VALIDITY OF THE STRUTINSKY METHOD, STUDIED WITHIN THE HARTREE - FOCK FRAMEWORK.

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Abstract:

The foundation of the Strutinsky method within the Hartree-Fock (HF) framework is discussed. Both the basic energy theorem and the energy averaging method are investigated theoretically and numerically. The equivalence of the averaging method with semiclassical expansions is exhibited. Numerical tests of the basic assumptions of the shell-correction approach are presented, which make use of the results of constrained HF calculations for various nuclei and with different effective interactions. The HF energy is decomposed into a smooth part which is shown to be very close to a liquid drop model energy, a first order shell-correction defined in the usual way, and higher order corrections which usually are neglected in standard Strutinsky calculations. These higher order terms are shown not to contribute more than $\sim$ 1 - 2 MeV to the total energy in medium and heavy nuclei. New results for the nucleus ^{40}Ca show that this is no longer the case for light nuclei. Alternative ways of defining the smooth part of the energy are also considered. It is particularly found that if the Strutinsky averaging is performed selfconsistently, the sum of the average energy plus the first order shell-correction extracted from the average potential reproduces perfectly well the exact HF energy.

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1. INTRODUCTION

The shell-correction method proposed by Strutinsky [1] may be considered as a perturbative approach to a selfconsistent theory of nuclear binding and deformation energies avoiding the explicit use of a two body interaction. Starting from Hartree-Fock (HF) theory with any effective nucleon-nucleon interaction, one can in fact show [2-4] that the main part of the shell fluctuations in the total nuclear binding energy is contained in the sum of occupied eigenenergies of the averaged self-consistent field. The nucleon interaction enters explicitly only in terms of second and higher orders in the fluctuating part $\delta\varrho$ of the selfconsistent density matrix, which can be expected to be small. The practical shell-correction approach consists in neglecting these terms and identifying the average part of the selfconsistent field with one of the available phenomenological shell model potentials.

Using various versions of deformed shell model potentials and of the liquid drop model, the shell-correction calculations have been very successful in reproducing nuclear ground state masses and in describing the details of the static deformation energy surfaces of medium and heavy nuclei. Especially the fact that the nature of the fission isomers could be explained and that many experimental fission barriers could be fitted within less than $\sim$1-2 MeV, belong to the remarkable successes of this method. For discussions of all the details of these calculations, their applications and comparisons with experimental data, we refer

to some review articles [3,5-7] which also contain extended reference lists to many other important publications.

Our present aim is to discuss the foundation of the Strutinsky method on the basis of the HF theory. The energy theorem is discussed theoretically in sect. 2. Because of its practical importance, the energy averaging method is shortly reviewed in sect. 3 and its relations to some statistical and semiclassical methods are discussed. In sect. 4, extended numerical calculations are presented which were performed in order to test the assumptions made in the usual shell-correction approach. Other related calculations are compared and in the conclusions, some approximations are mentioned which allow to study the effects of various forces in a more economical way than by doing fully selfconsistent constrained HF calculations.

2. THE STRUTINSKY ENERGY THEOREM

We shall in this section discuss the theoretical derivation of the Strutinsky method in the framework of the Hartree-Fock (HF) theory. Since the paper of Strutinsky in 1968 [2], this derivation has been re-investigated many times by various authors [3,4,8-14] and we shall therefore restrict ourselves to a short presentation of the main steps and assumptions.

One starts from the HF-energy, expressed in terms of the density matrix ϱ corresponding to a Slater determinant wave-function:

$$E_{HF}(\varrho) = \mathrm{tr}\, T\varrho + \tfrac{1}{2}\mathrm{tr}\,\mathrm{tr}\,\varrho v\varrho \,. \qquad (2.1)$$

Here τ is the matrix of the kinetic energy operator and v the antisymmetrized matrix of an effective two body interaction which we for the moment assume to be local and density independent (In eq.(2.1) and henceforth, trtr means the double trace). The density matrix ρ is normalized to the number N of particles

$$\mathrm{tr}\,\rho = N. \tag{2.2}$$

(We consider here only one kind of particles). The selfconsistency is given through the HF equation

$$[T + V_{HF} + \lambda\hat{q}]\,\varphi_i = \varepsilon_i \varphi_i . \tag{2.3}$$

In eq. (2.3) V_{HF} is the HF-potential

$$V_{HF} = \mathrm{tr}\,\rho v \tag{2.4}$$

and $\lambda\hat{q}$ is a constraint (with Lagrange multiplier λ) which is introduced in order to give solutions with a fixed quadrupole moment Q

$$Q = \mathrm{tr}\,\hat{q}\rho\,, \tag{2.5}$$

$\hat{q}$ being the quadrupole operator. (Of course, other constraints can be used to fix different,or several, moments.) In terms of any basis $|\alpha\rangle$, we can write the single particle states as

$$\varphi_i = \sum_\alpha C_\alpha^i |\alpha\rangle, \tag{2.6}$$

and the coefficients C_α^i build the density matrix

$$\rho_{\alpha\beta} = \sum_{i=1}^{N} C_\alpha^{i*} C_\beta^i\,, \tag{2.7}$$

where the summation goes over the lowest occupied states of the selfconsistent spectrum $\{\varepsilon_i\}$.

The first step is now to write the selfconsistent density matrix as a sum of two terms

$$\rho = \bar{\rho} + \delta\rho \,. \tag{2.8}$$

Here $\bar{\rho}$ is the average part of ρ which is assumed to generate the bulk part of the total binding energy in the sense of the liquid drop model (LDM, see e.g.ref. [15]). Practically, $\bar{\rho}$ may be obtained by a statistical averaging over many neighbouring nuclei or by a semiclassical expansion (see the discussion in sect. 3 below). The shell fluctuations in the energy are then coming from the term $\delta\rho$ which is assumed to be a small correction to ρ, at least in heavy nuclei.

One then defines an average potential $\bar{V}$ by

$$\bar{V} = \mathrm{tr}\,\bar{\rho}\,v \tag{2.9}$$

which also varies smoothly with nucleon number and therefore may be identified with a shell-model potential. It determines the"shell-model" states $\{\hat{\varepsilon}_i, \hat{\varphi}_i\}$ by

$$[T + \bar{V}]\,\hat{\varphi}_i = \hat{\varepsilon}_i\,\hat{\varphi}_i \,, \tag{2.10}$$

and a density matrix $\hat{\rho}$ analogous to eqs. (2.6) and (2.7). In terms of these quantities one can then show,e.g. by first order perturbation theory [2,3] that

$$E_{HF} = \sum_{i=1}^{N} \hat{\varepsilon}_i - \tfrac{1}{2}\,\mathrm{tr}\,\mathrm{tr}\,\bar{\rho}\,v\,\bar{\rho} + O[(\delta\rho)^2]. \tag{2.11}$$

This equation, which in fact just relies on the stationarity of the HF solution against changes of the density ρ , tells us that all contributions to the energy of first order in $\delta\rho$ are contained in the sum of "shell-model" energies $\hat{\varepsilon}_i$. If the higher order terms can be neglected, the sum $\sum_{i=1}^{N} \hat{\varepsilon}_i$ contains all shell effects of the HF-energy. Eq. (2.11) thus gives the basis to the Strutinsky energy theorem

$$E_{HF} = \bar{E} + \delta E_1 + O((\delta\rho)^2), \tag{2.12}$$

where

$$\delta E_1 = \sum_{i=1}^{N} \hat{\varepsilon}_i - \overline{\sum_i \hat{\varepsilon}_i} \quad , \tag{2.13}$$

$$\bar{E} = \overline{\sum_i \hat{\varepsilon}_i} - \tfrac{1}{2} \text{ tr tr } \bar{\rho} v \bar{\rho} \, . \tag{2.14}$$

The quantity $\overline{\sum_i \hat{\varepsilon}_i}$ is the average part of the exact sum of the occupied levels $\hat{\varepsilon}_i$ and will be defined in sect. 3 below. In the practical shell-correction calculations [2-7], the energy $\bar{E}$, which by definition is a smoothly varying quantity, is replaced by the energy obtained from the liquid drop model (see e.g. ref. [15]); δE_1 is obtained substituting for $\hat{\varepsilon}_i$ the energy levels from a phenomenological deformed shell model potential (e.g. Nilsson model), and the higher order terms in $\delta\rho$ are neglected. Thus, the two body interaction v and the density matrices $\rho, \bar{\rho}$ never appear explicitly in such calculations.

