# TEST OF STRUTINSKY'S METHOD USING HARTREE-FOCK RESULTS*

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## Abstract

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New results of Hartree-Fock (HF) calculations are used to estimate the validity of Strutinsky's shell-correction method in a way which is independent of the shell and liquid-drop models usually involved. Strutinsky writes the total binding energy E of a nucleus as sum of a classical liquid-drop (LD)-model energy $E_{LD}$ and a shell correction energy $\delta E$, which is extracted from a sum of shell model energies $\epsilon_i$. Here the HF energy is decomposed into three terms: $E_{HF} = \overline{E} + \delta E_1 + \delta E_2$, where $\overline{E}$ is an average binding energy, $\delta E_1$ is a first order shell correction and $\delta E_2$ contains all higher order corrections, which usually are neglected in the Strutinsky method. By explicitly calculating $E_{HF}$, $\overline{E}$, and $\delta E_1$, these higher order corrections are evaluated and the reliability of the shell-correction method from the HF point of view is estimated. The HF results were obtained using the effective $\delta$-interaction of Skyrme in a new parametrization (SIII) which was recently demonstrated to give excellent fits to experimental ground-state energies, deformations and radii throughout the periodic table. A quadratic constraint of the quadrupole moment Q was used to obtain deformation energy curves. Pairing effects were included. Having calculated the self-consistent density matrix $\rho$, its average part $\overline{\rho}$ is determined by the usual energy averaging procedure. The HF energy can then be decomposed into the three terms stated above, of which $\overline{E}$ is solely dependent on smooth quantities like $\overline{\rho}$, $\delta E_1$ contains the first-order and $\delta E_2$ all higher order terms in $\delta\rho = \rho - \overline{\rho}$. As a result of these computations, it is found that the quantity $\overline{E}$ indeed behaves exactly like a LD model energy as a function of deformation. This, in itself, strongly confirms Strutinsky's renormalization method. The corrections $\delta E_2$ are found to have values of ~0.5 to ~3.0 MeV for nuclei with $A \geq 100$. Since only their oscillations contribute to the shell corrections, a reliability of the Strutinsky-calculated shell corrections to ground-state energies of ~1-2 MeV is concluded for medium and heavy nuclei. Similarly, the Strutinsky-calculated fission barriers are found to be affected by less than ~1 MeV. Fission lifetime estimates are expected to be lowered by inclusion of the second order correction.

## INTRODUCTION

The present paper is devoted to an analysis of the shell-correction method introduced by Strutinsky [1,2], in terms of Hartree-Fock (HF) theory. Ever since the shell-correction method was used in calculations of nuclear deformation energies, the question has been asked to what extent this method is consistent with entirely microscopic descriptions of the nucleus using realistic effective nuclear interactions. Strutinsky pointed out [2] that the shell-correction expression for the total nuclear binding energy $E = E_{LD} + \delta E$

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can be obtained from a HF solution by defining an average part $\bar{\varrho}$ of the self-consistent density matrix $\varrho$ and expanding the HF energy around $\bar{\varrho}$. In this way, one finds

$$E_{HF} = \bar{E} + \delta E_1 + \delta E_2 + \dots , \tag{1}$$

where $\bar{E}$ depends only on smooth quantities like $\bar{\varrho}$, and the corrections $\delta E_1$, $\delta E_2$, etc. are of increasing order in the difference $\delta\varrho = \varrho - \bar{\varrho}$:

$$\delta E_n \propto O[(\delta\varrho)^n] . \tag{2}$$

The fluctuations $\delta\varrho$ of the density matrix are expected to be relatively small [3] and the shell-correction expansion (1) should therefore converge rapidly.

So far, in all practical applications of the method, the second and higher order terms have been neglected. Usually, the smooth part $\bar{E}$ is replaced by a liquid-drop (LD) energy $E_{LD}$, and the first order shell correction $\delta E_1$ (often also written as $\delta U$) is extracted from the eigenenergies $\varepsilon_i$ of an average shell model potential [2-5]. An explicit expression for the second order shell correction $\delta E_2$ has been given in terms of shell model quantities only [3,5]. Bunatyan et al. [5] calculated $\delta E_2$ using Migdal's theory for a series of nuclei in the lead region and found $\delta E_2$ to be of the order of 0.5 to 3 MeV. Compared to the first order shell correction $\delta E_1$ which varies in that region from +5 to -13 MeV, these numbers are indeed quite small. Knowing that the shell effects are largest in spherical nuclei and extrapolating the quoted results to deformed nuclei, one would not expect the higher order terms to affect the usually calculated fission barriers by more than $\pm$0.5 to 1 MeV.

No consistent test of the shell-correction expansion (1) has so far been performed using HF results only. Bassichis et al.[6] proposed a method which differs slightly from the one outlined by Strutinsky and which will be discussed in this paper; but no results have been published yet. The same authors [7] recently compared HF results to a shell-correction calculation in which the parameters of a Nilsson potential and the liquid-drop model were fitted to give the least deviations from the HF results. However, they did not include the pairing interaction which is known to smooth out the shell effects in deformed nuclei. Furthermore, their test is dependent on the choice of a LD and a shell model, and therefore their conclusions, quoting a 30% unreliability of the first-order shell correction, cannot be considered to be very significant.

Within the last few years, the effective $\delta$-interaction of Skyrme [8] has been successfully applied in HF calculations of both spherical [9] and deformed nuclei [10-14]. Encouraged by their success, we have used these results to perform the decomposition of the HF energy into the shell-correction

series (1). By explicitly calculating its first two terms $\bar{E}$ and $\delta E_1$, we can determine the sum of all higher order terms and check the convergence of the series (1) numerically. In addition, we can see whether the smooth part $\bar{E}$ really behaves like a LD model quantity. This test is thus entirely independent of any LD or shell model parameters; on the other hand, it only tests the Strutinsky method within the HF framework. The only quantity which has to be defined ad hoc and exceeds the HF theory is the smooth part $\bar{\varrho}$ of the density matrix. We define it here consistently by applying Strutinsky's energy-averaging method [1-5].

In the first part of this paper we will present the detailed formalism of our calculations and in the second part present some numerical results and discuss their consequences.

## THE METHOD

We first repeat here the main equations of the constraint Hartree-Fock (CHF) method using Skyrme's effective interaction, as described in detail in earlier publications [9-11].

