STATIC DEFORMATION ENERGY CALCULATIONS: FROM MICROSCOPICAL TO SEMICLASSICAL THEORIES

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Abstract

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Various methods of calculating static potential energy surfaces are reviewed. Their uncertainties and limitations for the prediction of fission barriers of heavy nuclei are evaluated. The relations of the Strutinsky shell-correction method to the microscopical Hartree-Fock theory, on the one hand, and to semiclassical approaches, on the other hand, are discussed. Some representative experimental results are compared with the theoretical predictions, and the differences are related to the uncertainties in the theoretical results themselves.

1. INTRODUCTION AND SYNOPSIS

It was forty years ago that the fission process was qualitatively understood in terms of a barrier in the static deformation energy surface of the nucleus. The theoretical model which was underlying this interpretation and used in the classical papers by Bohr and Wheeler [1] and Frenkel [2], is the liquid drop model (LDM), familiar to every nuclear physicist. However only thirty years later, the first quantitative agreement between experimental and theoretical fission barrier heights could be achieved due to the shell-correction method (SCM) proposed by Strutinsky [3]. Since then, important progress has been made in the understanding of shell structure effects, especially in heavy deformed nuclei. The SCM has been confirmed by purely microscopical Hartree-Fock calculations with various effective interactions. Some promising progress has also been made in the refinement of semiclassical theories which are closely related to the Strutinsky method.

The aim of this paper is a comparison of the different methods used for the calculation of static deformation energy surfaces of heavy nuclei. In particular we try to give a critical evaluation of their suitability and their limitations for the theoretical prediction of fission barriers. As the title is indicating, we shall not follow the historical development of the theory, but rather start at a purely microscopical level.

In Section 2, microscopical calculations are reviewed. We discuss the constrained Hartree-Fock (CHF) method, its physical and technical limitations, and a recently improved time-saving approximation to it. The semimicroscopical shell-correction method (SCM) still being the most powerful

tool for systematic calculations of deformation energy surfaces, it is natural that an entire Section 3 is devoted to it. Here we first discuss the theoretical and numerical justification of the SCM within the HF framework. Some possible uncertainties inherent in the practical SC-approach, using phenomenological shell model potentials and LDM parameters, are evaluated. Then some extensions of the method applicable to excited nuclei and the possible inclusion of correlations through the Migdal theory are shortly summarized. Finally, the most important practical ingredient of the SCM, namely the Strutinsky energy averaging procedure, is discussed. Though a technical detail, it is essential and has provoked repeated criticism especially in connection with the use of finite depth potentials. Its uncertainties are carefully studied and several alternative methods and recent improvements are reviewed. In particular, we shall emphasize the complete equivalence between the (traditional) Strutinsky energy averaging and the extended Thomas-Fermi (ETF) model. Finally, with the help of some recent experimental results for actinide fission barriers, we shall establish the kind of agreement that is obtained by the most typical shell-correction calculations. The discrepancies are then compared to the uncertainties presented in the theoretical results themselves. The two most persisting cases where the disagreement with experiment clearly exceeds the theoretically expected error limits, namely the so-called Pb-and Th-anomalies, are discussed. We emphasize in particular the connection between the Pb-anomaly and the apparent lack of selfconsistency between the commonly used finite depth shell model potentials and LDM parameters.

In the final section 4 we shall summarize our conclusions and shortly mention some recent progress in the development of semiclassical methods which are very useful in determining average nuclear properties. We will outline an iteration procedure with which it should soon be possible to determine average potentials and deformation energies selfconsistently in a purely semiclassical way.

2. MICROSCOPICAL METHODS

2.1 Selfconsistent (CHF) calculations

The only practically feasible ways of describing heavy deformed nuclei on a purely microscopical level are using the indpendent particle (Hartree-Fock, HF) approximation or - when including pairing correlations - the independent quasiparticle (HF-Bogolyubov, HFB) approximation. Even in the HF framework, the technical problems are rather immense due to the non-linearity and the (in general) integro-differential character of the HF-equations. It is therefore only the development of fast computers on one hand and of mathematically sufficiently simple effective nucleon-nucleon interactions on the other hand, that made selfconsistent microscopical calculations possible for heavy deformed nuclei. For an extensive general review of HF-calculations of nuclear properties with phenomenological effective forces, we refer to a recent article of Quentin and Flocard [4].

An important development was initiated some ten years ago with the revival of the effective interaction of Skyrme by Vautherin and Brink [5]. The simplicity of this interaction consists in a zero-range expansion, where the finite range of the force is expressed through gradient dependent terms. The parametrization of the Skyrme force and its application to constrained Hartree-Fock (CHF) calculations was further developed by the Orsay group [6,7,19] and resulted in the first selfconsistently calculated fission barrier of ^{240}Pu [7]. Although the agreement with the experiment was not too good - several reasons for this will be discussed below

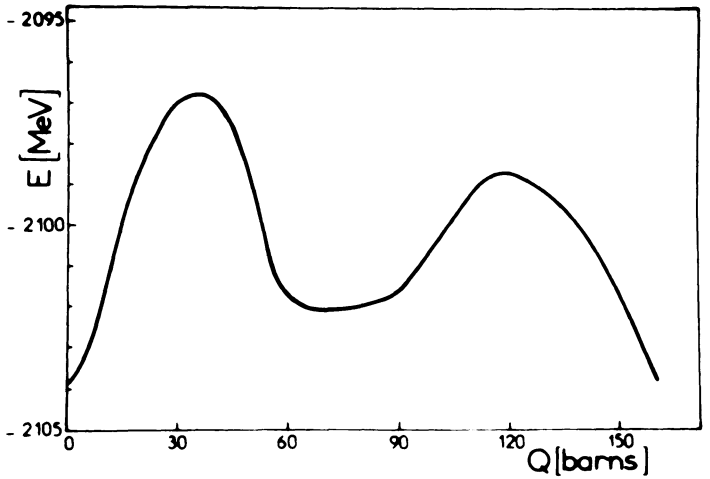

FIG.1. Fission barrier of the hypothetical super-heavy nucleus $^{298}114$, obtained with the Skyrme force, SIII, and the CHF method [8]. Q is the (mass) quadrupole moment.

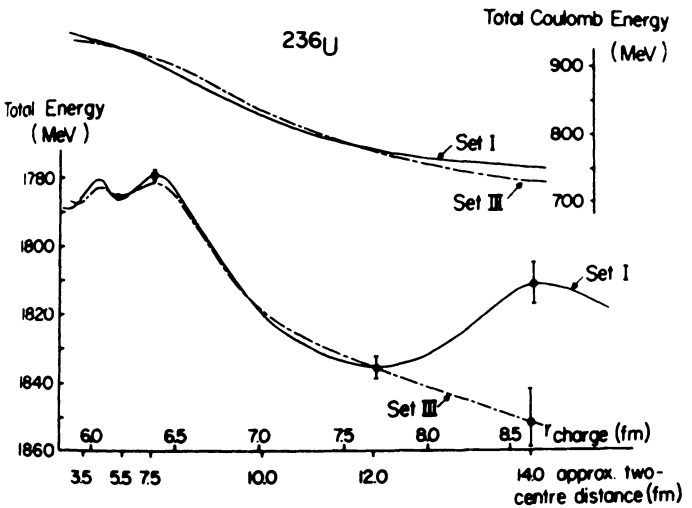

FIG.2. Fission barrier of ^{236}U, obtained with the self-consistent K-matrix model [12]. Mass asymmetry is included at and beyond the second saddle. Only four points have been calculated.

in sect. 2.2 - it was quite exciting to see the familiar double-humped shape emerging from a purely microscopical calculation. Due to the large computer times needed for these calculations, no systematical CHF-investigation of actinide fission barriers has been performed up to date. However, some selected calculations were done for the barriers of hypothetical superheavy nuclei [8,9]. As an illustration, we show in Figure 1 the barrier of $^{298}114$ obtained with the Skyrme III force [8]. In refs. [7,9], the dependence of the barrier heights on the force parameters has also been investigated (for some results, see the discussion below).

In another group, a selfconsistent K-matrix model [10] initiated by Meldner [11] was applied to a CHF-calculation for the asymmetric fission of ^{236}U by Kolb et al. [12]. In this case, the deformation energy curve was continued from the saddle point down to the scission region, see Figure 2. One notes here that two sets of parameters, which give similar results for spherical nuclei [12], lead to different predictions of the barrier heights and, especially, of the deformation energy curve near scission.

In both these sets of calculations, a quadratic constraint was used to obtain points of the deformation energy curves away from local minima. Pairing correlations were included in the BCS approximation using a pheonomenological gap parameter Δ or an average pairing matrix element G. This is a rather severe restriction of the consistency of these models: The paring matrix element is added ad hoc, and not calculated from the same effective interaction which determines the average (HF) field of the nucleus. As a consequence, the familiar dilemma concerning the deformation dependence of G (or the average gap $\tilde{\Delta}$) arises, which already caused a lot of discussion and uncertainties in the shell-correction calculations of fission barriers (see Sect. 3 below). Indeed, a drastic dependence of the barrier height on constant or surface-pairing was demonstrated in the CHF-calculations [7], too (see also 2.2.d below).

The right thing to do - but a lot more complicated - is to use an effective interaction which allows to perform true HFB calculations. With the present-day Skyrme forces [6] this is not possible due to their unrealistic behaviour at high momentum transfer. (This defect can, however, be removed by adding a few more exchange terms [13].) Recently, Gogny succeeded in designing a phenomenological finite range force (with a zero-range density dependent term) which is suited for HFB-calculations [14,15] in spite of the rather enormous technical problems involved. The results obtained in ref. [15] show a remarkable agreement between theoretical and experimental pairing properties of Sn-isotopes and various rare-earth nuclei. Simultaneously, the total binding energies and density distributions obtained in these calculations for spherical nuclei are at least of the same quality as those of the best earlier HF-calculations with effective forces. The first fission barrier calculations with the Gogny force will be presented in the subsequent paper at this Symposium [16].