In contrast to the findings of refs. [8,9], the energy theorem (2.12) is also true for density dependent effective interactions as obtained from nuclear matter G-matrix calculations in the local density approximation [16, 17], if the rearrangement terms are included consistently in all quantities defined above, esp. also in the averaged potential $\bar{V}$ (2.9)(see ref. [4] for a detailed discussion of this point). Three or more body forces are treated readily in the same way. Moreover, the pairing correlations can be easily included in the BCS approximation (see refs. [2], [6]). For a discussion of the energy theorem within the HF-Bogolyubov approximation, we refer to ref. [18].

A point of special interest has been the question [10,19] whether one should include a constraint in the shell-model Hamiltonian eq. (2.10). If so, it is clear that one has to

constrain the shell model solution $\hat{\varrho}$ in such a way that $\mathrm{tr}(\varrho-\hat{\varrho})\hat{q}=0$. But the consideration in δE_1 of energies $\hat{\varepsilon}$ either with or without the external field contribution, does not affect significantly the numerical results for the total energy, as found in Ref. [20] (see also sect. 4 below).

Let us summarize at this point the different aspects of the basic assumptions which underly the usual shell-correction approach:

1) The selfconsistent density matrix ϱ can be split into a smooth part $\bar{\varrho}$ and an oscillating part $\delta\varrho$ in such a way, that all energy terms containing only $\bar{\varrho}$ vary slowly with nucleon number and deformation.
2) The terms of second and higher orders in $\delta\varrho$ in the total HF energy are negligible. Since the typical shell-corrections δE_1 one deals with are of order $\pm$5-10 MeV, the neglected terms should not contribute more than ~1-2 MeV.
3) The average potential $\bar{V}$ eq. (2.9) can be represented by one or the other of the usual phenomenological shell-model potentials.
4) The average energy $\bar{E}$ eq.(2.14) can be represented by some liquid drop model energy.
5) The smooth part $\overline{\sum_i \hat{\varepsilon}_i}$ of the single-particle energy sum in eq.(2.13), which in principle is related to the smooth matrix $\bar{\varrho}$, can practically be defined in a unique way.

Whereas the last point 5) is rather a technical problem which can be discussed independently of HF calculations - this will be done in sect. 3 -, the assumptions 1) - 4) can only be tested in numerical calculations explicitly using an effective interaction v. In sect. 4, we will discuss such numerical calculations which were recently performed in order to check the validity of the Strutinsky method. An indirect evidence for the

smallness of the neglected terms is given by the close agreement found between experimental and theoretical fission barriers, ground state mass corrections and deformations, as well as between their various theoretical predictions using rather different shell model potentials and nuclear shape parametrizations.

Before concluding this section, we will discuss a slightly different form of the energy theorem, which is not directly related to the practical application of the Strutinsky method, but which might give some insight into the role of the quantities defined above. For that, we have to anticipate that a practical way of defining the smooth density matrix $\bar{\rho}$ is found by introducing the averaged occupation numbers $\bar{n}_i$ which will be defined in sect. 3 below. One may thus define (cf. eq.(2.7))

$$\bar{\rho}_{\alpha\beta} = \sum_i C_\alpha^{i*} \cdot C_\beta^i \bar{n}_i ; \quad \mathrm{tr}\,\bar{\rho} = \sum_i \bar{n}_i = N . \tag{2.15}$$

Consistently with this, one can define the smooth part of the sum of occupied HF levels ε_i:

$$\overline{\sum_i \varepsilon_i} = \sum_i \varepsilon_i \bar{n}_i . \tag{2.16}$$

(Eq.(2.16) is only true with some restriction to be discussed in sect. 3 below).

Using eqs. (2.1), (2.3) one can easily see that

$$\sum_i \varepsilon_i \bar{n}_i = \mathrm{tr}\, t \bar{\rho} + \mathrm{trtr}\, \rho v \bar{\rho} + \lambda\, \mathrm{tr}\, \hat{q} \bar{\rho} , \tag{2.17}$$

and that E_{HF} is exactly given by

$$E_{HF}(\rho) = E(\bar{\rho}) + \delta E_1^{HF} - \lambda \mathrm{tr}\hat{q}\delta\rho - \tfrac{1}{2}\mathrm{tr}\,\mathrm{tr}\,\delta\rho v \delta\rho \tag{2.18}$$

where

$$E(\bar{\rho}) = \mathrm{tr}\mathcal{T}\bar{\rho} + \tfrac{1}{2}\mathrm{trtr}\,\bar{\rho}\mathcal{V}\bar{\rho} \tag{2.19}$$

and

$$\delta E_1^{HF} = \sum_{i=1}^{N} \varepsilon_i - \sum_i \varepsilon_i \bar{n}_i . \tag{2.20}$$

The difference between δE_1^{HF} (2.20) and δE_1(2.13) is that in the former quantity, the selfconsistent energy levels ε_i are used. Since they are obtained with a constraint (see eq.(2.3)), an extra term appears in eq.(2.18). It is easy to show that the difference between δE_1 eq.(2.13) and the two first order terms in eqs. (2.18) is of second order in $\delta\rho$.

Eq. (2.18) explains the result of ref. [21] , where it was found that the curvatures around two minima in the selfconsistently calculated deformation energy curve of ^{32}S, as well as the energy difference between the minima, were well reproduced in a Strutinsky calculation using the HF levels ε_i.

One should, however, not confuse the fact that the shell-correction may be found from the HF levels directly (up to second-order terms) with the wrong statement, that the sum of occupied HF levels $\sum_{i=1}^{N} \varepsilon_i$ should contain <u>all</u> first order contributions. This misinterpretation of the Strutinsky energy theorem has repeatedly lead to erroneous conclusions, when the sum $\sum_{i=1}^{N} \varepsilon_i$ and the constrained HF energy E_{HF} were found to behave differently as functions of deformation [10,19,22] . The reason why $\sum_{i=1}^{N} \varepsilon_i$ contains too strong fluctuations can be seen from the equations above. The formally smoothed quantity $\sum_i \varepsilon_i \bar{n}_i$ eq.(2.17) contains also an oscillating term linear in $\delta\rho$, namely $\mathrm{trtr}\,\delta\rho\mathcal{V}\bar{\rho}$. This term cancels a part of the fluc-

tuations contained in $\sum_{i=1}^{N} \varepsilon_i$, such that the difference δE_1^{HF} defined by equation (2.20) contains all essential fluctuations (up to the constraint and higher order terms in eq. (2.18)). Contrarily, if the eigenvalues $\hat{\varepsilon}_i$ of the smoothed one body Hamiltonian are used to define δE_1, as shown in eqs.(2.9)-(2.14) above, all fluctuations of first order in $\delta\rho$ are contained in the sum $\sum_{i=1}^{N} \hat{\varepsilon}_i$. The numerical results discussed in sect. 4 will further illustrate this point.

The form (2.18) of the Strutinsky energy theorem corresponds to a Taylor expansion of the HF energy functional around the smooth value $\bar{\rho}$ of the density matrix. We may thus speak of an expansion of E_{HF} into a "shell-correction series", the zeroth order term of which is the average (LDM) binding energy, the other terms being the first and higher order shell-corrections. The fact that no third order term appears in eq.(2.18) is due to the special choice of the interaction; this will no longer be so in the presence of e.g. a three body force. The convergence of the shell-correction series may depend on the special definition of $\bar{\rho}$ and of δE_1 (or δE_1^{HF}), the interaction used, the specific nucleon number, etc. The numerical results presented in sect. 4 below will show that by a suitable choice of the first two terms of the shell-correction series, one may minimize the sum of the remaining higher order corrections even for rather light nuclei.

3. THE STRUTINSKY ENERGY AVERAGING METHOD

For the definition of the smooth part of the single particle energy sum appearing in the definition of the shell-correction δE_1 (2.13) above, Strutinsky introduced a special energy-averaging technique [1,2] which is very convenient for practical use. We refer again to the literature for the details and discuss here mainly its relation to some alternative methods which have been proposed. We ignore in this section the difference between the selfconsistent energies ε_i and the shell-model energies $\hat{\varepsilon}_i$ made in the last section, and assume just that ε_i are the eigenvalues of the single particle Hamiltonian H with some potential V:

$$H\varphi_i = (T+V)\varphi_i = \varepsilon_i \varphi_i . \tag{3.1}$$

The smooth single particle energy is defined in terms of an average level density $\bar{g}(E)$ obtained by smearing the spectrum ε_i over an energy range γ :

$$\bar{E} = \overline{\sum_i \varepsilon_i} = \int_0^{\bar{\lambda}} E\bar{g}(E)dE, \tag{3.2}$$

$$\bar{g}(E) = \frac{1}{\gamma}\sum_i f_M\left(\frac{E-\varepsilon_i}{\gamma}\right) \tag{3.3}$$

In eq. (3.2), $\bar{\lambda}$ is the Fermi energy determined by the particle number conservation

$$N = \int_0^{\bar{\lambda}} \bar{g}(E)dE ; \tag{3.4}$$

hereby the bottom of the potential V has been normalized to zero energy. In eq. (3.3), $f_M(x)$ is some smooth distribution function, normally taken to be a Gaussian, including the curvature-correc-

tions. These corrections are an essential ingredient of the procedure; they guarantee that any smooth part of the level density through the definition (3.3) is implicitly approximated by the first 2M+1 terms of its Taylor expansion.