The total binding energy of a nucleus with neutron and proton numbers N,Z and the total (mass-) quadrupole moment Q is found by minimizing the following functional:

$$\delta\left\{\langle T+V_{Sky}\rangle + f(\mu,\langle Q\rangle) + E_{pair}(\lambda_q, n_i^q)\right\} = 0, \qquad (3)$$

In eq.(3), $V_{Sky}$ is the Skyrme interaction including spin-orbit term and Coulomb interaction [9,10]; $f(\mu,\langle Q\rangle)$ is a constraint of the quadrupole moment [11] and $E_{pair}(\lambda_q, n_i^q)$ is a pairing energy functional [10] depending on the single-particle occupation numbers $n_i^q$. The index q labels the isospin state of the nucleons, i.e. neutrons or protons. The Lagrange parameters $\mu$ and $\lambda_q$ in (3) are used for the constraints

$$\langle Q\rangle = Q, \qquad (4)$$

$$\sum_i n_i^p = Z, \quad \sum_i n_i^n = N \qquad (5)$$

The expectation values are taken between Slater determinants of orthonormalized single-particle wavefunctions $\Phi_i^q(\underline{r})$ which are expanded in a deformed harmonic oscillator basis $\{\varphi_\alpha(\underline{r})\}$:

$$\Phi_i^q(\underline{r}) = \sum_{\alpha=1}^{\infty} C_\alpha^{qi}\varphi_\alpha(\underline{r}) \qquad (q = n, p) \qquad (6)$$

The expansion coefficients $c_\alpha^{qi}$ and the occupation numbers $n_i^q$ define the density matrices $\rho_{\alpha\beta}^q$:

$$\rho_{\alpha\beta}^q = \sum_i n_i^q (c_\alpha^{qi})^* c_\beta^{qi}, \qquad (q = n, p)$$
$$\rho_{\alpha\beta} = \rho_{\alpha\beta}^n + \rho_{\alpha\beta}^p. \tag{7}$$

One of the advantages of the Skyrme interaction is that the expectation value of the total Hamiltonian $H = T + V_{Sky}$ for an even-even nucleus can be written as integral over an energy density $\mathcal{E}(\underline{r})$ [9]:

$$\langle H \rangle = \int d^3\underline{r}\, \mathcal{E}(\underline{r}). \tag{8}$$

Here $\mathcal{E}(\underline{r})$ is a relatively simple algebraic function of the spatial densities $\rho_q(\underline{r})$, the kinetic energy densities $\tau_q(\underline{r})$ and the spin-orbit densities $\underline{J}_q(\underline{r})$ defined by

$$\rho_q(\underline{r}) = \sum_i n_i^q |\Phi_i^q(\underline{r})|^2 = \sum_{\alpha,\beta} \rho_{\alpha\beta}^q \varphi_\alpha^*(\underline{r}) \varphi_\beta(\underline{r}),$$
$$\tau_q(\underline{r}) = \sum_i n_i^q |\underline{\nabla} \Phi_i^q(\underline{r})|^2 = \sum_{\alpha,\beta} \rho_{\alpha\beta}^q \underline{\nabla}\varphi_\alpha^*(\underline{r}) \cdot \underline{\nabla}\varphi_\beta(\underline{r}), \tag{9}$$
$$\underline{J}_q(\underline{r}) = (-i)\sum_i n_i^q \Phi_i^q(\underline{r})^* (\underline{\nabla}\times\underline{\sigma}) \Phi_i^q(\underline{r}) = (-i) \sum_{\alpha,\beta} \rho_{\alpha\beta}^q \varphi_\alpha^*(\underline{r}) (\underline{\nabla}\times\underline{\sigma}) \varphi_\beta(\underline{r}),$$

and

$$\rho(\underline{r}) = \rho_n(\underline{r}) + \rho_p(\underline{r}), \quad \tau(\underline{r}) = \tau_n(\underline{r}) + \tau_p(\underline{r}), \quad \underline{J}(\underline{r}) = \underline{J}_n(\underline{r}) + \underline{J}_p(\underline{r}).$$

The explicit expression for $\mathcal{E}(\underline{r})$ is [9,10]

$$\begin{aligned}
\mathcal{E}(\underline{r}) = {} & \frac{\hbar^2}{2m}\tau(\underline{r}) + t_3 \cdot \frac{1}{4} \rho_n(\underline{r}) \rho_p(\underline{r}) \rho(\underline{r}) \\
& + \tfrac{1}{2} t_0 \left[ (1 + \tfrac{1}{2} x_0) \rho^2(\underline{r}) - (x_0 + \tfrac{1}{2}) (\rho_n^2(\underline{r}) + \rho_p^2(\underline{r})) \right] \\
& + \tfrac{1}{4}(t_1 + t_2) \rho(\underline{r}) \tau(\underline{r}) + \tfrac{1}{8}(t_2 - t_1)(\rho_n \tau_n + \rho_p \tau_p) \\
& + \tfrac{1}{16}(t_2 - 3t_1) \rho(\underline{r}) \nabla^2 \rho(\underline{r}) + \tfrac{1}{32}(3t_1 + t_2)(\rho_n \nabla^2 \rho_n + \rho_p \nabla^2 \rho_p) \\
& - \tfrac{1}{2} W_0 (\rho(\underline{r}) \underline{\nabla} \cdot \underline{J}(\underline{r}) + \rho_n \underline{\nabla} \cdot \underline{J}_n + \rho_p \underline{\nabla} \cdot \underline{J}_p) \\
& + V_{CD}(\underline{r}) \rho_p(\underline{r}) + \tfrac{3}{4} V_{CE}(\underline{r}) \rho_p(\underline{r}),
\end{aligned} \tag{10}$$

with the Skyrme parameters $t_0$, $t_1$, $t_2$, $t_3$, $x_0$ and $W_0$. $V_{CD}(\underline{r})$ and $V_{CE}(\underline{r})$ are the direct and the exchange part of the Coulomb potential; the former is given by

$$V_{CD}(\underline{r}) = \int d^3\underline{r}'\, \rho_p(\underline{r}')\, \frac{e^2}{|\underline{r} - \underline{r}'|} \tag{11a}$$

and the latter by

$$V_{CE}(\underline{r}) = -\left(\frac{3}{\pi}\right)^{1/3} e^2\, \rho_p^{1/3}(\underline{r}), \tag{11b}$$

where the Slater approximation has been used [15].