2.2 Discussion of error sources and limitations

When comparing the fission barriers obtained in CHF calculations to experimental ones, one should consider several restrictions made in the models discussed above. Let us first discuss the physical restrictions.

a) Spurious energies.
A well-known deficiency of the HF-approximation is the fact that Slater determinants (or BCS wavefunctions) are neither good eigenstates of the total centre of mass momentum $\vec{P}$ nor of the total angular momentum $\vec{J}$. As a

consequence, the HF energy contains spurious kinetic energy contributions of translational and rotational motion. The former can reasonably well be taken care of (at least in heavy nuclei) by the direct part of

$$\Delta E_{cm} = \langle \vec{P}^2 \rangle / 2mA$$

leading to a slight rescaling of the total single-particle kinetic energy [6,19]. Since this correction is very little deformation dependent (even including the exchange part [17]), it leads to no serious errors in deformation energies. The spurious rotational energy, however, is harder to determine. Exact angular momentum projection being much too cumbersome in heavy nuclei, one often approximates its contribution by the expectation value (see, e.g. [20]):

$$\Delta E_{rot} = \hbar^2 \langle \vec{J}^2 \rangle / 2\mathcal{J}$$

where $\mathcal{J}$ is the moment of inertia. In heavy deformed nuclei, ΔE_{rot} easily amounts to ~ 3-6 MeV at the ground state [17,19,21] and further increases with increasing deformation. It thus leads to an overestimation of the fission barriers. Since in the above expression, the moment of inertia is needed, it is cumbersome to calculate and can only approximately be estimated. Using the cranking model values, one obtains for typical actinides a correction of ~ 1 MeV to the inner (E_A) and ~ 2-3 MeV or more to the outer barriers (E_B). The safest estimate is perhaps possible for the correction to the isomer excitation energy (E_{II}), using the experimental values of $\mathcal{J}$, and amounting here to ~ 1 MeV. (All these corrections are relative to the ground state energy E_I). We anticipate here that the correction ΔE_{rot} (as well as $\Delta E_{C.M.}$) plays no important role in the shell-correction approach, since it can be argued there [21] that only its - safely negligible - fluctuating part must be considered.

b) Coulomb exchange energy.
Since an exact calculation of the Coulomb exchange energy E_{CEX} is very time-consuming, it has in most cases been taken into account only approximately. In ref. [12] e.g., the statistical estimate

$$E_{cex} = -\frac{5}{4\pi}\left(\frac{3}{2\pi^2}\right)^{2/3} E_{CD}$$

was used, where E_{CD} is the direct Coulomb energy. A somewhat more refined (local density) Slater approximation is [22,23]

$$E_{cex} = -\frac{3}{4} e^2 \left(\frac{3}{\pi}\right)^{1/3} \int d^3r\, \rho_p^{4/3}(r)$$

$\rho_p(r)$ being the proton density, and was used in most of the Skyrme-HF calculations [5-9]. Both these approximations (and others) were checked against exact calculations and found to be satisfactory at ground state deformations [24, 19]. More recent investigations of E_{CEX} using analytical deformed harmonic oscillator results [25] indicate, however, that the Slater approximation may have the wrong deformation dependence in some cases (namely practically none), whereas the statistical approximation (where E_{CEX} is proportional to E_{CD}) seems more justified. For the Skyrme-HF results, this would lead to a positive correction at the second barrier of ~ 0.5 - 1 MeV for actinides and ~ 1-1.5 MeV for super-heavy nuclei [9].

c) Dependence of barriers on the force parameters
In most phenomenological effective interactions, there is some freedom left in the choice of the parameters, if one restricts oneself to ground-state properties only. In the case of the Skyrme-forces there is, in fact, an infinite choice of parameters (see Beiner et al. [6]) in the sense that any value of the density dependent term (t_3) may be chosen. The rest of the parameters can then still be chosen such as to give reasonably good fits to ground state properties of all spherical

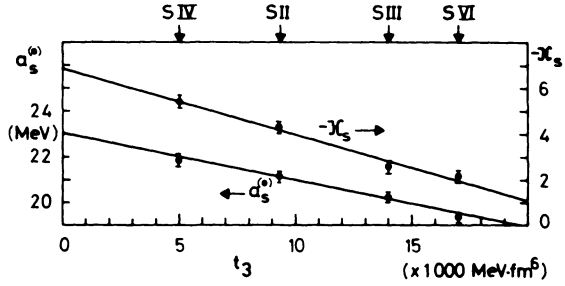

FIG.3. Surface energy $a_s^{(0)}$ and surface asymmetry coefficients κ_s for different Skyrme interactions (with theoretical error bars), obtained by a semiclassical variational calculation [40]. No spin-orbit contribution is included. Note the linear dependence of $a_s^{(0)}$ and κ_s on the Skyrme force parameter t_3.

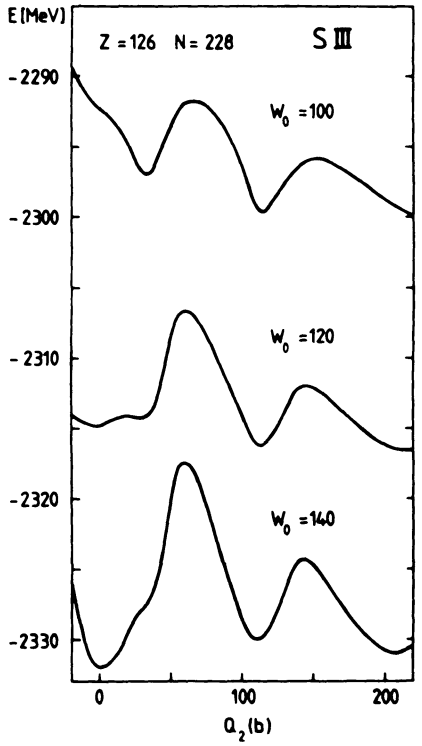

FIG.4. Deformation energy curves for the hypothetical nucleus $^{354}126$, obtained with the expectation value method (see Section 2.3). The spin-orbit force parameter W_0 (in units of MeV·fm^5) is varied, the other parameters of the force Skyrme III are kept constant. W_0 = 120 MeV·fm^5 is the standard value (from Ref. [9]).

nuclei; hereby, the forces with a larger density-dependent term t_3 turn out to have a larger effective nucleon mass m*(r). It is thus important to know how the properties at large deformations depend upon this variation of parameters.

In the thesis of Flocard [7] (p. 37), a comparison is made of the barriers of ^{240}Pu obtained with the Skyrme forces SIII and SIV. Both barrier heigths are larger by ~ 5-6 MeV with S IV than with S III. A similar difference (6 MeV) was found for the inner barrier of the super-heavy candidate $^{354}126$ with the same forces [9]. One may argue that the S III force has to be preferred because of its more realistic value of the effective nucleon mass in the interior of the nucleus (m*/m = 0.75 for S III and 0.5 for S IV) and its better single-particle spectra of deformed nuclei [19, 26]. Still, the sensitivity of the fission barriers to the force parameters is rather severe. These results are substantiated by independent investigations of the liquid drop parameters inherent in the Skyrme interaction. It was found, indeed, that the surface and surface asymmetry parameters of the different Skyrme forces do vary appreciably, those of S III being very close to the standard LDM values. This is illustrated in Fig. 3.

A similar variation of barrier heights was observed in the calculations of Kolb et al. [12] reported already in Fig. 2 above. In particular, the difference obtained near scission is rather drastic. Note, however, that only four points were calculated along these curves. A more recent calculation, using a newer version of the K-matrix model [27], is reported in ref. [4] (see fig. 11 there). It seems to substanciate the curve labeled "Set III" in Fig. 2, although with a second barrier of more than ~ 15 MeV (as estimated from that figure).

So far, we have been discussing the freedom in the parameters for the central parts of the effective interactions used. An even more drastic - and actually alarming - dependence of the results is found, when it comes to varying the spin-orbit force. The latter has, in all HF (and HFB) calculations mentioned above, been added purely phenomenologically and adjusted such as to give the spin-orbit splittings of the single-particle levels observed experimentally in spherical nuclei. Note that the central part of the Skyrme forces has been linked back to density dependent Brückner-HF calculations with the Reid soft core nucleon-nucleon potential [23], and can therefore be said - as well as the K-matrix models - to be one degree less phenomenological than the spin-orbit force which, in this respect, is to be put at the same level as the simple shell model.

In Figure 4 we show three fission barrier curves for the superheavy nucleus $^{354}126$, obtained with the same force Skyrme III, but with three different values of the spin-orbit parameter W_0 [9]. These curves are not obtained fully selfconsistently, but with the expectation value method [18] to be discussed below. The lack of self-consistency leads to an uncertainty of ~ 1-2 MeV up to the second minimum and does in any case not affect the dramatic variation of the barrier heights with W_0. Note that for W_0 = 120 MeV fm^5 (the standard value for S III) and W_0 = 140 MeV fm^5, the nucleus is spherical in the ground state, whereas for W_0 = 100 MeV fm^5 it becomes deformed. The height of the first barrier varies from 5 to 15 MeV in the three cases. Of course, it is no surprise that the spin-orbit force plays an important - if not the decisive - role for the magnitude and the phase of the shell effects. However, a variation of ± 10 % of the constant W_0 could easily be absorbed by a readjustment of the other Skyrme parameters without spoiling the nice results for ground-state properties. And its determination by fitting the

HF-levels to experimental single-particle (or hole) states in magic nuclei may be disputed, since the latter are known to receive appreciable contributions from couplings to vibrational modes, which are missing in the HF approach, and which are especially large in spherical closed-shell nuclei (see, e.g. ref. [28]). It is therefore no large overstatement to say that one can obtain almost any barrier one wants by exploiting the freedom in determining the spin-orbit parameter. Taken together with the ambiguities in the rest of the force, uncertainties of many MeV are present in the heights of fission barriers.

In future HF-calculations, fission barriers must definitely be taken into account in pinning down the force parameters. Furthermore, a better understanding of the spin-orbit force is highly desirable. In this respect we refer to an interesting recent attempt to link the spin-orbit force back to simple model nucleon-nucleon potentials by fully relativistic Hartree-calculations [29].

d) Treatment of pairing correlations

We have already discussed the lack of consistency of HF plus BCS calculations as performed by the Orsay group [5-9] and Kolb et al. [10,12]. Of course, for the ground-states this is no severe restriction since their pairing properties can usually be fitted reasonably well by the phenomenological constants Δ or G. The deformation dependence of Δ and G is, however, not known well enough. We may deduce some hints from the result of the Gogny group [15]. There, a deformation energy curve of ^{152}Sm was obtained in a full HFB-calculation (using a linear constraint) and compared to two approximate (HF plus BCS) calculations. At large deformations, the prescription of a constant gap Δ clearly gave a better agreement with the HFB result than a pairing interaction G proportional to the surface. If this trend persists for heavy nuclei, it might have very interesting consequences for fission barriers. Note that in the Skyrme-HF-BCS calculations of Flocard et al. [7], the constant Δ prescription led to a second barrier of ^{240}Pu which was $\sim$ 8 MeV higher than the one obtained with the other prescription. The newest HFB-results with the Gogny force seem to confirm, indeed, the trend of a constant average pairing gap Δ [16]. We also remark here that some interesting attempts have been made to treat the pairing correlation in a classical (Thomas-Fermi) approximation [30]. When applied to deformed nuclei, this approach might also provide some valuable information.

Let us now turn to some technical limitations of the CHF calculations, which are mainly due to their time consuming character.

e) Truncation effects from finite basis expansion.

For spherical nuclei, the HF-equation can be solved directly and relatively fast in coordinate space (i.e. in the radial variable) with standard numerical procedures [5,6,10,14,23]. In deformed nuclei, however, the two-or three-dimensional, nonlinear partial (integro-) differential equations pose severe numerical problems. The standard way out is projection on a deformed harmonic oscillator basis and diagonalization of the hamiltonian matrix. We need not explain this method which is well-known from shell-correction calculations (see, e.g. ref. [31]). So far, all CHF calculations for fission barriers with realistic interactions have been performed by this projection method, recently renewed attempts in coordinate space [32] not withstanding. The difference to the SCM is that the truncation effects are present in the total HF-energies with

their full weight. The time and space limitations of computer calculations set lower bounds on the induced errors. For spherical nuclei, they can be studied carefully by comparison to the exact (r-space) results (see, e.g. ref. [19]) and extrapolated to small deformations. At large deformations one has to content oneself with observing the convergence of the (relative) deformation energies under variations of the size (number N_0 of major oscillator shells) and the parameters (oscillator strength $\hbar\omega$ and ratio q of principal axes) of the deformed basis. In the fission direction (symmetry axis), a single oscillator well (with $N_0 \simeq$ 13 to 15) is just about sufficient for deformations up to the second saddle point of actinide nuclei. In ref. [7], the remaining truncation error was estimated to be ~ 1-2 MeV at the second barrier of ^{240}Pu. When going beyond the outer barrier, a two-center basis of some kind becomes indispensable [8,12,16] (see also refs. [33,34]).

f) Restrictions on symmetries and degrees of freedom

Even with projection on a finite basis, the computer time and space limitations force one to keep some symmetries of the variational space. Whereas left-right (mass) asymmetry can be allowed for at a relatively low cost [12,16], the abandonment of axial symmetry is still too expensive in HF-applications to heavy nuclei. (For triaxial HF-calculations in light nuclei see, e.g. ref. [35].) The corresponding errors in the deformation energies can only be estimated from comparison with the results of SCM-calculations. Thus, in the ^{240}Pu results of Flocard et al. [7], the first and second barrier heights may be reduced by ~ 1 MeV and ~ 4 to 5 MeV due to the lack of non-axial and left-right asymmetric degrees of freedom, respectively.