The procedure has been formulated in ref. [23] in terms of a general class of averaging functions $f_M(x)$ and it has been shown that, independently of the specific shape of $f_M(x)$, the smooth energy $\bar{E}$ eq.(3.2) can be written as

$$\bar{E} = \sum_i \varepsilon_i \bar{n}_i + \gamma \frac{d\bar{E}}{d\gamma} \tag{3.5}$$

for all values of γ and M. The average occupation numbers $\bar{n}_i$ are given by

$$\bar{n}_i = \frac{1}{\gamma} \int_0^{\bar{\lambda}} f_M\left(\frac{E-\varepsilon_i}{\gamma}\right) dE \Rightarrow \sum_i \bar{n}_i = N . \tag{3.6}$$

Practically, the second term in eq.(3.5) does not contribute, since $\bar{E}$ and with it the shell-correction δE, defined by

$$\delta E = \sum_{i=1}^{N} \varepsilon_i - \bar{E} , \tag{3.7}$$

have to fulfill the plateau-condition, i.e. they have not to depend on γ in a region of values somewhat larger than the mean distance Ω of shells in the spectrum $\{\varepsilon_i\}$. The plateau condition may be written in an infinitesimal form [23] as

$$\left.\frac{d\tilde{E}}{d\gamma}\right|_{\gamma_c} = - \left.\frac{d(\delta E)}{d\gamma}\right|_{\gamma_0} = 0 \tag{3.8}$$

and is usually fulfilled for values of M and γ_0 given by

$$0 < M \lesssim 6 - 12; \qquad \Omega \lesssim \gamma_0 \lesssim 2\Omega \ll \lambda . \tag{3.9}$$

For realistic finite depth potentials, the distance of the Fermi level λ from the continuum region is normally of the order of the main shell spacing Ω, such that non-negligible contributions to $\bar{g}(E)$ come from this region. If no continuum states are included in the sums in eqs.(3.3) and (3.5), the level density suddenly drops to zero there and the values of $\bar{g}(E)$ close to the Fermi level become too low. This problem is usually circumvented [3,23,24] by including some artificial unbound states in the lower part of the continuum. This leads, however, to some ambiguities in the determination of $\bar{E}$. (For numerical estimates of these ambiguities, see the discussion below.) A more correct method would be to include the resonances, as demonstrated by Ross and Bhaduri [25], but this is practically not realizable for realistic deformed potentials.

Mainly due to this continuum problem and the uncertainties related to it, several alternative methods have recently been proposed for the definition of the smooth energy $\bar{E}$ or the average level density $\bar{g}(E)$.

In the thermodynamical-statistical theory of a system of independent particles (see,e.g. ref. [26]), it is a well-known feature that the shell-effects disappear at large temperatures (i.e. at large excitation energies). Some asymptotic relations between entropy S and excitation energy E^* can be obtained in which the ground state shell-correction appears as a parameter [27]. Ramamurthy et al. [28] have used this fact and proposed a method to extract the shell-correction energy by calculating S and E^* for large temperatures and extrapolating their average parts back to zero temperature. The shell-corrections found in this way for a Nilsson model spectrum agreed well with the values

of δE given by eq.(3.7). In order to find unique values one has, however, to use the same kind of curvature-corrections as in the Strutinsky averaging method. In fact, one can show that the two methods are analytically equivalent, as was established independently by Kolomiets [18] and Bhaduri and Das Gupta [29] . The fact that the average quantities obtained in the temperature method have to be extrapolated back to zero temperature, makes evident that the Strutinsky smoothing leads to a cold average (i.e. without excitation). This can also be seen qualitatively from eq. (3.5) above (see also ref. [13]). With the identification $\gamma = T$, the Strutinsky-smoothed energy $\bar{E}(3.2,3.5)$ fulfils an equation analogous to the equation for the free energy

$$F = E - TS = \sum_i \epsilon_i \cdot n_i - T \frac{dF}{dT} . \qquad (3.10)$$

Thus, the quantity $\frac{dE}{d\gamma}$ in eq. (3.5) corresponds to the negative entropy. If, however, the plateau-condition (3.8) is fulfilled - which is only possible for curvature-corrections with $M > 0$ - this entropy is zero.

The temperature method has the same deficiency as the Strutinsky averaging in finite depth potentials, due to the continuum region, and is not more practical in use than the latter.*)

A method, which also relies upon statistical mechanics, but is formulated in a different mathematical way, was proposed by Bhaduri and Ross [31] and further developed by Jennings and Bhaduri [32, 33]. It consists in expressing the level density, the particle number and the single particle energy sum in terms of the partition function and expanding the latter in a series of powers of $\hbar$. Such a semiclassical expansion is indeed possible for any smooth local potential and has been developed by Wigner and Kirkwood [34]. Using only the first few terms of the expanded

*) For a compilation of several practical realizations of the temperature method, see Ref. [30] .

partition function, one obtains the average parts of level density and single-particle energy sum. These average quantities have been shown [32] to be the same as those obtained in the extended Thomas-Fermi model [35,36] or those obtained by Balian and Bloch [37] in an asymptotic expansion for large nucleon numbers. The partition function method allows to determine the average single-particle energy $\bar{E}$ to an accuracy of less than ~ 1 MeV for an arbitrarily deformed realistic local potential. The inclusion of a spin-orbit potential is possible [38], and a generalization of the method to rotating nuclei has also been proposed [39]. Jennings [40] has shown that for an infinite potential, the partition function method is equivalent to the Strutinsky averaging method, if in the latter the stationary equation (3.8) and the inequalities (3.9) for the smoothing width γ_0 are fulfilled.

For finite potentials, the partition function method has the advantage that the continuum region is never used in the numerical calculations. This allows therefore to test the validity of the commonly practised inclusion of artificial unbound states in the Strutinsky averaging procedure. Such a test has been done in ref. [35] for realistic Woods-Saxon potentials, both spherical and deformed up to a typical saddle point shape of heavy nuclei. The smooth energies $\bar{E}$ there obtained with the two methods for nuclei with $A \gtrsim 70$ agree within ~ 1MeV . This is also the order of the uncertainties coming from the truncation of the semiclassical expansion in one method and from the determination of the stationary points γ_0, eq. (3.8), in the other method.

An asymptotic expansion similar to that of Balian and Bloch [37] was proposed for the sum of occupied single-particle energies

by Bohr and Mottelson [41] :

$$\sum_{i=1}^{N} \varepsilon_i = a_v N + a_s N^{2/3} + a_c N^{1/3} + a_0 + \ldots + \delta E, \tag{3.11}$$

where a_v, a_s .... are constants which depend on the form of the potential, and δE is the shell-correction collecting all oscillating terms. The volume coefficient a_v is determined by the Thomas-Fermi result for the smooth energy, and the surface coefficient has been given by Siemens and Sobiczewski [42] in terms of phase shifts. For the curvature coefficient a_c no general analytical expression has been given so far; it may however be found by a numerical fit for the smooth part of eq. (3.25). This method is, however, met with some difficulties for realistic, deformed potentials. For spherical Woods-Saxon potentials without spin-orbit terms, numerical calculations of the coefficients in eq. (3.11) are in progress [43] . Since the results depend only on the occupied bound states ε_i ($i \leq N$), such calculations give also the opportunity to check the Strutinsky-averaged energies in finite potentials (see the discussion above).

4. NUMERICAL TESTS OF THE ENERGY THEOREM

4.1. Usual shell-correction expansion

In this section we will discuss numerical calculations performed in order to test the basic assumptions of the shell-correction method within the Hartree-Fock (HF) framework. We have earlier [20] presented some results obtained with the Skyrme effective interaction SIII for nuclei in the rare-earth region.

These calculations have since been extended (see also ref. [44]) to a larger number of nuclei and to other interactions as Skyrme II and the interaction of Negele in the density matrix expansion (DME) [45] . We do not here need to introduce these interactions, since they are discussed extensively at this conference.