The quadrupole moment Q of the nucleus can be written in terms of the densities $\rho_q(\underline{r})$ and the quadrupole operator $\hat{q}_{op}$ as

$$\begin{aligned} Q &= \langle Q_p \rangle + \langle Q_n \rangle , \\ \langle Q_q \rangle &= \int d^3\underline{r}\; \hat{q}_{op}\, \rho_q(\underline{r}) . \end{aligned} \tag{12}$$

A variation of the wavefunctions $\Phi_i^q(\underline{r})$ in (3) leads to the following Schrödinger equation which defines the single-particle energies $\varepsilon_i^q$:

$$\begin{aligned} &\left[-\underline{\nabla}\, \frac{\hbar^2}{m_q^*(\underline{r})} \cdot \underline{\nabla} + U_q(\underline{r}) + \underline{W}_q(\underline{r}) \cdot (-i)(\underline{\nabla} \times \underline{\sigma}) + \hat{q}_{op} \left.\frac{\partial f(\mu,\nu)}{\partial \nu}\right|_{\nu=0}\right] \Phi_i^q(\underline{r}) \\ &\quad = H_q\, \Phi_i^q(\underline{r}) = \varepsilon_i^q\, \Phi_i^q(\underline{r}) . \end{aligned} \tag{13}$$

The effective masses $m_q^*(\underline{r})$, the local HF potentials $U_q(\underline{r})$ and the spin-orbit form factors $\underline{W}_q(\underline{r})$ are given by

$$\frac{\hbar^2}{2m_q^*(\underline{r})} = \frac{\hbar^2}{2m} + \tfrac{1}{4}(t_1 + t_2)\rho(\underline{r}) + \tfrac{1}{8}(t_2 - t_1)\rho_q(\underline{r}) , \tag{14}$$

$$\begin{aligned} U_q(\underline{r}) = {} & t_0\left[(1 + x_0\tfrac{1}{2})\rho(\underline{r}) - (x_0 + \tfrac{1}{2})\rho_q(\underline{r})\right] + \tfrac{1}{4} t_3 (\rho^2 - \rho_q^2) \\ & + \tfrac{1}{4}(t_1 + t_2)\tau(\underline{r}) + \tfrac{1}{8}(t_2 - t_1)\tau_q(\underline{r}) \\ & + \tfrac{1}{8}(t_2 - 3t_1)\nabla^2\rho(\underline{r}) + \tfrac{1}{16}(3t_1 + t_2)\nabla^2\rho_q(\underline{r}) \\ & + \delta_{q,p}\left(V_{CD}(\underline{r}) + V_{CE}(\underline{r})\right) - \tfrac{1}{2} W_0\left(\underline{\nabla} \cdot \underline{J}(\underline{r}) + \underline{\nabla} \cdot \underline{J}_q(\underline{r})\right) , \end{aligned} \tag{15}$$

$$\underline{W}_q(\underline{r}) = \tfrac{1}{2} W_0\left(\underline{\nabla}\rho(\underline{r}) + \underline{\nabla}\rho_q(\underline{r})\right). \tag{16}$$

Variation of the occupation numbers $n_i^q$ in (3) under the constraints (5) leads to a set of "generalized BCS equations" whose explicit form depends on the pairing functional chosen [10]. For the functional

$$E_{pair} = -\sum_q G_q \left\{ \sum_i \sqrt{n_i^q (1-n_i^q)} \right\}^2 \tag{17}$$

with constant pairing strengths $G_n$ and $G_p$, one obtains the familiar BCS equations [16]

$$\frac{2}{G_q} = \sum_i \frac{1}{\sqrt{(\varepsilon_i^q - \lambda_q)^2 + \Delta_q^2}} , \tag{18}$$

$$n_i^q = \frac{1}{2}\left[ 1 - \frac{\varepsilon_i^q - \lambda_q}{\sqrt{(\varepsilon_i^q - \lambda_q)^2 + \Delta_q^2}} \right] \tag{19}$$

Vautherin [10] and Flocard et al. [11-14] chose in some calculations a different pairing functional

$$E'_{pair} = -2 \sum_q \Delta_q \left( \sum_i \sqrt{n_i^q (1-n_i^q)} \right) , \tag{20}$$

in which the gaps $\Delta_q$ are kept constant and the $n_i^q$ are again given by eq.(19).

As discussed in ref. [11], a quadratic constraint

$$f(\mu, \langle Q \rangle) = \frac{1}{2} c \left( \mu - \langle Q \rangle \right)^2 \tag{21}$$

is suitable to describe the deformation energy curve $E_{HF}(Q)$ in a monotonic way with the Lagrange parameter $\mu$. In eq.(21), c is a constant which can be chosen once and for all in a certain region of nuclei [11].

Once a selfconsistent solution of the HF equations (13) is found, the total binding energy of the nucleus under consideration is given by (8) and (10):

$$E_{HF} = E_{kin} + E_{pot} + E_{pair} , \tag{22}$$

where the kinetic energy $E_{kin}$ is the integral over the first term in eq.(10) and the potential energy $E_{pot}$ is the integral over the sum of all other terms in (10). The HF energy can also be expressed in terms of the single-particle energies $\varepsilon_i^q$, by means of eq.(13):

$$E_{HF} = \sum_{q,i} \varepsilon_i^q n_i^q - E_{pot} + E_R - E_{const} + E_{pair} . \tag{23}$$

In eq.(23) $E_R$ is a rearrangement energy term coming from the density-dependent part of the Skyrme interaction and the Coulomb exchange part; $E_{const}$ is a constraint energy. In detail

$$E_R = -\frac{1}{4} t_3 \int d^3\underline{r}\, \rho_n(\underline{r})\rho_p(\underline{r})\rho(\underline{r}) - \frac{1}{2}\int d^3\underline{r}\, V_{CE}(\underline{r})\rho_p(\underline{r}), \quad (24)$$

$$E_{const} = Q \cdot \frac{\partial f(\mu,\nu)}{\partial \nu}\Big|_{\nu=Q} . \quad (25)$$