For the same practical reasons, more than one constraint can hardly ever be included in full CHF calculations for heavy nuclei. Mainly two physical quantities have been constrained: 1) the quadrupole moment Q_2 [6-9, 15,16] which may be a reasonable fission mode up to the second barrier, and 2) the distance r between the two halves of the nucleus (i.e. the "nascent fragments") [12] which certainly is more appropriate beyond the saddle and especially around scission. Thus, real deformation energy surfaces have not been obtained with the CHF method, but rather their projections along a one dimensional path which is hoped to be close enough to some adiabatic fission trajectory. The question which constraint to choose in which portion of the deformation space can only be (approximately) answered using a lot of intuition and experience; its ultimate answer can, of course, only be given in the framework of dynamical calculations where the inertial mass tensor is taken into account [36].

g) Final remarks

To conclude this discussion of CHF calculations, we compile in Table I the various corrections, estimated according to a) - f) above, which have to be added to the fission barriers of ^{240}Pu obtained by Flocard et al. [7]. We see that after these corrections and ignoring the uncertainties in the force parameters themselves, the agreement with experiment is not too bad, if the prescription of an average pairing matrix element G proportional to the surface is used. With the constant gap Δ prescription, much too high barriers would result.

As to the results of Kolb et al. [12] shown in Figure 2, the corrections b) and f) do not apply (mass assymmetry was included and the Coulomb exchange energy taken in the statistical approximation). The truncation error should also be smaller here since a two-center basis was used. Thus, subtracting the spurious rotational energy of ~ 2-3 MeV,

TABLE I. FISSION BARRIERS OF ^{240}Pb OBTAINED BY FLOCARD ET AL. [7] AND SEVERAL ERROR ESTIMATES (ALL QUANTITIES IN MeV). EXPERIMENTAL RESULTS FROM Ref. [37]. RESULTS IN PARANTHESES ARE OBTAINED WITH A CONSTANT AVERAGE PAIRING GAP Δ

		E_A	E_B
	CHF, S III, G$\propto$surf. (Δconst.)	9 (11)	13 (21)
a)	spur. rotat. energy corr.	- 1	-2 to -3
b)	Coulomb-exch. energy corr.	$<$ + 0.5	+0.5 to +1
e)	truncation error	$<$ - 0.5	-2
f)	γ- and mass asymmetry energy	- 1	-4 to -5
c)	uncertainty in force parameters	several MeV	several MeV
	resulting barriers with S III	7 (9)	4-6 (12-14)
	experimental barriers	6.0 $\pm$ 0.3	5.35 $\pm$ 0.2

a second barrier of $\sim$ 4 to 7 MeV results, depending on the set of parameters. Note that a constant (average) gap was used in this caluclation, which thus leads to a lower result than the corresponding one of Flocard et al. [7]. The more recent result of Cusson and Kolb quoted in ref. [4] (Fig. 11), however, would also lead to a barrier of E_B of $\sim$ 13-14 MeV.

A similar result has now also been obtained in the newest Gogny-HFB calculations [16]. Together with the other results, this might indicate that an essential component is missing in the large-deformation behaviour of the effective forces in use.

Our conclusions should not be taken from a too pessimistic side: It is true that the experimental fission barriers are not yet well reproduced. On the other hand one should not forget that these CHF calculations represent a completely parameter-free (apart from the pairing problem) extrapolation from calculations where many ground-state properties of most stable nuclei are explained consistently with very few parameters of the effective interaction. As such, and considering the technical problems involved, they represent a remarkable progress.

We have clearly demonstrated that there is by far enough freedom in the force parameters to allow for a simultaneous inclusion of the correct barrier heights in a fit of the ground-state properties. It is also clear that this has to be done in the future - as well as it was necessary in the more phenomenological LDM plus shell-correction calculations. Such new fits in HF-calculations will, of course, require a lot of calculation time. It is therefore important to realize that some much more rapid, but still reasonably accurate approximations to the CHF method exist or are being developed, and will be valuable for the inclusion of

the large deformation behaviour in the selfconsistent description of nuclei with effective interactions. One purely microscopical approximation is discussed in the following subsection, others that make use of semiclassical methods will be presented in Sect. 4 .

Finally we should also mention the merit of the CHF calculations to have provided a purely microscopically based quantitative confirmation of the shell-correction approach. This aspect will be discussed in Sect. 3.1 below.

2.3. The Expectation-Value Method (EVM)

At the same time as the CHF calculations with Skyrme forces were developed, a non-selfconsistent, but microscopical approach was studied by Ko et al. [17]. This method consists in approximating the total binding energy by the expectation value of the two-body Skyrme Hamiltonian between Slater determinants built of eigenstates of a deformed Woods-Saxon (WS) potential. Practically it corresponds thus exactly to one iteration of a HF-calculation, using a suitably chosen (deformed) potential. In ref. [17], this potential was taken from a standard shell-correction calculation [38] with the generalized WS-Potential of ref. [31], using a two-dimensional (axially and left-right symmetric) family of nuclear shapes (c,h). (For details, see ref. [38].) The deformation parameters (c,h) play in this method the role of the constraint. The deformation energy surfaces obtained this way in ref. [17] for heavy nuclei had the correct shell structure (two saddle points, second isomer minimum). However, the mean part of the deformation energies was increasing too fast, leading to far too high fission barriers.

Recently, we proposed a new version of the EVM [18]. Two essential improvements over ref. [17] were made: 1) An effective mass $m^*(r)$ was included in the diagonalization of the WS-potential (it was put equal to the free nucleon mass in ref. [17]). 2) The parameters of the WS-potential (as well as effective mass and spin-orbit potential) were fitted to reproduce as well as possible the results of spherical HF calculations. (In this way no free parameters are left, those of the Skyrme force remaining fixed.) Thirdly, an improved relation was used to determine the basis deformation parameter q at each point (c,h) instead of the prescription of refs. [31,38].

The method thus consists of the following steps:

1) Fit the central nuclear potentials V(r), the effective masses $m^*(r)$ and the spin-orbit potentials W(r) obtained in a spherical HF-calculation by Woods-Saxon functions, such as to reproduce the correct half-value radii, surface thicknesses and mean values in the interior of the nucleus (independently for protons and neutrons).
2) Deform these WS-functions according to the prescription of ref. [31] along a suitable path in deformation space (c,h) (or any other given shape parametrization).
3) Diagonalize the one body-Hamiltonian (for each kind of nucleons)

$$\hat{H} = -\vec{\nabla} \cdot \frac{\hbar^2}{2m^*(\vec{r})} \vec{\nabla} + V(\vec{r}) - i\,\vec{\nabla} W(\vec{r}) \cdot (\vec{\nabla} \times \vec{\sigma})$$

compute the densities $\rho(r)$ and $\tau(r)$ and from them the total Skyrme energy. Minimize it with respect to the basis size parameter $\hbar\omega$ at each deformation. (This can be done analytically, see Vautherin, (1973), ref. [5].)

In order to compare the results to CHF calculations, the quadrupole moment Q_2 is easily computed at each point. We show such a comparison for ^{240}Pu in Figure 5 , taken from ref. [18]. The EVM curve was here obtained by

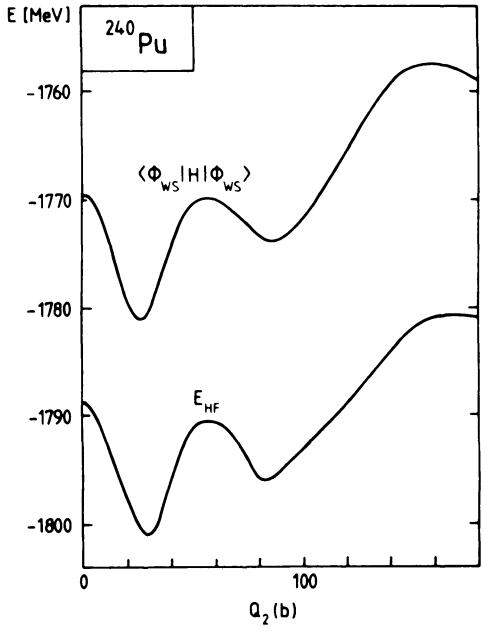

FIG.5. Fission barriers of ^{240}Pu obtained with the EVM (above) and the CHF method (below) using the force Skyrme III. A constant average pairing gap was used (from Ref. [18]).

minimizing the energy for each Q_2 with respect to the deformation parameters c and h. (The lowest path is not far from h=0 as in the results of shell-correction calculations [38].)

We see that up to the second barrier, the deformation energy obtained with this method reproduces the selfconsistent CHF result within ~ 1-2 MeV. (A constant average pairing gap $\tilde{\Delta}$ was used here.) Hereby, a factor of at least ~ 5 to 10 was saved in computation time. Similar results were obtained for other nuclei, too [18]. The lack of selfconsistency leads mainly to an almost constant shift of the deformation energy (here of ~ 20 MeV), the local minima and maxima being unaffected.

The error of ~ 1-2 MeV in the EVM results as compared to the CHF results is reasonably small in view of the various overall uncertainties, which we discussed above. (For the Skyrme force S IV, where the nuclear HF-potential has much larger oscillations in the interior than with S III, the discrepancies are larger, ~ 3-5 MeV [9].) The EVM is therefore an efficient tool for exploratory calculations in unknown regions of nuclei. It has been applied for an investigation of super-heavy nuclei [9], a result of which was shown in Figure 4 above.

Of course, this method requires some knowledge of the most important deformation degrees of freedom relevant for the desired application. It is therefore especially well suited in connection with a shell-correction calculation. If full selfconsistency is required, the EVM provides an excellent starting point for CHF-iterations. (As a rule, only ~ 2-5 iterations were required to obtain a well-converged energy.)

Note that in ref. [18], the Coulomb potential was not included in the diagonalization of the proton Hamiltonian $\hat{A}_p$. The Coulomb energy was thus treated fully in lowest order perturbation. Including a reasonable (e.g. LDM-) guess for the Coulomb potential in $\hat{A}_p$ should improve the method and might, in fact, remove most of the remaining smooth error.

The step 1) described above - although it is simple and straight forward - might be a little cumbersome, in particular if many different nuclei and force parameters are investigated. It is hoped that the potentials V(r), W(r) and m*(r) may soon be obtained in semiclassical variational calculations. In fact, for spherical nuclei such investigations have already been performed [39,40] and the EVM was applied there with a similar success.