The idea of these tests is to perform numerically the program outlined by Strutinsky [2] to justify the shell-correction method, as discussed in sect.2 above. Let us first summarize the different steps involved and their practical realization.

1. Full HF calculations are performed for different nuclei. A quadratic constraint on the quadrupole moment Q is used to obtain selfconsistent deformation energy curves $E_{HF}(Q)$ (see ref. [46]). The variational equations are solved by diagonalization of the HF Hamiltonian in a deformed harmonic oscillator basis $|\alpha\rangle$. Pairing correlations are included consistently (see ref. [47]). Hereby the uniform gap method [2,3], which allows to use one single parameter $\tilde{\Delta}$ for all nuclei and deformations, was applied in determining the pairing strengths $G_{n,p}$ for protons and neutrons.

2. At each deformation Q of a given nucleus, the selfconsistent density matrix ϱ is numerically smoothed using the Strutinsky averaging method to obtain

$$\bar{\varrho}_{\alpha\beta} = \sum_i \langle \alpha | i \rangle \langle i | \beta \rangle \bar{n}_i \qquad (4.1)$$

(independently both for protons and neutrons). Here $\bar{n}_i$ are the occupation numbers defined by eq. (3.6) in terms of the HF single-particle energies ε_i and $\langle i | \alpha \rangle$ is the projection of the i-th HF single-particle state on the

basis state $|\alpha\rangle$. (Note that with ε_i, we mean always the variational energies which contain contributions from the constraint, and not the physical removal energies!)

3. From the average density matrix $\bar{\rho}$ an average HF-Hamiltonian ("shell model" Hamiltonian) is calculated and its eigenvalues $\hat{\varepsilon}_i$ found by diagonalization.

4. The average energy $\bar{E}$, defined analogously to eq.(2.14) including the rearrangement terms, and the first order shell-correction δE_1 eq.(2.13) are explicitly calculated and can separately be compared to the LDM energies and shell-corrections obtained in the usual approach.

5. By taking the difference between E_{HF} and the sum of $\bar{E}$ and δE_1, one obtains the sum of all higher order shell-corrections, which we here call δE_2:

$$E_{HF} = \bar{E} + \delta E_1 + \delta E_2 . \qquad (4.2)$$

Explicit expressions for all these quantities, including the constraint and pairing terms, have been given for the Skyrme force in ref. [20] and need not be repeated here. In the Strutinsky averaging of the spectra ε_i and $\hat{\varepsilon}_i$, the stationary condition (3.8) is used so that no single parameter enters the decomposition (4.2) of the HF energy. We shall in the following present some selected results, which supplement those of ref. [20]. An extended compilation of all results with discussions of the technical details will be published elsewhere [48].

Fig. 1 shows different deformation energy curves calculated for the nucleus ^{240}Pu with the interaction Skyrme III. The solid line is the HF energy E_{HF} which has been published before [49]. The

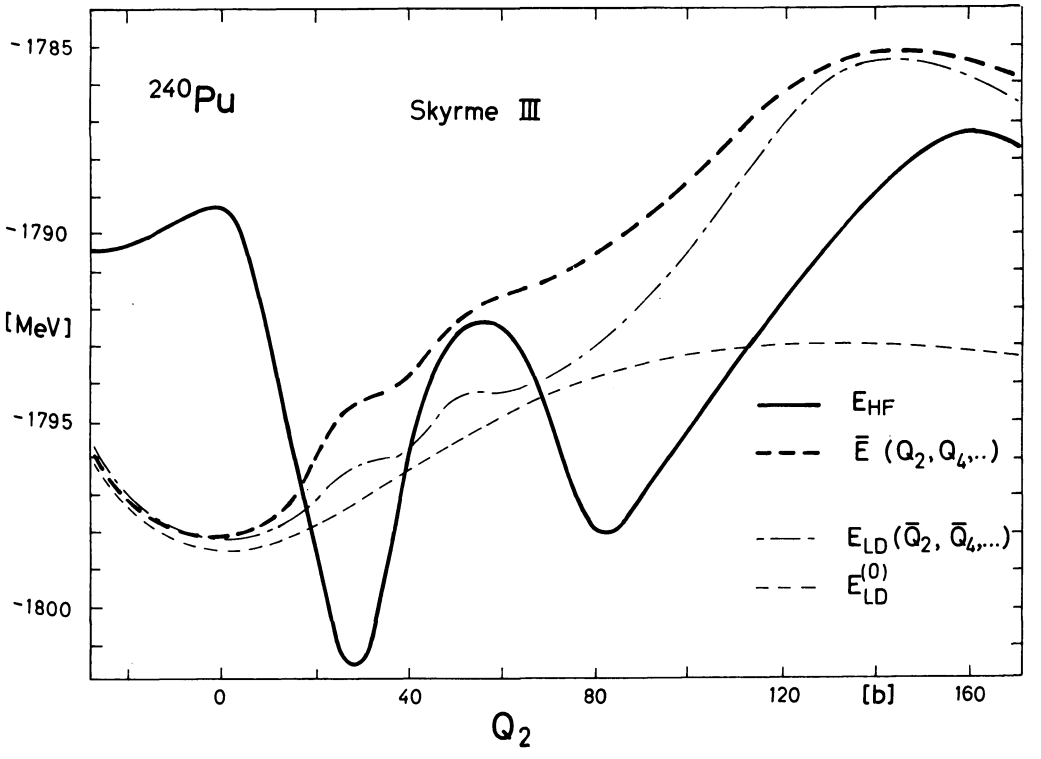

Fig. 1: Deformation energy curves of ^{240}Pu obtained with the Skyrme III interaction. Q is the mass quadrupole moment in barn. Pairing is included. Solid line: HF energy E_{HF}. Heavy dashed line: average energy $\bar{E}$. The thin lines are LDM deformation energies. The dashed-dotted curve E_{LD} is taken along the path $\bar{Q}_2$, $\bar{Q}_4$ in deformation space as $\bar{E}$. The dashed thin line $E_{LD}^{(o)}$ is taken along the LD-valley (see text), leading over the LD saddle point.

heavy dashed curve is the smooth energy $\bar{E}$ obtained in the way outlined in sect.2 (see eq.(2.14)). It exhibits none of the shell-structure of the HF curve, but is very smooth as a function of deformation with one minimum at spherical shape. The energy $\bar{E}$ thus behaves very much like a LDM energy. The small wiggles around the deformation of the ground state and the first barrier of the curve $E_{HF}(Q)$ are explained by the fact that the path in the deformation space, along

which $\bar{E}$ is obtained, does not follow the path of lowest energy in the LDM energy surface (the so-called "LD-valley"). This is demonstrated with the two thin curves in fig. 1. They are calculated with a simple liquid drop model consisting of surface and Coulomb energy only, using the Myers-Swiatecki LDM-parameters [15]. The thin dashed line $E_{LD}^{(o)}$ is the energy along the LD valley going over the "true" saddle point (limiting the shapes to β_2 and β_4 deformations only), whereas the dashed-dotted line $E_{LD}(\bar{Q}_2,\bar{Q}_4)$ is calculated along the same path $(\bar{Q}_2, \bar{Q}_4)$ along which the smooth energy $\bar{E}$ has been obtained. The wiggles and the barrier height in the latter curve are well reproduced by this LDM calculation. There is, however, a smooth discrepancy of ~1 - 2.5 MeV between the two curves around the first barrier region, which may be due to one or several of the following reasons. In comparing the curves $\bar{E}$ and E_{LD}, one should remember that the HF wavefunctions, which are Slater determinants, are not eigenstates of linear and total angular momentum. Consequently, the HF-energy contains spurious center of mass motion and rotational contributions (see also refs. [49]). The average parts of these spurious energies are also contained in the quantity $\bar{E}$, but certainly not in the experimental binding energies to which the LDM parameters are fitted. Their magnitude and deformation dependence are not easy to determine, but an estimate of ~ 2-3 MeV of the rotational energy around the ground state and isomer minima is reasonable [49] . Other effects on the HF energy curve in ^{240}Pu might come from dynamics, the unknown dependence of the pairing strength on deformation and, technically, from the truncation [49] . All these effects go also into the smooth energy $\bar{E}$ (and are not, as in the Strutinsky method, renormalized on the average!) Bearing this in mind, one may consider the curve $\bar{E}(Q)$ to be fitted reasonable well by a standard LDM calculation.