It is the expression (23) from which one has to start [2,3,5] in order to obtain the shell-correction expansion (1). For this purpose we must introduce a smooth part of the density matrix $\rho$. "Smooth" here means slowly varying with deformation Q and nucleon numbers N and Z. Strutinsky's energy-averaging procedure [1,2] here immediately suggests itself. With this, the average density matrices are given by

$$\bar{\rho}^q_{\alpha\beta} = \sum_i \bar{n}^q_i \,(C^{qi}_\alpha)^* C^{qi}_\beta ,$$
$$\bar{\rho}_{\alpha\beta} = \bar{\rho}^n_{\alpha\beta} + \bar{\rho}^p_{\alpha\beta} , \quad (26)$$

where the HF occupations numbers $n^q_i$ in eq.(7) are replaced by some averaged occupation numbers $\bar{n}^q_i$. These are defined using an averaging function $f_M(x)$ (which includes curvature-corrections of order M) [3-5]:

$$\bar{n}^q_i = \frac{1}{\gamma}\int_{-\infty}^{\bar{\lambda}_q} dE\, f_M\left(\frac{E-\varepsilon^q_i}{\gamma}\right) . \quad (27)$$

The Fermi energies $\bar{\lambda}_q$ are determined by equations analogous to (5).

Using eqs. (9),(12),(14)-(16), we now define analogous averaged quantities $\bar{\rho}_q(r)$, $\bar{\tau}_q(r)$, $\underline{\bar{J}}_q(r)$, and in turn $\bar{Q}$, $\bar{m}^*_q(r)$, $\bar{U}_q(r)$, and $\underline{\bar{W}}_q(r)$ by replacing $\rho^q_{\alpha\beta}$ everywhere by $\bar{\rho}^q_{\alpha\beta}$. Inserting the average quantities in the single-particle Hamiltonian $H_q$ defined by eq. (13), we find a smoothed Hamiltonian $\bar{H}_q$ :

$$\bar{H}_q = -\underline{\nabla}\cdot\frac{\hbar^2}{2\bar{m}^*_q(\underline{r})}\underline{\nabla} + \bar{U}_q(\underline{r}) + \underline{\bar{W}}_q(r)\cdot(-i)(\underline{\nabla}\times\underline{\sigma}) + \hat{q}_{\sigma\tau}\cdot\frac{\partial f}{\partial \nu}(\nu,\bar{Q}), \quad (28)$$

which may be considered as a "shell model" Hamiltonian [2,3,5]. We shall denote here its eigenvalues by $\hat{\varepsilon}^q_i$ and its eigenfunctions by $\hat{\Phi}^q_i(\underline{r})$

$$\bar{H}_q \hat{\Phi}^q_i(\underline{r}) = \hat{\varepsilon}^q_i \hat{\Phi}^q_i(\underline{r}) . \quad (29)$$

Now, if the density oscillations $\delta\rho^q_{\alpha\beta} = \rho^q_{\alpha\beta} - \bar{\rho}^q_{\alpha\beta}$ are sufficiently small - which will be checked numerically below - one can treat the difference $\delta H_q = H_q - \bar{H}_q$ as a small perturbation of $H_q$. Then the energies $\varepsilon^q_i$ and $\hat{\varepsilon}^q_i$ can be related in first order perturbation theory by

$$\varepsilon^q_i \simeq \hat{\varepsilon}^q_i + \int d^3\underline{r}\, \hat{\Phi}^q_i(\underline{r})^*\, \delta H_q\, \hat{\Phi}^q_i(\underline{r}) . \quad (30)$$

Multiplying eq.(30) by $n_i^q$ and summing over i gives

$$\sum_{qi} \varepsilon_i^q n_i^q = \sum_{qi} \hat{\varepsilon}_i^q n_i^q + \int d^3\underline{r}\, \delta H_q \rho_q(\underline{r}) + O[(\delta\rho)^2] \quad (31)$$

Expanding the terms $E_{pot}$ and $E_R$ in eq.(23) around $\bar{\rho}_{\alpha\beta}^q$ and using eq.(31), the first order terms in $\delta\rho_{\alpha\beta}^q$ cancel each other so that

$$E_{HF} = \sum_{qi} \hat{\varepsilon}_i^q n_i^q - \bar{E}_{pot} + \bar{E}_R - E_{const} + E_{pair} + O[(\delta\rho)^2], \quad (32)$$

where $\bar{E}_{pot}$ and $\bar{E}_R$ are defined again in terms of the averaged densities.

Note in eq.(32), $E_{const}$, $E_{pair}$ and the $n_i^q$ are still the HF quantities. We now introduce the occupation numbers $\hat{n}_i^q$ which are defined by eqs.(5) and (19), but in terms of the "shell model" energies $\hat{\varepsilon}_i^q$, and define the corresponding pairing energy $\hat{E}_{pair}$:

$$\hat{E}_{pair} = E_{pair}(\hat{\lambda}_q, \hat{n}_i^q) \quad (33)$$

With these we can rewrite eq. (32) as

$$E_{HF} = \sum_{qi} \hat{\varepsilon}_i^q \hat{n}_i^q - \bar{E}_{pot} + \bar{E}_R - \bar{E}_{const} + \hat{E}_{pair} + \delta E_{pair} - \delta E_{const} + O[\delta\rho^2] \quad (34)$$

where

$$\delta E_{pair} = \sum_{qi} \hat{\varepsilon}_i^q (n_i^q - \hat{n}_i^q) + (E_{pair} - \hat{E}_{pair}), \quad (35)$$

and the constraint energy $E_{const}$ has been split into a smooth part and a small correction term:

$$\bar{E}_{const} = \bar{Q} \cdot \frac{\partial f}{\partial \nu}(\mu,\nu)\Big|_{\nu=\bar{Q}}, \quad (36)$$

$$\delta E_{const} = E_{const} - \bar{E}_{const} \simeq \delta Q \cdot \frac{\partial f}{\partial \nu}(\nu,\mu)\Big|_{\nu=\bar{Q}}. \quad (37)$$

Since the occupation numbers $n_i^q$ and $\hat{n}_i^q$ are expected to differ only slightly (only in the energy region $\sim\lambda_q \pm \Delta_q$ do they differ at all), the quantity $\delta E_{pair}$ should be very small. Similarly, $\delta E_{const}$ (37) is expected to be small, being the product of $\delta Q = Q - \bar{Q}$ ($\sim$1-2 barns, see ref. [3] ) times the slope of a LD-like deformation energy curve [11] (< 1 MeV/barn ). Indeed, we will see numerically below that both quantities $\delta E_{pair}$ and $\delta E_{const}$ do not exceed $\sim$0.5 MeV in magnitude in a medium-heavy nucleus, and therefore we treat them as quantities of second order.