3. THE SHELL-CORRECTION METHOD (SCM)

Swiatecki and Myers [41, 42] emphasized the close connection between the shell-effects in the nuclear binding energies and the non-uniformities of the single-particle spectra of the shell model. In the LDM fits of ref. [42], the energy shell-corrections were phenomenologically parametrized as functions of nucleon masses and deformation.

Strutinsky [3] gave the first microscopical definition of the shell-correction δE, pointing out that it can be extracted from the sum of occupied levels ε_i^{SM} of the (deformed) shell model (separately for neutrons and protons):

$$\delta E_{n,p} = \sum_{i=1}^{N(Z)} \varepsilon_i^{SM} - \left\langle \sum_{i=1}^{N(Z)} \varepsilon_i^{SM} \right\rangle_{aver} \tag{3.1}$$

Here, the second term is a suitably averaged part (see Sect. 3.3) of the single-particle sum. The ansatz

$$E_{tot} = E_{LDM} + \delta E \quad (\delta E = \delta E_n + \delta E_p) \tag{3.2}$$

was justified by Strutinsky [3] from HF-theory using a (formal) decomposition of the HF density matrix ρ^{HF} into a smooth part $\bar{\rho}$, which is responsible for the averag (LDM) energy, and a fluctuating part $\delta\rho$, which to lowest order is contained in δE:

$$\rho^{HF} = \bar{\rho} + \delta\rho \tag{3.3}$$

(For simplicity we omit indices for neutrons and protons and consider only one kind of nucleons.)

The shell-correction method (SCM) [3] - on the other side of the Atlantic Ocean also called "microscopic-macroscopic method" - is based on eqs. (3.1,3.2) and the use of phenomenological LD models (e.g. ref. [42]) and deformed shell-model potentials (e.g. of Nilsson [43]). It has initiated a revolutionary development in the understanding of the shell structure in deformed nuclei. In particular, it led to the first qualitative and quantitative explanation of the fission isomers [44] in terms of the by now famous double-humped fission barrier (see also refs. [45, 46]). It is not our aim here to review the numerous calculations made using the SCM with different macroscopic and microscopic ingredients; for that we refer to some representative review articles [38, 47] where many details and applications can be found.

Presently, we shall rather be concerned with the numerical verification of what has been termed the "Strutinsky energy theorem" [48]. Later in this section, some extensions of the method and the technical ways of performing the averaging in eq. (3.1) shall be discussed.

3.1 Numerical tests of the SCM within the HF-framework

a) The Strutinsky energy theorem

The original derivation of eq. (3.2) from HF-theory by Strutinsky [3] has been discussed and reformulated by numerous authors [38,48-52]. Expanding the HF-energy (in matrix notation)

$$E_{HF} = \mathrm{tr}\, T\rho^{HF} + \tfrac{1}{2}\,\mathrm{tr}\,\rho^{HF}\left(\mathrm{tr}\,\rho^{HF}\bar{v}\right) \tag{3.4}$$

where $\bar{v}$ is the (antisymmetrized) two-body matrix element of the effective interaction, into a Taylor series around the average part $\bar{\rho}$ in eq. (3.3), one can easily show using perturbation theory arguments that

$$E_{HF} = E[\rho^{HF}] = E[\bar{\rho}] + \delta E_1 + O[(\delta\rho)^2] \tag{3.5}$$

where

$$E[\bar{\rho}] = \mathrm{tr}\, T\bar{\rho} + \tfrac{1}{2}\,\mathrm{tr}\,\bar{\rho}\left(\mathrm{tr}\,\bar{\rho}\,\bar{v}\right) \tag{3.6}$$

and δE_1 is the first-order shell-correction, which can be written as in eq. (3.1). Using the occupation numbers n_i^{HF} and $\tilde{n}_i$ (see Sect. 3.3), it reads

$$\delta E_1 = \sum_i \hat{\varepsilon}_i\, n_i^{HF} - \sum_i \hat{\varepsilon}_i\, \tilde{n}_i = \sum_i \hat{\varepsilon}_i\, \delta n_i \tag{3.7}$$

Hereby $\hat{\varepsilon}_i$ are the eigenvalues of the averaged HF-Hamiltonian $\bar{H}$ defined by

$$\bar{H} = H_{HF}[\bar{\rho}] = \left.\frac{\partial E_{HF}}{\partial \rho}\right|_{\bar{\rho}} \tag{3.8}$$

The point is that the term δE_1 in eq. (3.5), and with it the sum of occupied levels $\hat{\varepsilon}_i$, contains all contributions of first order in $\delta\rho$. This is true for any density dependent effective interaction, in contrast to the findings of ref. [48] where the rearrangement terms were not correctly included in the definition of the average field (see the detailed discussions in refs. [51,53]).

The practical shell-correction approach consists in the following basic assumptions (see also refs.[3,52]):

1. The average HF energy $E[\bar{\rho}]$ (3.6) can be approximated by a phenomenological LDM energy E_{LDM}:

$$E[\bar{\rho}] \Longrightarrow E_{LDM} \tag{3.9}$$

2. The levels $\hat{\varepsilon}_i$ of the averaged HF-Hamiltonian $\bar{H}$ eq. (3.8) can be approximated by shell-model levels ε_i^{SM}:

$$\sum_i \hat{\varepsilon}_i\, \delta n_i \Longrightarrow \sum_i \varepsilon_i^{SM}\, \delta n_i \tag{3.10}$$

3. The "shell-correction expansion" eq. (3.5) is converging fast enough, so that the terms of second and higher order in $\delta\rho$ can be neglected.
4. In the points 1. and 2. it is assumed that $\bar{\rho}$ and the corresponding average quantities derived from it are smooth as functions of nucleon numbers and of deformation.

As a particular point of criticism, the argument was made [54] that in the identification (3.10), a constraint should be added to the shell-model potential, since a constraint is also necessary in the HF-calculation to obtain points away from local minima. It was shown, however, in refs. [49, 52,53,55] that this is not true. This misunderstanding was based, in fact, upon the erroneous assumption that all first-order shell-effects should be contained in the sum of occupied Hartree-Fock levels ε_i^{HF} [50,54] (which led to much too negative conclusions about the validity of the SCM [50,54,56]). That this is not so, is easily seen noting that

$$\delta E_1^{HF} = \sum_i \varepsilon_i^{HF} n_i^{HF} - \sum_i \varepsilon_i^{HF} \tilde{n}_i \qquad (3.11)$$

does contain all first-order contributions in $\delta\rho$. (δE_1^{HF} differs from δE_1 (3.7) only to second order in $\delta\rho$.) Since the second sum in eq. (3.11) also contains an oscillating term linear in $\delta\rho$ (which was actually observed in ref. [50]!), this term is missing - or rather double-counted - in the sum of the occupied HF-levels ε_i^{HF}.

Before turning to numerical tests of the energy theorem (3.5), we remark that pairing effects are usually included in the BCS-approximation in the SCM (see, e.g. refs. [3,38]). A derivation of the energy theorem within the HFB-theory was given by Kolomietz [57].

b) Numerical tests.

At the time when the SCM was developed, no reliable HF-calculations were available to test the above assumptions. Bunatian et al. [51] exploited the fact that the second-order shell-correction δE_2 (containing all terms quadratic in $\delta\rho$ in the expansion (3.5)) can be expressed explicitly in terms of the two-body interaction or the scattering amplitude (see also ref. [38]). They calculated the term δE_2 in perturbation, using different parameter sets of Migdal's universal quasiparticle amplitude [58] and Woods-Saxon single-particle wavefuntions. In their results for a series of spherical nuclei around ^{208}Pb, the quantity δE_2 did not vary more than by $\pm \sim 1$ MeV around a mean value of ~ 2 MeV.

Another preliminary test was performed by Bassichis et al. [59], comparing first-order CHF-results for ^{108}Ru [50] obtained with the Tabakin potential [60] to some ad hoc fits of Nilsson levels and LDM parameters. Their conclusions cannot be taken on their face values due to the lack of self-consistency and the omission of pairing effects in these investigations.

The first consistent test of the energy theorem (3.5) was presented at the Rochester fission symposium by Brack and Quentin [55]. There, CHF-calculations were performed mainly for rare-earth nuclei with the Skyrme force S III. Later, these tests were extended in refs. [61-63] for light and heavy nuclei, using also the Skyrme force S II and the Negele-DME force [23] (see also refs. [4,19,53]). In these calculations, the average density matrices $\bar{\rho}$ were calculated with the Strutinsky averaging procedure, using everywhere the local plateau condition (see Sect. 3.3), so that no single free parameter was used. The averaging of ρ was done either once on top of the converged CHF results [55,61] or self-consistently in each iteration [62,63].

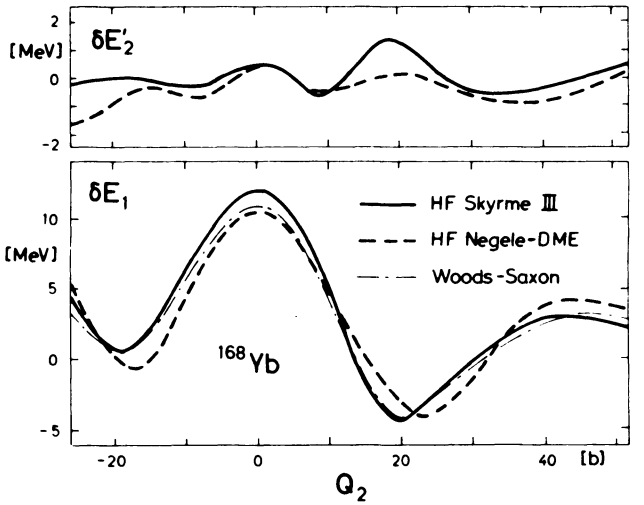

FIG. 6. First-order (δE_1) and sum of higher-order shell-corrections ($\delta E_2'$) obtained for ^{168}Yb with the forces S III and Negele-DME using the shell-correction expansion (3.5) of the HF energy [62]. The shell-correction δE_1 obtained from a Woods-Saxon potential is shown for comparison. Note that the scale for $\delta E_2'$ is twice as large as that for δE_1.

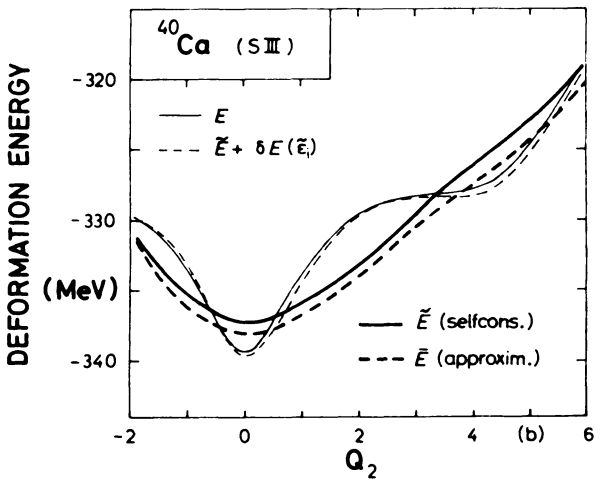

FIG. 7. Deformation energies for ^{40}Ca obtained with the force S III [61]. Thin solid line: HF energy. Heavy solid line: self-consistently averaged energy. Heavy dashed line: energy, averaged once after HF-iteration. Thin dashed line: 'Strutinsky' approximation to HF energy, differing everywhere less than by 0.5 MeV from the latter.