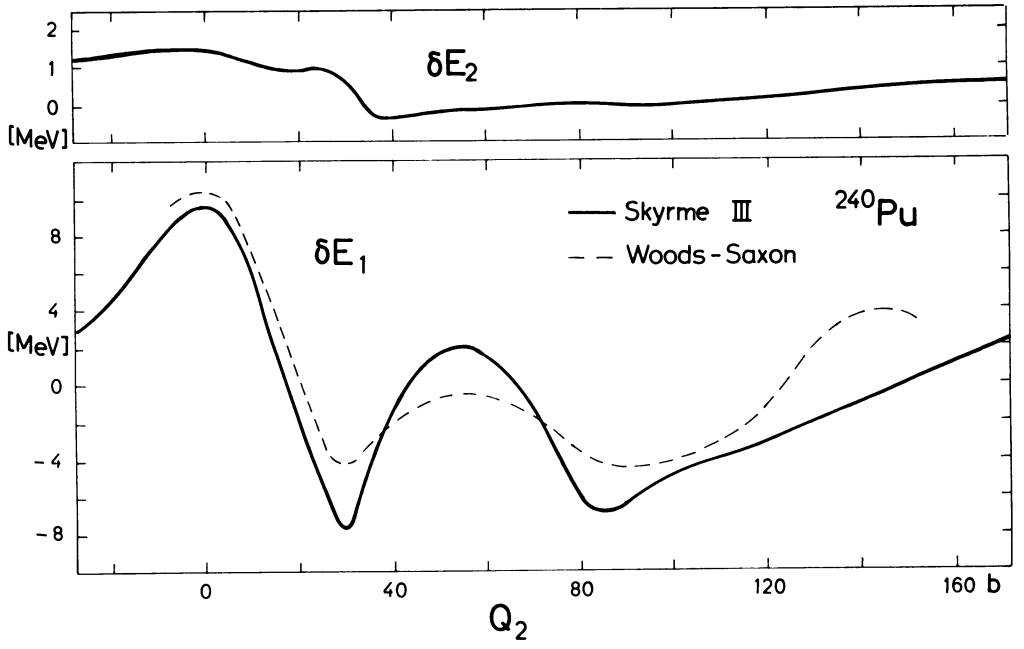

Fig. 2: First order shell-correction δE_1 and sum of higher order corrections δE_2 of ^{240}Pu (Skyrme III). (Note that the scale of δE_2 is twice as large as that of δE_1!) The thin dashed curve δE_1 is obtained from a standard Woods-Saxon potential.

Fig.2 shows the shell-corrections δE_1 and δE_2, defined by eqs. (2.13) and (4.2), for the same case. Clearly δE_1 contains all important fluctuations of more than 15 MeV, whereas δE_2 oscillates by less than $\sim \pm 1$MeV around a constant average value of ~ 0.5 MeV (Note that the scale of δE_2 is twice as large as that of δE_1!) In the lower part of fig. 2(dashed curve) is also added the shell-correction δE_1 obtained from a Woods-Saxon potential used in extended Strutinsky type calculations [3,6].

It does not agree very well with the curve δE_1 extracted from the HF calculation. This is, however, not surprising, since the Skyrme - HF results overestimate the barriers of ^{240}Pu - partially due to the various effects mentioned above - whereas the Woods-Saxon-Strutinsky calculations give the correct experimental barrier heights [3,6] . (In both calculations presented here, only axially and left-right symmetric shapes are considered).

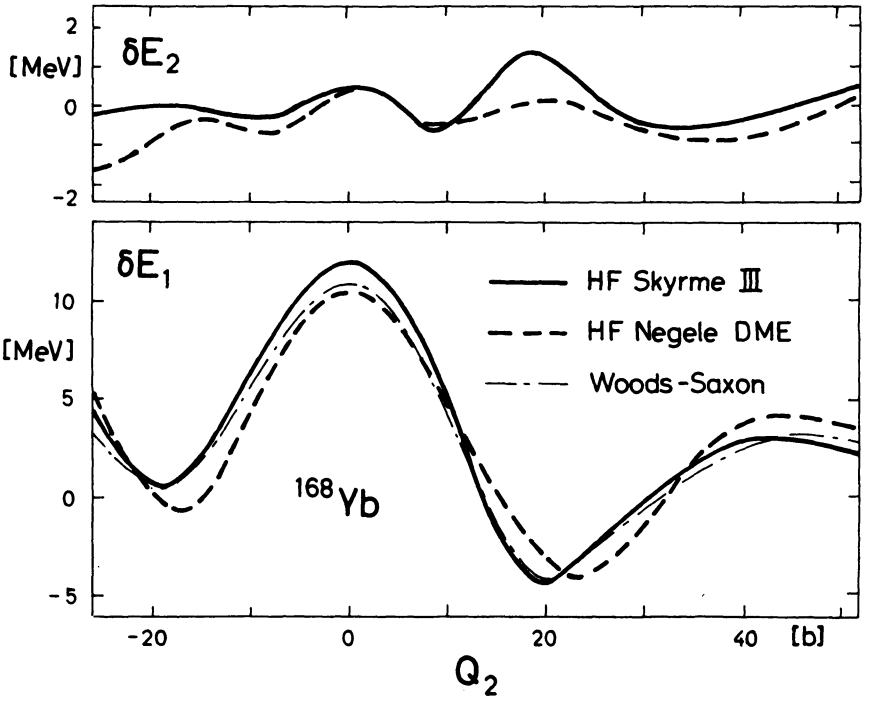

Fig. 3: The same as in fig. 2, but for ^{168}Yb and both the interactions SIII and Negele-DME. (Note the different scales for δE_1 and δE_2!) The parameters of the Woods-Saxon Strutinsky calculation [2] (dashed-dotted line) were not fitted to this special case.

Fig. 3 shows the shell-corrections δE_1 and δE_2 obtained for the nucleus ^{168}Yb both with the Negele-DME and the Skyrme SIII interaction. (See fig. 7 below for the Skyrme III curves E_{HF} and $\bar{E}$ and ref. [44] for the DME curves). Here, too, the oscillations in δE_2 are much smaller than those in δE_1, amounting in the upper case to $\pm \sim 1$ MeV. Furthermore, both quantities obtained with the two different forces agree within 1.5 MeV at all deformations. This seems to indicate the weak dependence of the shell-corrections on the detailed form of the interaction. The dashed-dotted curve E_1 obtained from a standard Woods-Saxon-Strutinsky calculation (not fitted to this special purpose!) agrees very well with those extracted from the HF results, especially with the SIII force. This excellent agreement might be accidental; it proves, however, at least that the averaged effective HF potentials $\bar{V}(\underline{r})$ may very well be fitted by a Woods-Saxon potential.

The results presented so far, which were confirmed for other nuclei and also with the force Skyrme II (see refs. [20, 46] and also fig. 6 below) allow us to draw the following conclusions.

1) The shell-correction expansion (4.2) converges rapidly for heavy and medium heavy nuclei. The sum of all higher-order shell-corrections δE_2 fluctuates not more than $\sim \pm 1$ MeV as a function of both deformation and nucleon number in nuclei with $A \gtrsim 100$.

2) The first order shell-corrections δE_1 contain therefore all important fluctuations. In particular, the locations of the stationary points of the deformation energy curves are correctly reproduced by the sum of $\bar{E}$ and δE_1.

3) The average energies $\bar{E}$ found numerically are smooth as functions of deformation and have all the expected features of LDM energies. This by itself confirms the adequateness of the Strutinsky averaging procedure in defining the smooth density matrix $\tilde{\rho}$ eq.(4.1).

4) The neglection of the higher order corrections δE_2 would affect the barrier heights in heavy nuclei by not more than ~1 MeV; it would not affect the equilibrium deformations at all.

5) The two well-known deficiencies which occurred in most shell-correction calculations, the so-called "Th-anomaly" (the inner barriers of Th-isotopes are ~2 MeV too high) and the "Pb-anomaly" (the ground-state shell-correction of ^{208}Pb is too low by ~ 2 - 5 MeV if finite depth potentials are used), can therefore <u>not</u> be explained by the neglection of higher-order shell-corrections.

6) In transition regions between spherical and deformed nuclei, where the first-order correction δE_1 is small, the higher-order terms might be decisive for finer details of the energy surface, like e.g. the prolate-oblate energy differences.

7) The constraint problem mentioned in sect. 2 has been settled in ref.[20] by doing the above numerical test both with and without including a constraint in

the averaged Hamiltonian (2.10). The changes in $\bar{E}$ and δE_1 were completely negligible and the higher order term δE_2 was changed by less than ~0.5 MeV. This proves that a shell-correction calculation without constraint is correct and closely reproduces the HF-energy also at deformations off equilibrium.