Collecting all terms of second and higher order in $\delta E_2$ - note the slight change of notation from eq.(1) - we define

$$\delta E_2 = \delta E_{pair} - \delta E_{const} + O[(\delta\rho)^4] \tag{38}$$

and obtain from (34)

$$E_{HF} = \sum_{qi} \hat{\varepsilon}_i^q \hat{n}_i^q + \hat{E}_{pair} - \bar{E}_{pot} + \bar{E}_R - \bar{E}_{const} + \delta E_2 . \tag{39}$$

The first two terms in (39) correspond exactly to the usual shell model energy sum plus pairing, and contain all first order contributions from $\delta\rho$. These are now extracted as the first order shell correction $\delta E_1$:

$$\delta E_1 = \sum_{qi} \hat{\varepsilon}_i^q \hat{n}_i^q - \bar{U} + \hat{E}_{pair} - \bar{E}_{pair} . \tag{40}$$

The uniform quantities $\bar{U}$ and $\bar{E}_{pair}$ are defined as in the usual shell-correction theory [2,3,4] by

$$\bar{U} = \sum_{qi} \hat{\varepsilon}_i^q \bar{n}_i^q , \tag{41}$$

$$\bar{E}_{pair} = -\frac{1}{2} \sum_q \bar{g}_q(\bar{\lambda}_q) \bar{\Delta}_q^2 , \tag{42}$$

where the $\bar{n}_i^q$ are defined by eq.(27) in terms of the $\hat{\varepsilon}_i^q$, $\bar{\Delta}_q$ are the average pairing gaps and $\bar{g}_q(E)$ are the uniform level densities defined by

$$\bar{g}_q(E) = \frac{1}{\gamma} \sum_i f_M\left(\frac{E - \hat{\varepsilon}_i^q}{\gamma}\right) \tag{43}$$

Collecting all smooth terms occuring in eqs.(39) and (40), we define the LD part of the HF energy by

$$\bar{E} = \bar{U} + \bar{E}_{pair} - \bar{E}_{pot} + \bar{E}_R - \bar{E}_{const} . \tag{44}$$

With the definitions (40) and (44) we thus have explicit expressions for the first two terms of the shell-correction expansion (1). Writing

$$\delta E_2 = E_{HF} - \bar{E} - \delta E_1 , \tag{45}$$

we can calculate $\delta E_2$ and thereby check the convergence of the series (1). $\bar{E}$ and $\delta E_1$ can separately be compared to the corresponding quantities found in the LD model and the usual shell-correction calculations.

A special point of interest is the argument that the smoothed constraint present in the definition of the "shell model" Hamiltonian $\bar{H}_q$ (28) should be omitted, since we want to check the use of ordinary shell model potentials

in which no constraint is present. However, we expect this not to affect the results - at least not the smooth and the first order terms, $\bar{E}$ and $\delta E_1$. The reason can easily be seen using perturbation theory. Switching off the constraint in $\bar{H}_q$ (28), which is a small disturbance, the i-th eigenvalue of $\bar{H}_q$ is changed by

$$\Delta \hat{\varepsilon}_i^q \simeq - \int \hat{\bar{\Phi}}_i^q(\underline{r})^* \frac{\partial f}{\partial \nu}(\mu, \nu = \bar{Q})\, \dot{q}_{op}\, \hat{\bar{\Phi}}_i^q(\underline{r}), \tag{46}$$

and therefore

$$\Delta \sum_{iq} \hat{\varepsilon}_i^q \hat{n}_i^q \simeq - \hat{Q} \cdot \frac{\partial f}{\partial \nu}(\mu, \nu = \bar{Q}), \tag{47}$$

where $\hat{Q}$ is the "shell model" quadrupole moment which is close to the HF value Q. The change in $\bar{U}$ (41) is then

$$\Delta \bar{U} = \sum_{qi} \Delta \hat{\bar{\varepsilon}}_i^q \hat{\bar{n}}_i^q \approx - \bar{Q} \cdot \frac{\partial f}{\partial \nu}(\mu, \nu = \bar{Q}), \tag{48}$$

so that the two contributions to $\delta E_1$ in (40) cancel up to a term comparable to $\delta E_{const}$ (37). Similarly, the contribution of the constraint to $\bar{U}$ is in eq.(46) cancelled in first order by the energy $\bar{E}_{const}$. Thus, all differences made by including or omitting the average constraint on $\bar{H}_q$ are expected to be of second order only. This will be confirmed by our numerical results below.

Before presenting the results, we want to compare our method briefly to the one proposed by Bassichis et al. [6]. These authors define a smooth density $\bar{\rho}_{\alpha\beta}$ and a "shell model" Hamiltonian $\bar{H}_q$ in a similar way to ours (not including the constraint in $\bar{H}_q$). The main difference in their approach lies in their explicit use of the "shell model" density matrix $\hat{\rho}^q_{\alpha\beta}$:

$$\hat{\rho}_{\alpha\beta} = \sum_i n_i^q \left(\hat{C}_\alpha^{qi}\right)^* \hat{C}_\beta^{qi} \tag{49}$$

the $\hat{c}_\alpha^{qi}$ being the expansion coefficients (cf. eq. (6) ) of the eigenfunctions $\hat{\bar{\Phi}}_i^q(\underline{r})$ of $\bar{H}_q$. Using the fact that the HF energy is stationary as a functional $E[\rho]$ of the density matrix $\rho$, they write

$$E_{HF}[\rho] = E[\hat{\rho}] + O[\delta c^2], \tag{50}$$

where $O[\delta c^2]$ is a term of second order in the changes of the wavefunctions, $\delta c = \hat{c}_\alpha^{qi} - c_\alpha^{qi}$. The right hand side of eq.(50) can then be transformed - without using perturbation theory - into a form which is similar to eq.(32), but in which one second order term is given explicitly. Thus the advantage of this method is that one part of the second order shell corrections can be

evaluated exactly. However, another part is still left in the term $\sigma[\delta c^{+}]$ in eq.(50) which can only be calculated indirectly. The advantage of our method is that one only needs to know the eigenvalues $\hat{\varepsilon}_i$ of the average Hamiltonian $\bar{H}_q$, and therefore one does not have to compute the densities $\hat{\rho}_q(\underline{r})$, $\hat{\tau}_q(\underline{r})$, etc. The numerical evaluation of the second order terms given by Bassichis et al. [6] is planned for future calculations.