The quantities $E[\rho]$ and δE_1 were then calculated directly according to eqs. (3.6), (3.7), and the sum of all second and higher order terms was obtained inclusively by the difference

$$\delta E'_2 = E_{HF} - E[\bar{\rho}] - \delta E_1 \qquad (3.12)$$

Pairing correlations were included consistently in the BCS-uniform gap method [3,38]. For details of the calculations, see refs. [55,62].

The main results of these investigations can be summarized as follows:

1. The shell-correction series (3.5) indeed converges very rapidly; the sum $\delta E'_2$ of higher order corrections is (for $A \gtrsim 100$) of the order $\sim$ 1-2 MeV and does not oscillate by more than $\sim \pm$ 1 MeV (both as function of deformation and nucleon number).
2. The first-order shell-correction δE_1 depends little on the effective interaction used[1] (this need not be so for $E[\bar{\rho}]$!). It is furthermore well reproduced (within $\sim$ 1-2 MeV) by a phenomenological (Woods-Saxon) potential. (See Fig. 6 below.)
3. The average energy $E[\bar{\rho}]$ (3.6) has the properties required for a LDM energy: it is smooth and has its minimum at spherical symmetry. If spurious energies and truncation errors are subtracted (see Sect. 2.2), it can well be fitted with suitably chosen LDM parameters. (In particular, the results extracted from the Skyrme III force were closely reproduced by the 1966 parameters of Myers and Swiatecki [42]), see refs. [55,61].) These results may also be viewed as a microscopical derivation of the LDM, which in itself is interesting.
4. An optimal convergence of the series (3.5) is reached, if the average densities ρ are determined selfconsistently. (This has been suggested independently by Tyapin [66] and further discussed by Strutinsky [52,67].) It was achieved in refs. [61-63] by averaging ρ in each step of the iteration, so that the quantities ρ, $E[\bar{\rho}]$ and $\bar{H}$ after convergence became selfconsistent. It was found, then, that $\delta E'_2$ is less than $\sim$ 0.6 MeV in magnitude at all deformations, even in such light nuclei as ^{16}O and ^{40}Ca. (See also Fig. 7 below.)
5. In light nuclei ($A \lesssim 40$), if the averaging of $\bar{\rho}$ is not done selfconsistently, $\delta E'_2$ is up to $\sim$ 3-4 MeV and of the same order as δE_1.
6. The sum of all oscillating terms is also reasonably well reproduced (to within $\sim$ 1 MeV) by the shell-correction δE_1^{HF} eq. (3.11) [62]. This had also been noted by Krieger and Wong [64].

We illustrate these results in Figs. 6 and 7. The first-order shell-correction δE_1 and the sum of all higher-order terms $\delta E'_2$ are shown for ^{168}Yb in Figure 6 (from ref. [62], Trieste 1975). The forces Skyrme III and Negele-DME were used. They lead to almost identical results (within $\sim$ 1-2 MeV), although the total energy $E[\bar{\rho}]$ is different by several MeV at larger deformations for these two forces [61]. We see also that the resulting δE_1 is well reproduced by the shell-correction obtained from a Woods-Saxon potential with the same Q_2-deformation [38]. (No adjustment was made of the W-S parameters!) Note the correlations between the oscillations in δE_1 and $\delta E'_2$, which seem to suggest that neglecting $\delta E'_2$ would affect differences between stationary points of the total energy surface (e.g. barrier heights) only by $\sim$ 1 MeV.

In Figure 7, deformation energies are shown for the nucleus ^{40}Ca (from ref. [61], Paris 1975), obtained with S III. The once averaged ($\bar{E}$) and selfconsistently averaged($\bar{\bar{E}}$) energies are shown to differ by $\sim$ 1-2 MeV; they

[1] Apart from the spin-orbit force, see Section 2.2c and Fig. 4.

are both perfectly smooth. The approximation $\tilde{E} + \delta E(\tilde{\varepsilon}_i)$, where the shell-correction (3.7) is now evaluated in terms of the eigenvalues of the self-consistent average field, is very close ot the HF energy E at all deformations. This implies that the sum $\delta E'_2$ of higher order corrections is everywhere smaller than ~ 0.5 MeV. The same was found also for medium and heavy nuclei [62,63]. We show the result for ^{40}Ca here because it demonstrates that the decomposition of the HF energy into a LD and a shell-correction part works even for very light nuclei (including ^{16}O [62]), which might not have been expected a priori.

Similar investigations were made by Bassichis et al. [65] along a program outlined in ref [50] and using the earlier HF-results for ^{108}Ru [50] mentioned above. However, they used an inconsistent averaging of the density matrix (without curvature-corrections) which, in fact, includes some excitation energy. Consequently, their results depend strongly on the averaging width. Disregarding this fact, they can be said to agree well with our above results.

c) Discussion of results and conclusions

We should not forget that the above investigations only can test the validity of the SCM within the HF-framework, i.e. to the extent that nature can be replaced by HF-claculations. The effects of correlations are therefore not included, or only as far as they can be mocked up by the effective force used in the HF-approximation. (For extensions beyond HF, see Sect. 3.2 below.).

As we have said in Sect. 2, however, the groundstate energies of most nuclei are very well described in the HF-approximation using the present-day effective interactions. We have also seen that, at least in principle, the deformation energies are reasonably well described. Hereby we emphasize that some of the most pertinent uncertainties of the CHF method discussed in Sect. 2.2, namely the spurious energy contributions and the truncation effects, essentally cancel out in the shell-correction δE_1. As to the uncertainties in the parameters of the (central) force, they are mostly taken care of in the SCM by the LDM parameters which are adjusted to fit experimental results. (The uncertainties in the spin-orbit force and the deformation dependence of the pairing parameters, however, mainly persist in the SCM.)

Keeping this in mind, we may draw the following conclusions from the above HF-tests of the SCM:

1. The rapid convergence of the shell-correction expansion (3.5) has been established. The second and higher-order terms which are neglected in the practical SCM, oscillate not more than $\sim \pm 1$ MeV. Their mean value depends somewhat on the definition of the average part $\bar{\rho}$ of the density matrix and is minimized if the averaging is done selfconsistently.
2. In transitional nuclei, where the first-order shell-correction δE_1 is small, the higher order terms might not be negligible, especially if finer details such as e.g. prolate-oblate energy differences are considered. The same is true in light nuclei if LDM and shell-model parameters are not determined selfconsistently.
3. The first-order shell-correction δE_1 is a rather stable quantity. It is little sensitive to the effective forces used (apart from the spin-orbit part!) and depends also not much on the selfconsistency of the treatment (see also Sect. 2.3).
4. The average part of the HF-energy is mainly determined by the properties of the force; hereby the selfconsistency is important.
5. Phenomenological LD models can in principle fit the average HF-energies well. For the validity of the SCM, it is essential how good such a fit

is and whether the average (shell-model) potential is consistent with the LDM parameters. This is, however, not easily checked in actual cases.

6. A particular case of an inconsistency between shell-model potential and LD-energy may be the Pb-anomaly. Since the (selfconsistent) shell-correction δE_1 extracted from Skyrme-HF calculations for ^{208}Pb is in agreement with the value found from a Woods-Saxon potential [38] (~ -18 to -20 MeV), the anomaly must be due to the LDM parameters used in the SCM calculations. (See also Sect. 3.5.)
7. We may invert the content of the points 3 and 4 above and state: A selfconsistent treatment using effective forces is only necessary for obtaining the average parts of deformation or binding energies. Shell effects can be treated in perturbation, if selfconsistent LD and shell-models are used. (This may be done either with the SCM or with the EVM discussed in sect. 2.3). This gives a strong renewed motivation for the improvement of semiclassical methods, as will be discussed in Sect. 4.
8. The possibilities of improving the phenomenological shell-model potentials towards selfconsistency in the above average (statistical) sense was discussed by Strutinsky in ref. [52], where also explicit correction formulae were derived. (See also Strutinsky's review talk [67].) These have, however, not yet been used in numerical calculations.

3.2 Extensions of the SCM

So far, all our considerations concerned nuclei without excitations. Two extensions of the SCM have been developed which allow to include excitations.

One of them is the treatment of intrinsic excitations within the statistical model [68,69]. It has been widely used in calculations of entropies and level density parameters [70]. The Strutinsky-renormalization eq. (3.2) is thereby usually made at temperature T = 0. The assumption implicitly made is then that both LDM and shell-model parameters do not depend on the excitation (temperature) of the nucleus. The temperature-dependence of the LDM parameters has been studied [71] and found to be rather weak. The effect of a finite temperature on the (selfconsistent) shell-model potential was investigated in HF-calculations using Skyrme forces by two groups [72,73]. Hereby not the intrinsic energy, but the thermodynamical potential

$$\Omega = \langle H \rangle - TS - \lambda \langle N \rangle$$

is minimized. The main result of these calculations is that, indeed, changes in the selfconsistent potential are negligible. The HF-energies ε_i^{HF} depend very little on the temperature up to T ~ 5-6 MeV. In particular, the physically relevant quantity, namely the entropy S as a function of the excitation energy E*, is extremely well reproduced when calculated from the "cold " spectrum (evaluated at T=0). (This result is qualitatively understood by extending the energy theorem (3.5) to finite temperatures, see ref. [72].) Together with the results quoted above in Sect. 3.1, this shows that the usual, non-selfconsistent thermodynamical-statistical approach [70] is well justified. (Strictly speaking, the conclusions of refs. [72,73] are only valid to the extent that the parameters of the effective interaction themselves do not depend on the temperature. As long as T is much smaller than the Fermi energy, this assumption should however be well fulfilled.)

The idea of renormalizing the grand canonical partition function Φ, from which all thermodynamical quantities can be derived consistently, was put forward by Gottschalk and Ledergerber [74]. They derived a shell-correction expansion of Φ which is of the same spirit as that of the HF-energy in eq. (3.5). The problem here is how to determine the "empirical" Φ_{LDM} by which the average part of the shell-model quantity is replaced. In ref. [74] this was done in terms of an average level density which, however, cannot be determined uniquely.

Another extension is that for nuclei with large angular momentum, which is done by minimizing the expectation value of the cranking Hamiltonian H_ω :

$$H_\omega = H - \omega J_x$$

for a rotation about, say, the x-axis. We do not need to give references to the extensive high-spin studies done by several groups over the past five years; they will be reviewed and discussed in the paper of the Lund group [75]. The selfconsistency of these calculations has not been tested so far. Due to the loss of time reversal symmetry of the cranking Hamiltonian, the corresponding HF-calculations become extremely time consuming for heavy nuclei. (For some cranked HF-calculations for ^{20}Ne, see e.g. ref. [76].) The problem of selfconsistency should, however, be kept in mind when using cranked shell-correction calculations for the prediction of yrast traps, which might depend rather crucially on the shell-model and LDM parameters.

We finally mention an important extension of the SCM which allows to go beyond the HF framework. Bunatian et al. [51] showed that in the Fermi liquid theories of Landau and Migdal (see ref. [58]), the first-order shell correction to the total nuclear binding energy can be cast in the same form as eq. (3.7), where this time ε_i are the quasiparticle energies. This has, however, not been used for actual shell-correction calculations so far [2] (apart from the estimation of the second-order terms in ref. [51]), although this would be interesting because it allows the inclusion of correlations (cf. also Dietrich's summary talk of the Rochester conference [77]).