8) The obtained results for the average energies $\bar{E}$ may be used to determine the "effective liquid drop parameters" of the interaction used. Some crude fits in medium and heavy nuclei indicate that the surface energy coefficient of the force Skyrme III could be close to the 1966 Myers-Swiatecki value a_s=18.56 MeV [15]; that of the Negele-DME force (without starting energy corrections) is somewhat larger.

It is interesting to perform similar calculations for light nuclei, because one cannot a priori expect the separation of the total energy into a liquid drop and a shell-correction part to work well in light nuclei. We have done some CHF calculations for the nucleus ^{40}Ca using the Skyrme III interaction. Since the strength of the pairing interaction is not well known in this case, we have done the calculations both without and with inclusion of pairing. In the latter case two different values of the constant average gap $\tilde{\Delta}$ have been used: $\tilde{\Delta}$ = 1 MeV and $\tilde{\Delta}$ = 2 MeV, corresponding to the roughly constant pairing strengths G ≈ 0.50 MeV and G ≈ 0.63 MeV, respectively. In the

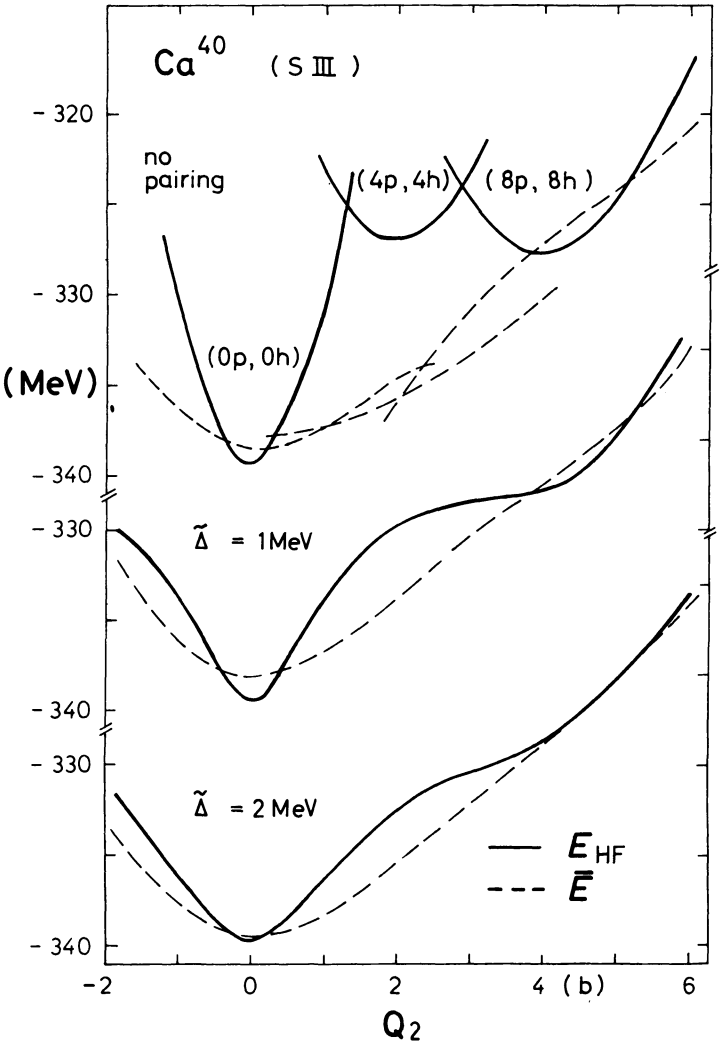

Fig. 4: Deformation energy curves of ^{40}Ca obtained with the Skyrme III interaction. HF energy and average energy $\bar{E}$ as in fig. 1. Three different pairing constants are used ($\tilde{\Delta}$=0, $\tilde{\Delta}$=1 MeV and $\tilde{\Delta}$=2 MeV). In the case without pairing, the three branches of the curves correspond to three different configurations (np,nh) with n particle-hole excitations with respect to the closed (s,d)-shell core of the ground state.

case without pairing, 3 different configurations were considered in different regions of the axially symmetric deformations, namely the closed s-d-shell as the ground state configuration (0 particles, 0 holes), the configuration with 2 neutrons and 2 protons in the $1f_{7/2}$, $K = \frac{1}{2}$ state (4p,4h) and the one with additionally 2 protons and 2 neutrons in the $1f_{7/2}$, $K = 3/2$ state (8p,8h).

Fig. 4 shows the HF energies together with the averaged energies $\bar{E}$ versus the quadrupole moment Q_2. We see that the secondary minima of the (4p,4h) and the (8p,8h) configurations are washed out already for a rather weak pairing constant ($\tilde{\Delta} < 1$MeV). The energy curves $\bar{E}(Q_2)$ behave like LDM curves also in this case. It is not surprising that the three branches in the case without pairing do not join smoothly, since the corresponding HF curves go along different paths in deformation space. The two curves $\bar{E}(Q_2)$ obtained with pairing closely agree: they differ only by the increase in the average pairing energy which is constant as a function of deformation and depends quadratically on the average gap $\tilde{\Delta}$.

Fig. 5 displays the shell-corrections δE_1 and δE_2 for the same three cases. (In contrast to figs. 2 and 3, both quantities are plotted in the same scale here!) It is immediately striking that the two quantities are of the same order. Even when the pairing is used to smooth out the cusps, δE_2 oscillates by almost the same amount as δE_1. Furthermore the oscillations of the two quantities are of opposite phases, such that the neglection of δE_2 would lead to a drastic overestimation of the shell effects (at most deformations by more than 100%).

We can conclude that the shell correction expansion (4.2) converges much slower in this case than in heavy nuclei, such that the higher order corrections may not be neglected. If

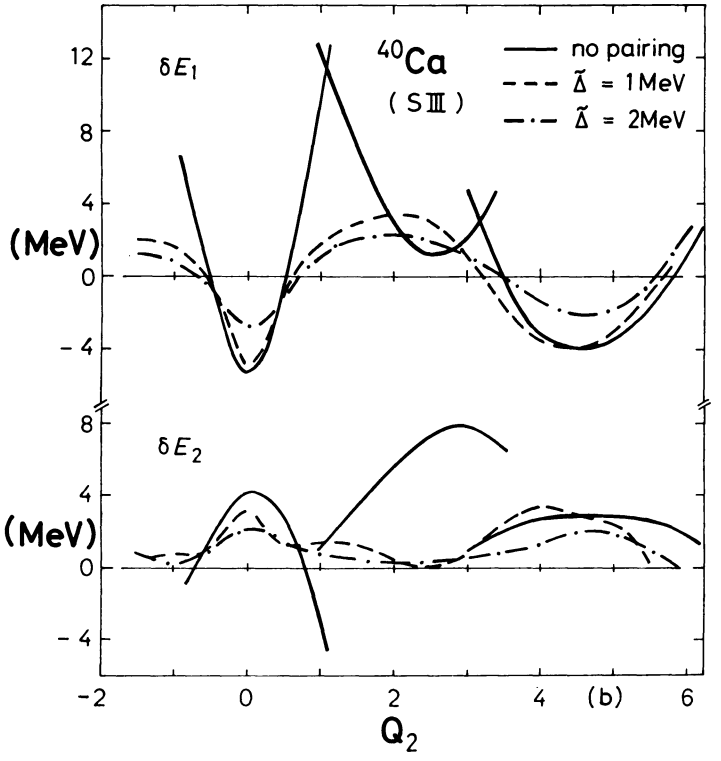

Fig. 5: First order δE_1 and sum of higher order shell-corrections δE_2 obtained for ^{40}Ca with the 3 different pairing strengths (Skyrme III interaction). Note the opposite phases of the oscillations in δE_1 and δE_2.

the shell model (e.g.Nilsson model) energies are to be identified with the $\hat{\varepsilon}_i$, this should give a warning to the blind application of the shell-correction method to the region of light nuclei (see e.g. ref. [50]):

4.2. Taylor series expansion

At the end of section 2, we have indicated the possibility of making a Taylor expansion of the HF energy functional $E_{HF}(\varrho)$ around the averaged value $\bar{\varrho}$ of the density matrix. This leads to an alternative form of the shell-correction expansion for E_{HF}, which we rewrite here for convenience:

$$E_{HF}(\varrho) = E(\bar{\varrho}) + \delta E_1^{HF} - \lambda \delta Q - \tfrac{1}{2} \mathrm{trtr}\, \delta\varrho\, v\, \delta\varrho . \quad (4.3)$$

In this equation which is exact for a density independent two body force v, δE_1^{HF} is the first order shell-correction defined in the usual way but in terms of the constrained HF single particle energies ε_i (see eq.(2.20)) and δQ is the shell-correction to the quadrupole moment:

$$\delta Q = Q - \bar{Q} = \mathrm{tr}\hat{q}\delta\varrho . \quad (4.4)$$

Although the term $\lambda\delta Q$ in eq.(4.3) is formally of first order in $\delta\varrho$, one can expect it to be rather small. From calculations with shell model potentials, one knows that δQ is of the order of ~1 - 2 barns (see ref. [3]). On the other hand, the Lagrange parameter λ , which is equal to the negative slope $-dE_{HF}/dQ$ of the HF curve $E_{HF}(Q)$, is not larger in magnitude than ~1 MeV per barn in medium and heavy nuclei, so that $\lambda\delta Q$ is of the order of $\pm$ ~1 - 2 MeV.