## NUMERICAL RESULTS AND CONCLUSIONS

In our numerical calculations we used the set "SIII" of Skyrme parameters. These were recently shown to give excellent fits of the ground-state energies, radii and deformations throughout the periodic table [13]. For completeness we give the parameters in Table 1.

To check the shell-correction expansion in a medium-heavy nucleus, we performed a complete CHF-calculation for the rare-earth element $^{168}$Yb. For the pairing effects we used the normal BCS treatment, thus choosing the pairing functional (17). As in ref. [3], a single parameter was used in the form of a uniform gap $\bar{\Delta}$, chosen here to be $\bar{\Delta}$ = 1.0 MeV which corresponds to the pairing strengths $G_n$ = 0.15 MeV and $G_p$ = 0.19 MeV (at all deformations).

Figure 1 shows the deformation energy curve $E_{HF}(Q)$ of $^{168}$Yb in a region containing the prolate ground-state, an oblate secondary minimum and the ascent towards the fission barrier. The curve $E_{W.S.}$ was obtained as a zeroth order approximation using the shell model wavefunctions found in a Strutinsky calculation with a deformed Woods-Saxon potential [3]. As recently described [17], these wavefunctions give an excellent approximation to the HF solutions. The total binding energy obtained in this approximation is at smaller deformations only $\sim$ 7 - 10 MeV higher than the HF energy, as can be seen also in Fig. 1. The dashed line in Fig. 1 is the smooth energy $\bar{E}$ obtained by eq.(44). This curve indeed behaves like a LD deformation energy. Within the numerical accuracy of our results, here $\sim \pm$ 0.5 MeV in the total energies, the curve is smooth. This result strongly supports Strutinsky's theory of renormalization of the LD energy part.

TABLE 1. PARAMETERS OF THE SKYRME INTERACTION SIII USED IN OUR CALCULATIONS

| $t_0$ | $t_1$ | $t_2$ | $t_3$ | $x_0$ | $W_0$ |
|---|---|---|---|---|---|
| - 1128.75 | 395.0 | -95.0 | 14000.0 | 0.45 | 120.0 |

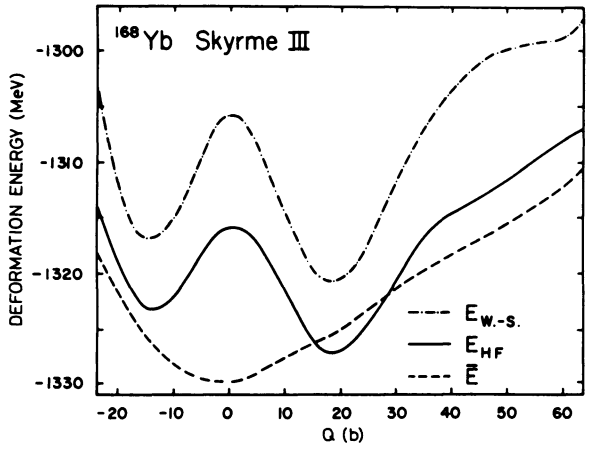


FIG. 1. Deformation energy curves E(Q) for $^{168}$Yb, obtained with Skyrme interaction SIII. Solid line: CHF result. Dashed-dotted line: approximation $E_{W.S.}$ with shell model wave functions. Dashed line: smooth part E of the HF energy.

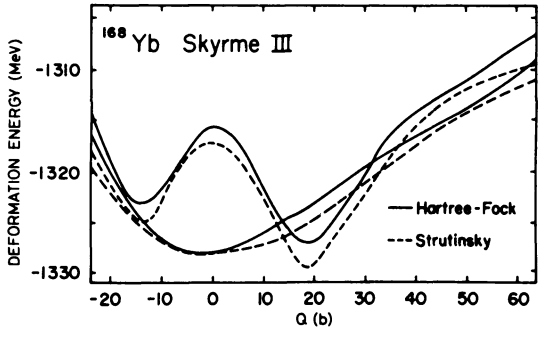


FIG. 2. Comparison of CHF and Strutinsky deformation energy curves for $^{168}$Yb. Solid lines: $E_{HF}$ and $\bar{E}$ obtained with interaction SIII (see Fig. 1). Dashed lines: total energy $E_{LD} + \delta E_1$ and LD energy $E_{LD}$ obtained in a shell-correction calculation with a deformed Woods-Saxon potential.

To check our arguments concerning the constraint in the smoothed Hamiltonian $\bar{H}_q$, we did the calculations twice, once with and once without the constraint. In both cases, the LD energy $\bar{E}$ turned out to be exactly the same.

In Figure 2 we compare the HF energy curve and its LD part to the curves obtained in a Strutinsky-type calculation. In the latter, the shell-correction $\delta E_1$ was found from a deformed Woods-Saxon potential already mentioned above (see ref.[3]). The deformation energy $E_{LD} + \delta E_1$ was taken along a path going through the two minima and approximately following the LD valley at larger

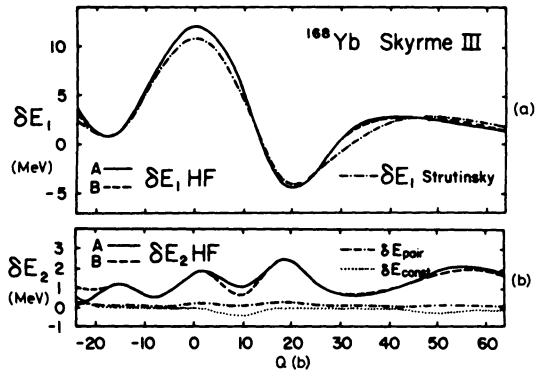


FIG. 3. (a) First order $\delta E_1$ and (b) higher order shell corrections $\delta E_2$ extracted from the HF energy. Solid lines (A): results obtained with constraint in the smooth Hamiltonian $\bar{H}_q$. Dashed lines (B): results obtained without constraint in $\bar{H}_q$. Figure 3b also shows the quantities $\delta E_{pair}$ and $\delta E_{const}$ contained in $\delta E_2$. In Fig. 3a, the dashed-dotted curve is the first order shell correction found with the Woods-Saxon potential (see Fig. 2).

deformations. The quadrupole moment was calculated at each point from the shell model wavefunctions as in eq.(12). The position of the Strutinsky curves is adjusted so that the values of $E_{LD}$ and $\bar{E}$ at zero deformation are the same. In $\bar{E}$, we have included here a constant of +1.7 MeV in order to take the average contribution of the higher order terms $\delta E_2$ into account (see below). We can see in Fig. 2 that the two models predict the same equilibrium deformations within a few percent.

