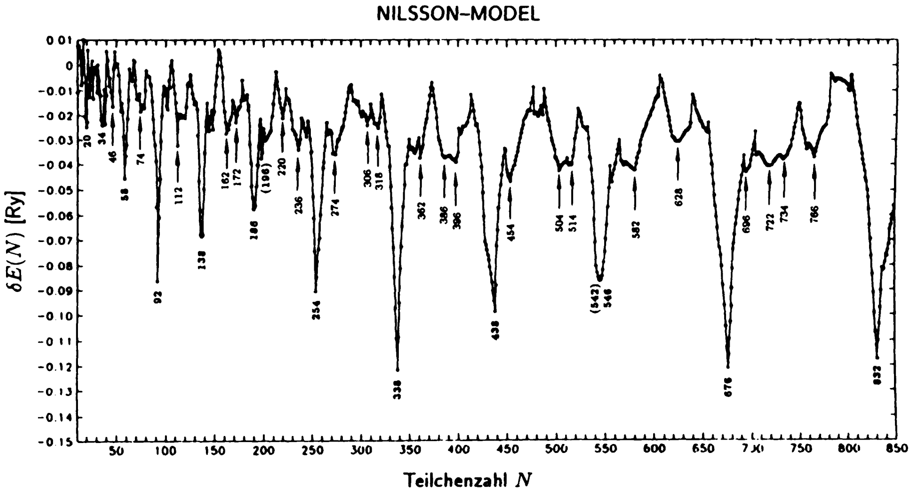

Fig. 10. Shell-correction energies δE of Na clusters versus number N of atoms (or valence electrons) at the corresponding (axially symmetric) ground-state deformations[64].

of states in the Hénon-Heiles potential[66] which has been intensively studied in connection with classical chaos (see, e.g., Ref.[67]). An interesting beating pattern in $\delta g(E)$ was found[65], even at energies where the classical orbits are mostly chaotic. This can be interpreted in terms of Gutzwiller's periodic orbit theory[39] – similarly to the super-shell beating just mentioned above – and demonstrates that long-range order in the energy spectrum can coexist with the short-range correlations that are typical for chaotic behavior.

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