We have checked numerically the different terms in eq.(4.3) It turned out that $E(\bar{\rho})$ is close to the quantity $\bar{E}$ above, the difference being not larger than 0.5 - 1 MeV. This is illustrated in Fig. 6 for the nucleus ^{150}Ce, calculated with the force Skyrme II. The solid and dashed lines show E_{HF} and $\bar{E}$ versus the (mass) quadrupole moment Q_2, as in the figures above.

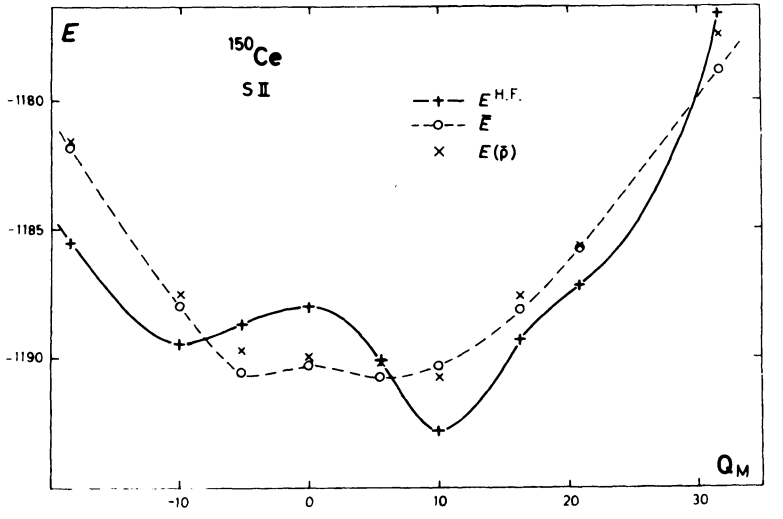

Fig. 6: The same as in fig. 1, but for ^{150}Ce and the Skyrme III force (no LD calculation shown). The crosses show the results for the average energy $E(\bar{\rho})$.

The crosses indicate the values of $E(\bar{\rho})$. The smooth bump in the curve $\bar{E}(Q)$ around the spherical point may be partially due to the anomalous behaviour of the Coulomb energy, which is connected with a slight breathing of the HF solution at these small deformations (see ref. [46]).

Numerically, the quantity $E(\tilde{\rho})$ turned out to be much more sensitive than $\bar{E}$ to the optimization of the basis parameters, the convergence of the HF result and the uncertainties discussed in sect. 3 in solving the stationary equation (3.8) which determines the smoothing width γ_c. Similar results for $E(\tilde{\rho})$ as shown in fig. 6 were also obtained in all the other nuclei considered.

In calculating the shell-correction δE_1^{HF} from the HF spectrum ε_i, we found in all cases that it agrees within less than ~ 0.5 MeV with the sum of the quantities $\delta E_1 + \delta E_2$ discussed above. (Remember that δE_1 is defined in terms of the eigenvalues $\hat{\varepsilon}_i$ of the averaged single particle Hamiltonian). The expansion (4.3) converges more rapidly than the standard shell-correction expansion, eq. (2.12), although it is numerically less stable.

This result is not of much practical use, since one needs the HF results to calculate δE_1^{HF}. But it illustrates the fact that by a suitable definition of the average energy and the first-order shell-correction the sum of the remaining corrections may be minimized. A more interesting way to achieve this is discussed in the next section.

4.3. Selfconsistent averaging

Another way of obtaining the smooth part of the total energy, which might have some practical consequences, is to perform the averaging of the density matrix in a selfconsistent way. The possibility of introducing a selfconsistent average energy has indeed been discussed theoretically by Tyapin [51] in connection with the Strutinsky energy theorem, but no numerical calculations were done. We present here some new results along these lines.

The (curvature-corrected) average occupation numbers $\bar{n}_i$ (3.6) can, in fact, be included in the iterative solution of the HF variational equation, as was discussed in a general way by Vautherin [47] in connection with the pairing treatment. This leads to a selfconsistent average energy $\tilde{E}$:

$$\tilde{E}(\tilde{\rho}) = \mathrm{tr}\, T\tilde{\rho} + \frac{1}{2}\mathrm{tr}\,\mathrm{tr}\,\tilde{\rho}v\tilde{\rho}. \tag{4.5}$$

The selfconsistent average potential $\tilde{V}$ is defined by

$$\tilde{V} = \mathrm{tr}\,\tilde{\rho}v, \tag{4.6}$$

and the variational equation has the form

$$[T + \tilde{V} + \tilde{\lambda}\hat{q}]\tilde{\psi}_i = \tilde{\varepsilon}_i\,\tilde{\psi}_i \tag{4.7}$$

with the condition

$$\mathrm{tr}\,\hat{q}\tilde{\rho} = \tilde{Q}_2 \tag{4.8}$$

for the constraint. (We have here, again, for simplicity written the formulae for a density independent force. Eqs.(4.5,6) can, however, immediately be reformulated for the Skyrme and Negele - DME forces.) The density matrix $\tilde{\rho}$ is defined exactly in the same way as $\bar{\rho}$ in eq.(4.1), but in the following we shall use the tilde "~" for the selfconsistently averaged quantities. The constraint in eq.(4.7) has to be used to fix the quadrupole moment $\tilde{Q}_2$(4.8). If it were missing, the solutions of eqs.(4.5)-(4.7) would always have spherical symmetry, since the energy $\tilde{E}$ (4.5) has the properties of a LDM energy.

In Fig. 7, the HF energy E_{HF} (thin solid line) and the average energy $\tilde{E}$ (thick solid line) are plotted against the

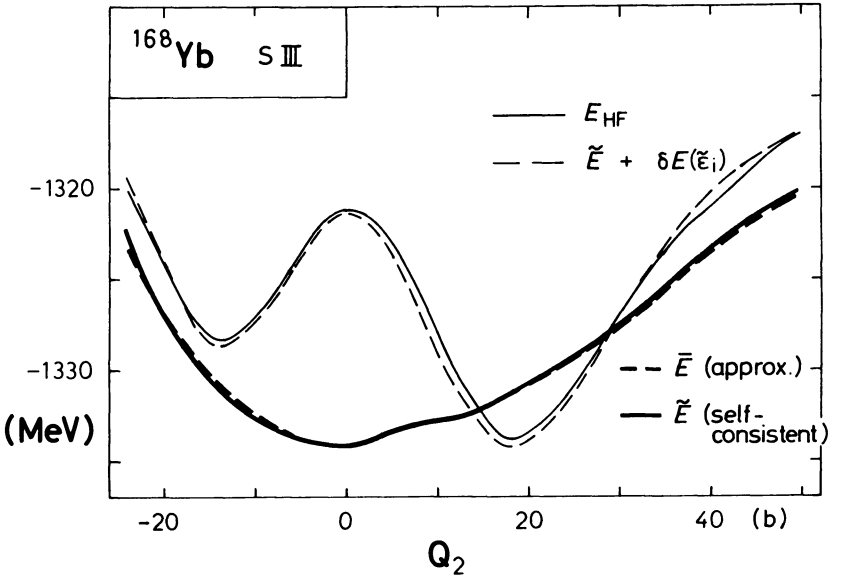

Fig. 7: Deformation energy curves for ^{168}Yb obtained with the Skyrme III force. The thin solid line is the HF energy and the heavy dashed line the average energy $\bar{E}$ as in figs. 1,2,4 and 6. The heavy solid line is the selfconsistent average energy $\tilde{E}$ and the thin dashed line is the approximation (4.10) to the HF energy.

quadrupole moment $Q_2 = \tilde{Q}_2$ for the nucleus ^{168}Yb (Skyrme III force). The energy $\bar{E}$, obtained as in the other calculations presented above, is shown by the heavy dashed line. It is striking that the two smooth curves agree with each other within less than 0.5 MeV over the whole range of deformations. This shows that the a priori not selfconsistent density matrix $\bar{\varrho}$, extracted from the HF solution, in fact is very close to the selfconsistent density matrix $\tilde{\varrho}$.