The first and higher order shell-corrections extracted from $E_{HF}$ according to eqs.(40),(45) are displayed in Fig. 3. The solid lines show $\delta E_1$ and $\delta E_2$ obtained with the average constraint included in $\bar{H}_q$, and the dashed lines show them without the constraint in $\bar{H}_q$. As expected, the two cases give essentially the same results. In the upper part of the figure, the small corrections $\delta E_{const}$ and $\delta E_{pair}$ are shown.

For the definition of the average densities $\bar{\varrho}_{\alpha\beta}$ by eqs.(25) and (26), a Gaussian averaging function with a fourth order curvature correction was chosen. The smearing range $\gamma$ was chosen to be $\gamma \simeq 1.1 - 1.4\ \hbar\Omega$, with $\hbar\Omega$ being the average separation of the main shells in the spectra $\varepsilon_i^q$. No significant change of the results shown in Figs. 1 - 3 was observed by varying $\gamma$ within the range mentioned.

In the lower part of Fig. 3, the shell-correction $\delta E_1$ found from the Woods-Saxon potential [3] is shown with the dashed-dotted curve. Its agreement with the HF curve is remarkable, in view of the fact that no adjustment at all has been made of the Woods-Saxon potential parameters.

The sum of the higher order shell corrections $\delta E_2$ is quite small as compared to the first order correction $\delta E_1$ (note the enlarged scale in the upper part of the figure!). They oscillate by $\sim \pm 1$ MeV around an average value of ~+1.7 MeV. Their relative smallness proves the rapid convergence of the shell-correction expansion (1). In looking closer at Fig. 3, we notice a clear correlation of the oscillations in $\delta E_1$ and $\delta E_2$: The maxima of $\delta E_2$ coincide with the extrema of $\delta E_1$. This can be understood by assuming that the terms of second order in $\delta\varrho$ are predominant in $\delta E_2$, as is made evident by the rapid convergence of the shell-correction expansion. Then it is clear that the "wavelength" of the oscillations in $\delta E_2$ must be one-half times that of the first order oscillations $\delta E_1$. This has two consequences for the calculations of deformation energies with the traditional shell correction method: 1) The inclusion of a second order correction affects the relative position of the stationary points of the curve only very little, since the values at the maxima of $\delta E_2$ vary only little around their average ($\pm \sim 0.6$ MeV in the present case). 2) The regions between the extrema of the deformation energy curve are lowered with respect to the stationary points, which tends to make the barriers thinner. Both effects can be seen in Fig. 2.

If the pattern of these results is confirmed in calculations for actinide nuclei and with different effective interactions - which will be carried out in the future - we can therefore conclude that the static fission barriers and the equilibrium deformations are sufficiently well described in a Strutinsky calculation. For the calculations of fission lifetimes, however, the second order corrections might be important, as the lifetimes are well known to be crucially dependent on the thicknesses of the barriers [3,18]. The second order effects thus tend to lower the calculated halflives, which is in favour of the results of refs. [3,18].

One should of course check these conclusions by applying our test to a heavy fissionning nucleus. However, in this region the Skyrme-CHF calculations do not yet reproduce the experimentally known fission barriers, the outer barrier being more than twice as large as its experimental value [14]. Since our test of the Strutinsky method is meaningless when the CHF results are in clear disagreement with experiment, we cannot expect to get conclusive results in this region.

At ground-state deformations and especially for spherical nuclei, however, the Skyrme-III interaction is very successful, as mentioned above. We therefore used these results to calculate the higher order corrections $\delta E_2$ for a series of nuclei in their ground states. The results are shown in Figure 4. The crosses show the values of $E_2$ evaluated for the nuclei $^{108}Ru$, $^{134}Ce$, $^{140}Ce$, $^{152}Sm$, $^{158}Gd$, $^{162}Dy$, $^{166}Er$, $^{168}Yb$, $^{174}Yb$, $^{178}Hf$, $^{184}W$, $^{190}Os$, $^{208}Pb$

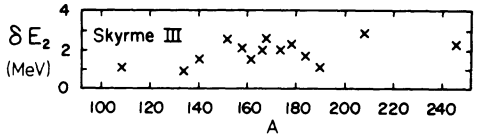


FIG. 4. Higher order shell corrections $\delta E_2$ for 14 nuclei in their ground state. Skyrme III interaction used; pairing effects included in all deformed nuclei.

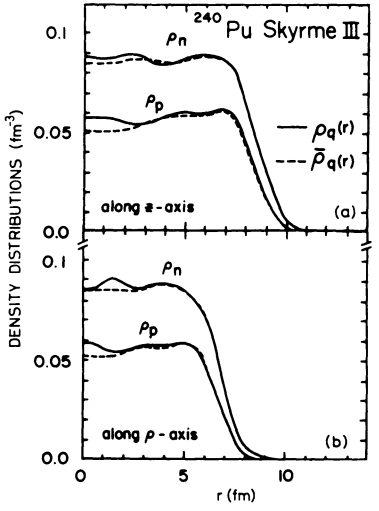


FIG. 5. Density distributions of $^{240}$Pu in the ground state. (a) along the z-axis (symmetry axis); (b) along the $\rho$-axis (perpendicular to the z-axis). Solid lines: HF results (Skyrme III). Dashed lines: energy-averaged densities $\bar{\rho}_q(\underline{r})$.

and $^{240}$Pu. In these calculations (except for $^{168}$Yb, see above) the pairing functional (17) was used and the gaps $\Delta_q$ chosen to be approximately equal to their experimental values. All values of $\delta E_2$ lie within $\sim 2.0 \pm 1$ MeV, including the doubly magic $^{208}$Pb. This result again demonstrates the smallness of the higher order effects, indicating that the first order shell corrections to the ground-state energies can be expected to be correct within $\sim \pm 1 - 2$ MeV.