3.3 The energy averaging method and alternative suggestions

a) Strutinsky energy averaging and the plateau condition

A lot has been published about the method which Strutinsky originally proposed in ref. [3] for the definition of the average part of the single-particle energy sum in eq. (3.1). This method of energy averaging was reformulated in various ways [38,49-51, 78-80] and repeatedly criticized [81] in connection with the so-called plateau-problem. Due to the abundant literature, we will be brief in discussing the method and emphasize those aspects from which new insight has been gained over the past six years.

According to the original prescription [3], the smooth part of the single-particle energy sum is expressed in the following way (for one kind of nucleons, say neutrons):

$$\left\langle \sum_{i=1}^{N} \varepsilon_i \right\rangle = \tilde{E} = \int_{-\infty}^{\lambda} E\,\tilde{g}(E)\,dE \qquad (3.13)$$

The average level density $\tilde{g}(E)$ in eq. (3.13) is obtained by folding the level spectrum ε_i over an energy range γ:

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[2] See, however, Werner, E., et al., paper IAEA-SM-241/C26, these Proceedings.

$$\tilde{g}(E) = \frac{1}{\gamma}\sum_i f\left(\frac{E-\varepsilon_i}{\gamma}\right) P_M\left(\frac{E-\varepsilon_i}{\gamma}\right); \quad \int_{-\infty}^{\lambda} \tilde{g}(E)\,dE = N \tag{3.14}$$

The (symmetric) folding function f(x) - usually taken as a Gaussian - may be of a rather general form, provided that it falls off sufficiently fast for large x [80]. The so-called curvature-correction polynomial $P_M(x)$ ensures that any smooth component of the level density, which is equal to a polynomial of order M in energy, is identically reproduced by the averaging procedure (3.14) independently of the value of γ and the precise shape of the averaging function f(x). Introducing occupation numbers $\tilde{n}_i$ by

$$\tilde{n}_i = \int_{-\infty}^{(\lambda-\varepsilon_i)/\gamma} f(x)\,P_M(x)\,dx \; ; \quad \sum_i \tilde{n}_i = N \tag{3.15}$$

one can rewrite the average energy $\tilde{E}$ (3.13) in the form [80,38]

$$\tilde{E} = \sum_i \varepsilon_i \tilde{n}_i + \gamma\,\frac{\partial \tilde{E}}{\partial \gamma} \tag{3.16}$$

For a harmonic oscillator potential, where the true average level density is a parabola (for E > 0), the energy $\tilde{E}$ (3.16) is independent of γ for $M \geq 4$ as soon as γ is somewhat larger than $\hbar\omega$, the level spacing, provided that $\lambda \gg \hbar\omega$ and sufficiently many levels are included above the Fermi energy λ. The curve $\tilde{E}(\gamma)$ thus shows an ideal "plateau". This also works approximately for the Nilsson-potential [46,78]. In more realistic potential wells, however, the average part of the level density is no longer a polynomial in E. Then the infinitesimal plateau conditions must be fulfilled

$$\left.\frac{\partial \tilde{E}}{\partial \gamma}\right|_{\gamma_0} = 0 \; ; \quad \left.\frac{\Delta \tilde{E}(\gamma_0)}{\Delta M}\right|_{M_0} = 0 \tag{3.17}$$

which corresponds to fitting the (true) average level density locally by an optimal Taylor expansion up to order M_0 [80]. In most cases, the conditions (3.17) can be fulfilled with values of the order

$$\gamma_0 \simeq (1.2 - 1.6)\,\hbar\Omega \; ; \quad M_0 \simeq 6 - 10 \tag{3.18}$$

where $\hbar\Omega$ is the average distance of the main shells in the spectrum ε_i.

Most of the trouble reported [81] was due to neglecting the simultaneous fulfilment of both conditions in eq. (3.17). Another problem is that of the contributions from states in the continuum for the case of finite depth potentials. The usual praxis of including the discrete levels obtained by diagonalisation of these potentials in a harmonic oscillator basis [38,79,80] is rediscussed in the review paper of Strutinsky [67]; we need therefore not discuss it here. We just mention that Ross and Bhaduri [82] showed that rather good plateaux can be obtained for a spherical Woods-Saxon potential, when sufficiently many resonances are included in the continuum region. On the other hand, the discrete states obtained with a typical restricted basis in the lower continuum (up to ~ 10 - 15 MeV in heavy nuclei) rather closely reproduce the positions of the resonances (see, e.g., ref. [72]).

With the plateau conditions (3.17) approximately fulfilled, the second term in eq. (3.16) can be omitted and the shell-correction δE then takes the form of eq. (3.7).

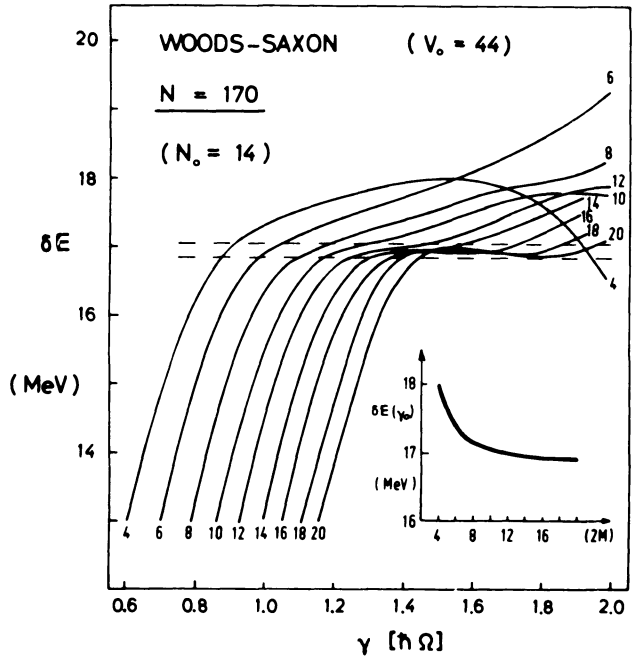

FIG.8. Shell-correction δE in a situation of high local level density (spherical Woods-Saxon potential without spin-orbit term, large positive value of δE), plotted versus averaging range γ for various orders 2M of the curvature-correction polynomial. Note that for $2M \gtrsim 12$, a rather well-defined value $\delta E \cong (17 \pm 0.15)$ MeV is found. The insert shows the stationary points (or points of deflection) $\delta E(\gamma_0)$ versus 2M. Using a typical standard value $\gamma \simeq 1.2\ \hbar\Omega$ and M = 4 or 6, the error made is still less than 1 MeV (from Ref. [83]).

In ref. [83], the plateau conditions (3.17) were carefully studied for a spherical Woods-Saxon potential (without spin-orbit term). The main results found there may be summarized as follows:

1. For medium and heavy nuclei, $A \geq 100$, the conditions (3.17) can usually be fulfilled up to an uncertainty in $\tilde{E}$ of $\Delta\tilde{E} \leq 1$ MeV.
2. For smaller particle numbers ($N \leq 50$) and in cases where the distance of the Fermi level λ from the continuum is smaller than $\hbar\Omega$, the uncertainty may be as large as $\Delta\tilde{E} \approx$ 1-2 MeV.
3. Difficulties are sometimes met in situations where the local level density at the Fermi energy is large, i.e. when δE is maximal (see also refs. [80,81]). In these cases it may help to go to rather large values of the curvature-correction order M ($\sim$ 14 - 16) to obtain a unique value of $\tilde{E}$. This is illustrated in Figure 8.
4. The optimal values γ_0 and M_0 are not necessarily smooth functions of the nucleon numbers N,Z. The error made in $\tilde{E}$ is thus discontinuous and rather random. The safest procedure is to determine γ_0 and M_0 for a couple of cases in a given region and then to fit a smooth interpolation formula γ_0 (N or Z) for systematic shell-correction calculations (see also ref. [80]).

5. In realistic cases, especially when deformations and spin-orbit term are included which tend to remove the largest degeneracies of the spectra ε_i, the uncertainty in $\tilde{E}$ should never be larger than $\Delta\tilde{E} \approx 1\text{-}1.5$ MeV, even if fixed standard values such as $\gamma_0 \approx 1.2$ $\hbar\Omega$ and $M_0 = 6$ are used.

b) Alternative methods

Mainly with the intention of overcoming the above-mentioned continuum and plateau problems, several alternative methods have been suggested to extract the smooth part of the sum of occupied levels. We shall here only discuss those methods which are of practical use or which have been studied in sufficient detail.

A modified energy averaging procedure with asymmetric smoothing functions, proposed by Bunatian et al. [51], turned out not to lead to unique values of $\tilde{E}$ [84].

The so-called temperature-method, proposed by Ramamurthy et al. [85], makes use of the fact that shell effects disappear at large temperatures. The idea is thus to calculate the (intrinsic) energy E(T) and the entropy S(T) as function of temperature T using the thermodynamical-statistical model. (For details see refs. [85-88].) For temperatures larger than $T_0 \sim 2\text{-}3$ MeV (k=1), the shell effects disappear (see also refs. [72,73]); E(T) and S(T) then become smooth functions $\tilde{E}(T)$ and $\tilde{S}(T)$, respectively. Thus, calculating $\tilde{E}$ and $\tilde{S}$ at same finite temperatures

$$T_o < T \ll |\lambda - V_o|$$

and extrapolating these functions back to zero temperature, one may isolate the energy shell effect at T = 0:

$$\Delta E_o = \sum_{i=1}^{N} \varepsilon_i - \tilde{E}(o) \qquad (3.19)$$

It was numerically verified that ΔE_0 is practically equal to the Strutinsky shell-correction δE (3.7) [85,87,88]. One important detail was to realize [85] that corrections to the asymptotic expansions of $\tilde{E}(T)$ and $\tilde{S}(T)$, containing the local derivatives of the average level density at the Fermi energy $\tilde{g}'(\lambda)$, $\tilde{g}''(\lambda)$, ..., must be included in order to obtain unique values of ΔE_0. Ignoring these corrections, one just obtains the "back-shifted Fermi gas model" results [86] (see also the discussion in the contribution of Junker et al. to this conference [89]). Including the terms containing derivatives of $\tilde{g}(E)$ corresponds exactly to the curvature-correction in the Strutinsky averaging method, as shown analytically in refs. [57,90]. We see this also by comparing the equation (3.16) for the Strutinsky-averaged energy $\tilde{E}$ with the equation for the free energy F:

$$\begin{array}{ccccc} \tilde{E} & = & \sum_i \varepsilon_i \tilde{n}_i & + & \gamma \dfrac{\partial \tilde{E}}{\partial \gamma} \\ \updownarrow & & \updownarrow & & \updownarrow \\ F & = & \sum_i \varepsilon_i n_i(T) & + & T \dfrac{\partial F}{\partial T} \end{array}$$

Both equations are identical in their form. The important physical difference is, however, that in the thermodynamical equation, $-\partial F/\partial T = S > 0$ for $T > 0$, whereas $\partial\tilde{E}/\partial\gamma$ is always zero (see eq. 3.17). Due to the curvature-corrections built into the $\tilde{n}_i$, the Strutinsky averaging is thus a "cold-averaging" (with zero "entropy" $\partial\tilde{E}/\partial\gamma$), in contrast to the temperature averaging which brings excitation energy into the system.