The thin dashed line in fig. 7 shows the sum of the smooth energy $\tilde{E}$ and the first order shell-correction $\delta E_1(\tilde{\varepsilon}_i)$ which is defined in terms of the solutions of eq.(4.7):

$$\delta E_1(\tilde{\varepsilon}_i) = \sum_{i=1}^{N} \tilde{\varepsilon}_i - \sum_i \tilde{\varepsilon}_i \tilde{n}_i . \tag{4.9}$$

The sum $\tilde{E} + \delta E_1(\tilde{\varepsilon}_i)$ agrees surprisingly well with the HF energy E_{HF}; the deviation is less than 500 keV at all deformations. The energy differences between the stationary points are even better reproduced (within $\sim$ 300 keV) by this approximation. Similar results are also obtained for ^{40}Ca, which is remarkable in view of the size of δE_2 found in Fig. 5 with the non-selfconsistent average density $\bar{\varrho}$.

With the same arguments as used in deriving the energy theorem in sect. 2, one can show that the sum of $\tilde{E}$ and $\delta E_1(\tilde{\varepsilon}_i)$ is equal to the exact energy E_{HF} up to second order terms in the difference $\varrho - \tilde{\varrho}$. The fact that these terms add up to less than $\sim$ 0.5 MeV is so far not clearly understood and the excellent quality of the approximation

$$E_{HF} \approx \tilde{E} + \delta E_1(\tilde{\varepsilon}_i) \tag{4.10}$$

has to be taken as a numerical result. More detailed discussions and further results will be presented in a forthcoming publication [48].

Let us summarize these results and draw some conclusions.

1) The average density matrix $\bar{\varrho}$ obtained by the non selfconsistent averaging of the HF density matrix is found numerically to be very nearly selfconsistent.

2) The shell-correction expansion of the HF energy converges better when the averaging is done selfconsistently. The exact HF energy is perfectly well repro-

duced by the sum of its first two terms, see eq.(4.10), the error being less than ~ 0.5 MeV even in the relatively light nucleus ^{40}Ca.

3) A practical application of eq.(4.10) might consist in calculating iteratively the selfconsistent average energy $\tilde{E}$ eq.(4.5) in a semiclassical model, such as the extended Thomas-Fermi model discussed in sect. 3. If this can be done with a sufficient numerical accuracy, a standard Strutinsky calculation added at the end would give an excellent approximation to the exact HF energy. Such a procedure - if technically realizable - would provide a fast and economical way to go around the very time consuming constrained HF calculations. Investigations along these lines are in progress.

4.4 Results of other related calculations

Bassichis et al. [10,19] performed first-order HF calculations with the Tabakin potential [52] which, in contrast to the effective interactions of Negele and Skyrme, is a realistic free nucleon-nucleon potential. In ref. [10] a program for testing the Strutinsky method was outlined, which is essentially based on the energy theorem (2.12) and differs from the one used in sect. 4.1 only in the explicit form of some second order terms. We shall not comment here on the conclusions drawn from a not selfconsistent test [53], where Nilsson levels and LDM parameters were fitted to some HF results.

In a more recent paper, Bassichis et al. [54] presented results of the selfconsistent test outlined in ref. [10], using a HF deformation energy curve obtained for ^{108}Ru with the Tabakin potential. The averaging of the density matrix ϱ was, however,

performed using BCS occupation numbers with a very large gap ($\Delta \sim 5$ - 12 MeV). Such a smoothing without curvature-corrections introduces some excitation in $\tilde{\varrho}$ and the average energies derived from it, as discussed in sect. 3, and is obviously not consistent with the averaging used in extracting the shell-correction δE_1 from the spectrum $\hat{\varepsilon}_1$. Consequently, all results strongly depend on the value of the smoothing gap Δ , which is clearly seen in fig. 2 of ref. [54] . Apart from this smooth dependence, the sum of all higher order corrections obtained there oscillates by $\sim\pm$ 1 MeV. Taking further into account that no pairing correlations were included in the HF calculation of ref. [54], these results are consistent with the ones presented in sect. 4.1. Unfortunately, no plot of the average energy $\bar{E}(Q)$ was shown in ref. [54] and the constraint problem (see sect.2) was not considered.

Prior to all these HF tests, Bunatian et al. [4] calculated the second order shell-corrections δE_2 in a way which does not require any HF results. This is in fact possible, as shown in ref. [4]. Extending the perturbation treatment which leads to the energy theorem (2.12) to second order, the quantity δE_2 (which here, in contrast to sect. 4.1, does not contain terms of third or higher order in $\delta\varrho$) can be expressed in terms of the shell model density $\hat{\varrho}$ and the scattering amplitude. Bunatian et al. [4] applied this to the Fermi liquid theory of Migdal [55] and calculated δE_2 using Migdal's quasiparticle amplitude and spherical Woods-Saxon shell model densities for a series of nuclei around ^{208}Pb. The results for δE_2 vary from ~0.3 MeV to ~ 3.4 MeV for the nuclei considered ($76 \leq Z \leq 88$ and $120 \leq N \leq 132$). Except for those nuclei far away from ^{208}Pb for which a spherical shape might not be appropriate, the fluctuations in δE_2 do not exceed ~1 MeV. This result is consistent with what was found in the HF calculations described above, although obtained from a rather different point of view.

5. Conclusions

We have seen that in three independent sets of calculations the second and higher order shell-corrections are found to contribute not more than ~1 MeV to the fluctuations in the total energy of medium and heavy nuclei. This has to be compared with the typical values of ± ~10 MeV of the first order shell-corrections on one hand, and with the uncertainties in extracting those from a given single particle spectrum on the other hand. These uncertainties were discussed in sect. 3 and are of the order of 0.5 - 1.5 MeV in finite depth potentials. We can thus conclude that the higher order shell-correction terms do not play an important role in most cases.

Different definitions of the average part of the HF energy lead for ^{40}Ca to different results for the higher order terms. A definite conclusion would therefore be premature for this nucleus.

The liquid drop like behaviour of the average energies exhibited in extensive results of sect. 4 and the smallness of the higher order corrections show that the Strutinsky method works well in medium and heavy nuclei and reproduces deformation energies obtained from HF calculations within ~1-2 MeV. When the average energy and the average potential are calculated self-consistently, the higher order terms are found to be completely negligible even in the nucleus ^{40}Ca. It will be a task for the future to construct liquid drop models and shell model potentials which fit as closely as possible the"ideal" ones extracted from HF results.

The comparison of the results obtained with different effective interactions seems to suggest that the shell effects are less sensitive to the details of the interaction but are determin-

ed by the shape of the average potential, whereas the interaction is important for the average energy, i.e. for the LDM parameters. This has, however, to be confirmed by similar calculations with finite range forces.

The results discussed in this talk might also have some practical applications in the search of approximative ways to calculate static deformation energy surfaces for a given effective interaction without going through the heavy and time consuming constrained HF calculations. One such way is to extract the optimal shell model and LDM parameters from HF calculations for some selected nuclei and deformations and to use those in normal Strutinsky calculations for extrapolations to other regions. Another way, strongly suggested by the numerical results presented in sect. 4.3 and already discussed there, would be to solve the selfconsistent problem for the average energy in some semiclassical approach and to add a Strutinsky calculation at the end of it. Another related approach has recently been proposed by Ko et al. [56] , in which the shell model wavefunctions obtained in standard Strutinsky calculations are used to calculate the expectation value of the many body (Skyrme) Hamiltonian. Especially for light nuclei, this method gives results rather close to those obtained in HF calculations.

The overall uncertainty of ~1-2 MeV in the usual shell-correction results, which may be concluded from these HF tests, is consistent with the fact that most experimental fission barriers and ground state mass corrections are reproduced within ~1-2 MeV in different Strutinsky calculations using various shell model potentials and rather different shape parametrizations.

We should finally like to mention that the Strutinsky method has also served as a basis in statistical calculations of excitation energies, entropies and level density parameters (see e.g.ref. [57]

and references quoted therein). The quiet assumption in such calculations is that the shell model and liquid drop parameters do not significantly depend on the nuclear temperature.

This has been investigated recently in some constrained HF calculations with inclusion of finite temperatures [58]. It was found that, indeed, the dependence of the selfconsistent field on the temperature is very weak and that the use of the level spectra obtained at zero temperature in calculating the entropy as function of excitation energy leads to an excellent approximation of the selfconsistent quantities. This result is in close relation to the one presented above in sect. 4.3, where the Strutinsky averaging was included selfconsistently. The connection between these two subjects is being further investigated [48].

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