We want to emphasize that the way in which we have defined the smooth part $\tilde{\varrho}^q_{\alpha\beta}$ of the density matrix is not the only possible one; other definitions may be tried. The Strutinsky averaging method is based on the belief that the most important shell effects come from the oscillations of the density of single-particle states in energy space, especially those in a region $\pm \hbar\Omega$ around the Fermi energy. This assumption might in our calculations be tested by the use of other averages for $\bar{\varrho}^q_{\alpha\beta}$. The averaging in energy space does not imply that the spatial density distributions $\bar{\varrho}_q(\underline{r})$ are completely smooth as functions of $\underline{r}$. This is illustrated in Figure 5, where the density distributions $\bar{\varrho}_q(\underline{r})$ of

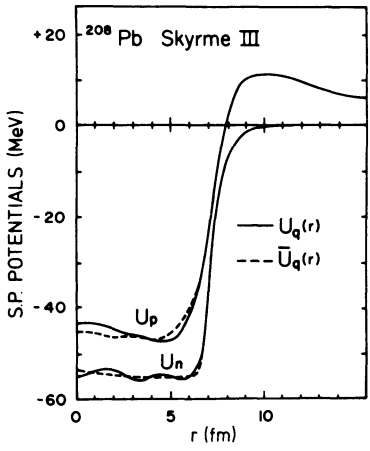


FIG. 6. Local parts $U_q(\underset{\sim}{r})$ and $\bar{U}_q(\underset{\sim}{r})$ of the HF and the averaged single-particle potentials, respectively, of $^{208}$Pb in the ground state (Skyrme III).

$^{240}$Pu in the ground state are shown. Although the densities $\bar{\rho}_q(\underset{\sim}{r})$ are much smoother than the selfconsistent ones, some oscillations still remain. These have been observed before [3,5] and are not believed to be responsible for shell effects. (For a detailed discussions of these remaining oscillations, see ref. [5].) Similarly, the smoothed single-particle potentials $\bar{U}_q(\underset{\sim}{r})$ still oscillate slightly inside the nucleus, as can be seen in Figure 6 where they are compared to the HF potentials $U_q(\underset{\sim}{r})$ for the case of $^{208}$Pb. (The proton potentials include the Coulomb potential (11a,b).) Results similar to those displayed in Figs. 5 and 6 where obtained for the rare-earth nuclei. The smooth potentials $\bar{U}_q(\underset{\sim}{r})$ look in general very similar to Woods-Saxon potentials, confirming the use of such potentials in Strutinsky calculations.

## SUMMARY

We have found that the definition of $\bar{\rho}$ yields an average part of the total HF energy which - at least for a nucleus like $^{168}$Yb - is perfectly smooth as a function of deformation. The shell-correction expansion (1) of $E_{HF}$, found by means of this smoothed density matrix $\bar{\rho}$, has been proved numerically to have rapid convergence. Our results for the higher order shell corrections are in good agreement with the results obtained previously by Bunatyan et al. [5] using a completely different method.

We conclude that first order shell corrections, calculated from a Woods-Saxon-type shell model potential, describe the stationary points of deformation energy curves sufficiently well: the higher order effects do not

affect them by more than $\sim \pm$ 0.5 - 1 MeV. The second order effects might be important in calculating fission lifetimes, tending to make barriers narrower and thus the lifetimes shorter. In transition regions from spherical to deformed nuclei, or from oblate to prolate nuclei, where the first order corrections are small, the second order effects might also play a decisive role.

We have seen that the inclusion of a constraint in the average potential has only a negligible effect on the single terms obtained in the shell-correction expansion.

These conclusions are drawn from the HF point of view, and are only relevant for the Strutinsky method to the extent to which HF calculations can be considered more fundamental than the shell-correction approach. We therefore plan to repeat this type of calculations using different interactions.

The extraction of a LD-like average part from the HF energy allows us to determine LD parameters, such as surface and symmetry energy coefficients, for a given effective interaction. The determination of the average potentials $\bar{U}_q(\underline{r})$ should also help to improve the shell model potentials to be used in shell-correction calculations. Such investigations are in progress and will be published elsewhere.

## ACKNOWLEDGEMENTS

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## DISCUSSION

K. DIETRICH: If the effective interaction depends on the density, a term linear in the fluctuation $\delta\rho$ arises which in general is not zero but would represent a correction to the Strutinsky term. You have told me that for the Skyrme interaction this term is zero. Is that fortuitous or is the Skyrme interaction so adjusted that this happens?

M. BRACK: One can easily verify that our method works for any density-dependent term of the form $\rho^{\alpha}(\underline{r})\,\delta(\underline{r}-\underline{r}')$ in the interaction with $\alpha$ being a real number. Furthermore, it was shown by Bunatyan and co-workers (Ref.[5] of our paper) that, for any density-dependent effective interaction, if one makes the local density approximation and stays within the HF framework, no term linear in $\delta\rho$ will appear, as long as the rearrangement energy is taken properly into account.

K. DIETRICH: The first two terms of your expansion

$$\left(E\left[\overline{\rho}\right] + \left(\frac{\delta E}{\delta \rho}\right)\delta\rho\right)$$

are not very sensitive to the details of the decomposition $\rho = \overline{\rho} + \delta\rho$ as long as $\overline{\rho}$ is reasonably smooth. In the phenomenological Strutinsky method, the term $E[\overline{\rho}]$ is replaced by the phenomenological droplet energy. It is very important here how $\delta\rho$ is defined. In your method you cannot check this aspect of the Strutinsky method.

M. BRACK: You are right in that we have not checked the correctness of the commonly used liquid-drop and shell models. Our test was concerned with the basic principle of Strutinsky's method, namely the possibility of obtaining a shell-correction expansion at all. Examining which phenomenological models have to be used to obtain the single terms $\overline{E}$ and $\delta E_1$ will be the next step.