We see thus that the backward-extrapolated value $\tilde{E}(0)$ in eq. (3.19) is equal to the Strutinsky averaged energy $\tilde{E}$ of eqs. (3.13, 3.16), and the two methods are completely identical - at least in principle. Practically, some minor differences occur due to the different technical ways of obtaining $\tilde{E}$ resp. $\tilde{E}(0)$. In some cases the Strutinsky $\tilde{E}$ is found less accurately than $\tilde{E}(0)$ with the temperature method, and vice versa [91]. Both methods do depend on the continuum contributions for finite potentials. Their results agree within the overall uncertainty of $\lesssim$ 1 - 1.5 MeV quoted above. A combination of the two methods which diminuishes somewhat the influence of the continuum states was recently proposed by Ofengenden et al. [92].

A different approach is replacing in eq. (3.13) the averaged level density $\tilde{g}(E)$ by an asymptotic expression $g_{AS}(E)$ valid for large values of E, i.e. for large nucleon numbers. The problem of finding $g_{AS}(E)$ for a given potential goes back to Weyl in 1911 [93] and has repeatedly been taken up again [78,94]. The use of $g_{AS}(E)$ for calculating the shell-correction was proposed in 1969 by Gaudin and Sajot [95] and applied for finite and infinite square-well potentials. In ref. [80], the case of an infinite box of cubic shape was investigated. It was found that with a careful use of the conditions (3.17) in the Strutinsky averaging (see point 4 in sect. 3.3a), the values for δE obtained by both methods agree within $\leq$ 0.2 MeV for $N \gtrsim 40$.

Bohr and Mottelson [69] proposed the direct asymptotic expansion of the single-particle sum:

$$\sum_{i=1}^{N} \varepsilon_i = E_{AS}(N) + \delta E$$

$$E_{AS}(N) = a_v N + a_s N^{2/3} + a_c N^{1/3} + a_o + \ldots . \qquad (3.20)$$

This is completely equivalent to the use of $g_{AS}(E)$ in eq. (3.13), but demonstrates the analogy with the LDM-expansion of binding energies more readily. The coefficients in $E_{AS}(N)$ are not easily evaluated in general. The volume term a_v is given in the Thomas-Fermi model [69], and the surface coefficient a_s can be related to the phase shifts of the bound state wave functions (due to the surface) in case of a local potential (no spin-orbit term!) [96]. The remaining coefficients must, however, be determined numerically by fitting $E_{AS}(N)$ to the exact sums of occupied ε_i for large values of N. This method was carefully investigated by Sobicewski et al. [83] for a local, spherical Woods-Saxon potential. The asymptotic series was found not to converge fast enough to allow for a unique determination of $E_{AS}(N)$ for realistic particle numbers. When chosen to fit the Strutinsky-averaged values $\tilde{E}(N)$ for very large N, however, agreement of E_{AS} and $\tilde{E}$ within $\leq$ 1 MeV was found for $N \geq 40$. Fulfilment of the stationary conditions (3.17) for E was important here, too (see also the discussion in sect. 3.3a above). This result is interesting because E_{AS} only depends on occupied states, thus demonstrating the correctness of the continuum treatment in the Strutinsky averaging. The method of the asymptotic expansion in itself is not able to give unique values of shell-corrections; in particular for potentials with spin-orbit terms and deformed shapes, where the phase shifts cannot be given analytically, it is not practically applicable.

The most successful alternative to the Strutinsky averaging, which is free from contributions of unoccupied states and is applicable for realistic deformed potentials, is the semiclassical partition function method proposed by Bhaduri and Ross [97] and further developed by Jennings and

Bhaduri [98,99]. It makes use of a semiclassical expansion of the partition function which goes back to Wigner and Kirkwood [100]:

$$Z(\beta) = Z_{CL}(\beta)\left\{1+\hbar^2\chi_2(\beta)+\hbar^4\chi_4(\beta)+\ldots\right\} \qquad (3.21)$$

In eq. (3.21), β is the inverse temperature (here simply treated as a mathematical variable); $\chi_n(\beta)$ are coefficients which depend on the potential and its first n gradients; and $Z_{CL}(\beta)$ is the classical partition function. By inverse Laplace transforming term by term of eq. (3.21), one obtains the smooth part of the level density g(E); the first (classical) term yielding the Thomas-Fermi result $g_{TF}(E)$. Correspondingly one obtains the particle number and the average single particle energy sum in the form

$$\begin{aligned} N &= N_{TF} + N_2 + N_4 + \ldots \\ E_{ETF} &= E_{TF} + E_2 + E_4 + \ldots \end{aligned} \qquad (3.22)$$

where the indices refer to the order of the corresponding terms in eq. (3.21) ($E_{TF} = E_{CL}$, etc.). For details of this method, we refer to refs. [98 - 101]. Since semiclassical corrections to the Thomas-Fermi expressions are evaluated here, the method is also referred to as the extended Thomas-Fermi (ETF) model; identical results can also be derived by other techniques [102,103]. The series for E_{ETF} (3.22) was shown in ref. [101] to converge very rapidly for realistic Woods-Saxon potentials; the term E_4 is of order ~ 1 MeV (for each kind of particles). The energy E_{ETF} can thus easily be evaluated to at least the same accuracy as the Strutinsky-averaged quantity $\bar{E}$. Hereby, the spectrum ε_i need not be known and only the classically allowed region $V(r) \leq \lambda$ is used to evaluate E_{ETF}.

The close connection between the Strutinsky energy averaging and WKB- or ETF-like methods was pointed out early [3,38,103]. In ref. [80] it was shown analytically that for a (deformed) harmonic oscillator potential, E_{ETF} and $\bar{E}$ are identical (independently of the exact shape of the averaging function f(x) in eq. (3.14)). Jennings [98,99] demonstrated the equivalence of the two methods for any (smooth) infinite potential, provided that a plateau can be found in the Strutinsky averaging. For realistic Woods-Saxon potentials, including spin-orbit term and deformations relevant for fission, the two methods have been compared carefully in ref. [101]. In all cases, E_{ETF} and $\bar{E}$ agree within $\leq$ 1 - 1.5 MeV, thus within the overall uncertainty of either method. This result not only demonstrates the complete equivalence of the two methods in the most general case; it also confirms the standard practice of including unbound discrete states in the lower continuum region. (In fact, using the results of ref. [82] where the resonances in the continuum were included and unique plateau values could be found in the Strutinsky energy $\bar{E}$, its agreement with E_{ETF} is within 0.25 MeV when E_{ETF} is evaluated to that accuracy.)

We finally mention very shortly a new averaging technique developed recently by Ivanyuk and Strutinsky [104,105] which makes use only of bound states and is derived directly from a least-square fit of the single-particle energy sum in powers of $N^{-1/3}$ (similar to eq. (3.20)). In the newest version of this method [105], perfect plateaux are found for the shell-corrections as functions of the number of (bound) levels included. This is illustrated in Figure 9. The method is discussed in the review paper by Strutinsky [67], to which we refer for details. It is important to note that this new method leads to some systematic differences in δE to the standard energy averaging results (see the arrows in Fig. 9). For deformed Woods-Saxon potentials, the difference in δE is roughly constant, ~ 1-2 MeV,

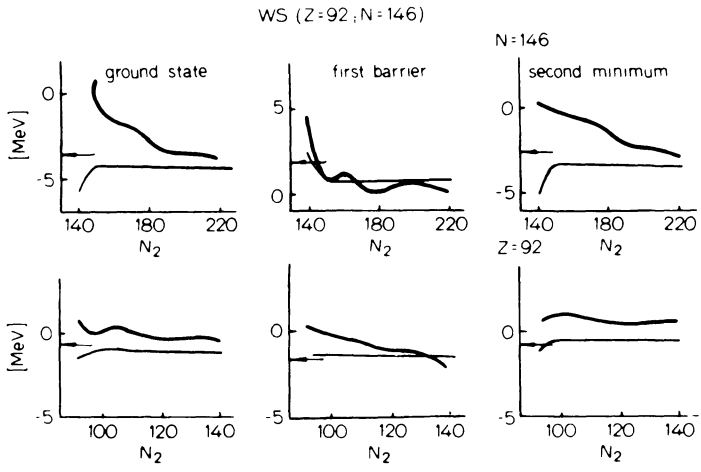

FIG.9. Shell-corrections obtained for deformed Woods-Saxon potentials with the new number-averaging method of Ivanyuk and Strutinsky [105], shown by the thin lines versus twice the number N_2 of the highest level included (see details in Ref. [105]). Fat lines are results from an earlier version [104]; arrows mark the values obtained with the standard energy-averaging technique. Note that in the caption of the original figure (Fig. 3 of Ref. [105]), the role of thin and fat lines was interchanged by mistake (private communication by F.A. Ivanyuk).

and affects relative barrier heights of actinides by less than ~ 1 MeV. For spherical nuclei, however, the difference amounts to several MeV, which has consequences for the so-called Pb-anomaly. (See ref. [67] for a detailed discussion.)

3.4 Summary of uncertainties in the SCM

Before turning to a comparison with experiments, let us now briefly recollect the sources and magnitudes of the main uncertainties in the shell-correction method, as discussed in this section.

a) Due to the numerical energy averaging:
- in infinite potentials (Nilsson etc.): $|\Delta \tilde{E}| \lesssim 0.5$ MeV.
- in finite depth potentials (Woods-Saxon, folded Yukawa): $|\Delta \tilde{E}| \lesssim 1 - 1.5$ MeV for $A \gtrsim 100$.
  However, larger uncertainties may arise in light nuclei or when the separation energy is small compared to $\hbar\Omega$ (e.g. in nuclei far off the β-stability line).

b) From the shell-correction expansion of the HF-energy:
- missing higher order terms: $|\Delta\delta E| \lesssim 1$ MeV for $A \gtrsim 100$.
  This error depends on the selfconsistency of the potential and the LD (droplet) model used; it may easily be several MeV in light nuclei.

- "quality" of commonly used potentials: $|\Delta\delta E| \lesssim 1 - 2$ MeV. This is merely an estimate, taken from comparisons of different calculations with both phenomenological and selfconsistent (HF) potentials.
- "quality" of liquid drop(let) models: an error of up to several MeV may be present, in particular in spherical cases. (Pb-anomaly! - see sect. 3.1c above and the discussion in ref. [67].) In contrast to the other uncertainties, this error should show up as a smooth function of N,Z and deformation!

(Note that in the last two items, the word "quality" is to be understood relative to the application in SCM calculations, as judged from the HF point of view. Nothing is said here against the merits and suitability of the phenomenological models in reproducing single-particle properties or average nuclear binding energies.)

Since it appears that most of the above errors or uncertainties are uncorrelated and rather random, one should not expect them to add up. As a rule, we may thus expect an overall uncertainty in SCM results of not much more than $\sim 1 - 2$ MeV. We emphasize that this should account for the realistic calculations as they were performed in particular for fission barriers, and neither for possible idealized cases where the errors could be somewhat smaller, nor for applications to extreme situations where much larger errors may occur (like e.g. in superheavy predictions [8,9] or heavy ion calculations [106]).

3.5 Comparison with experiment

It would lead beyond the scope of this paper to give an extended review of SCM calculations, which are well covered up to 1973 in refs. [38,47]. In the mean time, not many extended compilations were done. One new feature in the results of fission barrier calculations is the appearance of a "second second" saddle which is mass symmetric, but γ-deformed and lies some $\sim 1 - 2$ MeV higher than the usual mass asymmetric but axially symmetric outer saddle. It was reported in one case by Gavron et al. [107] and, independently, studied systematically over the whole actinide region by Junker and Hadermann [108]. The schematic picture of a typical mid-actinide fission barrier and the role of symmetries is now that shown in Figure 10. The structure at the mass-asymmetric outer saddle, reported for the first time by Möller and Nix at Rochester [47], is now confirmed by other results [109, 67]. It develops to a real third minimum especially for the lighter actinides and may have interesting consequences for the Th-anomaly (see below).

Besides fission barriers, the SCM can, of course, also be applied to (and tested against experimental) ground-state masses [47], moments [110], fission life times [111], fission fragment distributions [112] and other properties, most of which are dealt with at this conference. For a review of fission isomer properties, see especially the paper by Metag [113]. We shall content ourselves here with a short discussion of the two chief applications, where also the two chief discrepancies with experiment have been found, and try to find out whether we can attribute these discrepancies to any of the uncertainties of the SCM discussed above.

a) Fission barrier heights and the "Th-anomaly"

The most recent experimental fission barriers have been compiled and compared to shell-correction calculations in the review by Britt [114]. The overall agreement between experiment and theory is essentially unchanged

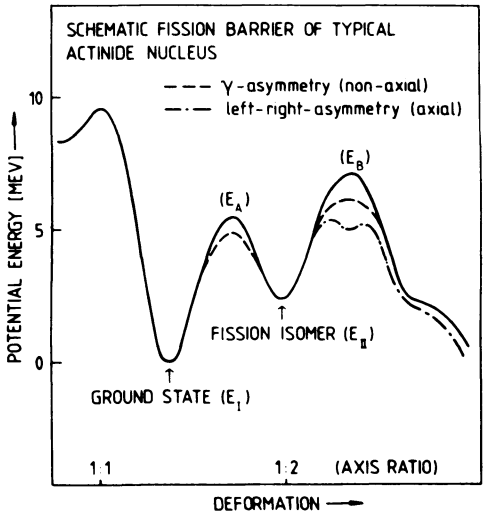

FIG.10. Systematic fission barrier of a typical even-even mid-actinide nucleus.

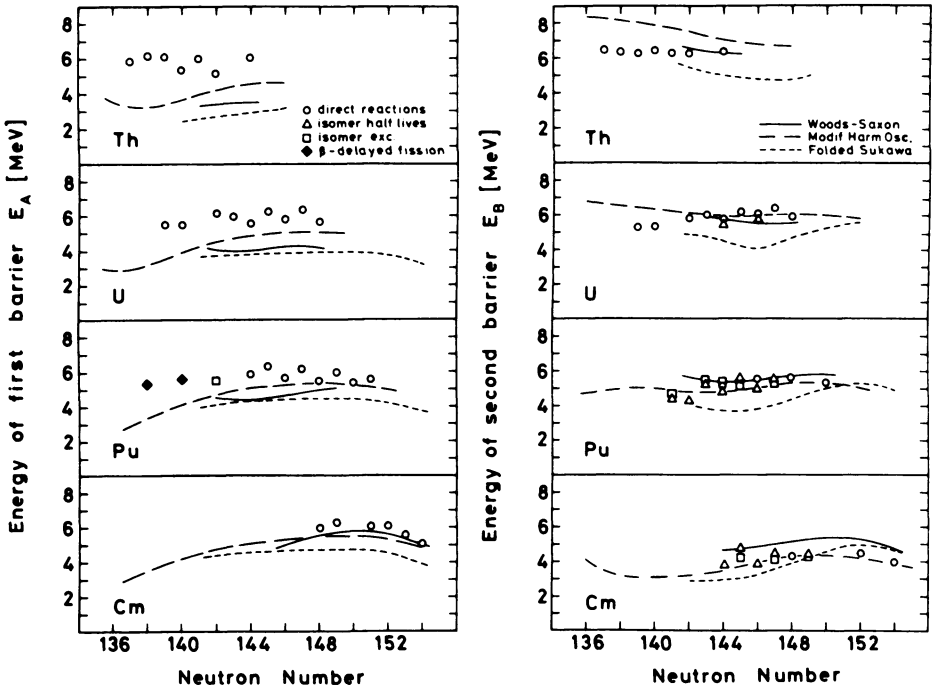

FIG.11. Heights of the inner (E_A) and outer (E_B) fission barriers of actinide nuclei, compiled by Habs et al. [115]. Circles, triangles and squares show experimental results obtained with different techniques. Solid, long dashed and short dashed lines show theoretical results obtained with the shell-correction method using a Woods-Saxon (Pauli, [47]), a modified harmonic oscillator and a folded Yukawa potential (both by Möller and Nix, [47]), respectively.

since Rochester (see, e.g., Möller and Nix [47]). In Figure 11, we show a comparison of fission barriers, taken from a recent article by Habs et al. [115]. For the outer barriers (E_B), the agreement between experimental and three different sets of theoretical results is in all cases within ~ 1-2 MeV. The same holds for the inner Barriers (E_A) of actinides with neutron numbers $N \geq 140$. However, there is a clear tendency of the theoretical inner barriers to be too low. This trend gets stronger for the lighter actinides with $N < 140$. In the lightest Th-isotopes, the discrepancy reaches up to ~ 4 MeV, which gave rise to the name "Th-anomaly" [38,47]. We see, however, clearly from Fig. 11, that this anomaly is not restricted to Thorium; there is a clear trend for all theoretical barriers E_a with $N \lesssim 144$ to decrease with decreasing N, whereas all measured values stay constant around ~ 5 - 6.5 MeV. This was emphasized in ref. [115] with the newly measured barriers of ^{232}Pu and ^{234}Pu. The former "Th-anomaly" is thus now a clear systematic discrepancy for all actinides (at least up to Pu) with neutron numbers $N \lesssim 140$.

For all the other cases, the agreement within ~ 1-2 MeV is very satisfactory. As we have summarized in sect. 3.4, the total of uncertainties in the SCM can hardly be expected to be smaller than ~ 1-2 MeV; the general agreement with experiment is thus the optimal one.

There have been proposed several explanations for the Th-anomaly (see, e.g., Möller and Nix [47], Pauli and Ledergerber [111], Larsson et al. [116]). The most popular is the one using the third minimum found by Möller and Nix [47] and will be much discussed at this conference. We do not want to comment on the possible experimental evidence for this third minimum, which is discussed extensively in several papers [117]. We note, however, that some care should be taken on the theoretical side with the quantitative interpretation of a (third) well with a depth of ~1 MeV, in view of the above uncertainty limits of the SCM itself. This is not meant to doubt the qualitative existence of a third minimum, which now seems well established [109,67]. On the other hand, when considering experimental consequences of the existence of this third well, one should not only think of ^{230}Th and ^{232}Th, where the original "Th-anomaly" was found, but one should look seriously at all those actinides where a third well is predicted (although this might not be easy experimentally).

In turn, from our point of view taken in this paper, we do not exclude an explanation of the systematic discrepancy in E_A of the actinides with $N \lesssim 140$ due to the uncertainty in the SCM alone (and thus compatible with the old double-humped picture also for the Th-isotopes!). As we stated in sect. 3.4 above, systematic smooth errors larger than ~ 1-2 MeV may arise in the SCM from a lack of selfconsistency of the shell-model potentials and liquid drop(-let) models employed. In fact, we shall see instantly that this explains the so-called "Pb-anomaly". And indeed, what started out as the Th-anomaly is an error in E_A which systematically increases as one approaches the Pb-region. To further substanciate - or disprove - this suspicion, it is therefore of great importance to investigate barrier heights of pre-actinide nuclei all the way dwon to ^{208}Pb (or even below), both theoretically and experimentally [118].

b) Ground state masses and the "Pb-anomaly"

We have now already several times touched upon the other - and largest - discrepancy between experimental data and results calculated with the SCM: a total binding energy of ^{208}Pb too low by ~ 4-7 MeV as found with the shell-correction δE in finite depth potentials. Nothing has changed in this

since 8 years (see the details in the reviews [38,47]), and no satisfactory explanation has been given. Our conclusions reached in sect. 3.3 clearly rule out an error of 4-7 MeV in δE due to the Strutinsky averaging method (also in finite depth potentials), as it was sometimes suspected.

We claim (see also ref. [119]) that the material presented in sect. 3.1 above gives a clear (not necessarily unique!) explanation of the Pb-anomaly: namely the fact that no such anomaly exists in the selfconsistent results of ref. [62] using the Strutinsky-smoothed HF-calculations. The "Pb-anomaly" appears thus as due to a lack of selfconsistency in the corresponding SCM calculations. Since the Skyrme-HF results support the value $\delta E \simeq -$ (18-20) MeV of the shell-correction in ^{208}Pb, found with a Woods-Saxon potential [38], the lack of selfconsistency must be sought in the LD model parameters used in ref. [38].

We note that Strutinsky [67] arrives essentially at the same result; we refer to his review for a further discussion of the LD model. A seemingly different explanation of the Pb-anomaly is given in the paper by Werner et al. [120] using Migdal theory. However, in as far as a large part of their effect is equivalent to the rearrangement in HF, their conclusions agree at least qualitatively with ours.

With the above explanation we have of course not yet given any remedy of the Pb-anomaly. Clearly, better selfconsistent sets of shell model and LD or droplet model parameters should be constructed. For that, more self-consistent (and preferentially semiclassical) calculations with realistic effective forces are needed. Since we argued above, that the old "Th-anomaly" also might be connected with the same effect, more than one problem might be cured in the event of a positive outcome, so that renewed efforts in these directions are certainly justified.

Apart from the region around ^{208}Pb, the theoretical binding energies obtained with the SCM agree generally with the experimental ones within $\sim$ 1-2 MeV; we thus have here the same satisfactory result as for most of the actinide fission barriers.

4. SUMMARY, CONCLUSIONS AND OUTLOOK

We have examined several methods of calculating nuclear deformation energies, with emphasis on fission barriers of actinides, and compared their results to experiment. We first discussed the constrained Hartree-Fock (CHF) method which makes use of effective nucleon-nucleon interactions fitted to nuclear ground-state properties. Without changing or adding any parameter, the total binding energy is then calculated at large deformations using a constraining external field. That double-humped fission barriers are obtained even qualitatively, is rather remarkable, since they represent only a permille effect in the total binding energy. With the results of HFB calculations by Berger et al. [16], confirming that the average pairing gap Δ is roughly constant up to the second barrier, three independent groups now have consistently obtained too high barriers E_B of ^{240}Pu or ^{236}U by roughly a factor of two. This need not be alarming. On one hand, we saw that the freedom in fitting the force parameters (in particular for the case of the Skyrme interaction) leaves enough room for quite appreciable variations in the barrier heights. Especially the spin-orbit force is too little known and leads to large uncertainties. On the other hand it is quite possible that an essential feature of the effective forces in use is generally missing and shows up only at large deformations. This problem in any case presents an interesting challenge for the next future. Clearly, in forthcoming

improvements of the effective interactions, the barrier heights should be carefully watched and incorporated in any adjustment of parameters. It may turn out that the long-range part of the forces needs to be essentially improved. Qualitatively, the inclusion of a second order tensor force should lower the binding energy; whether it brings the desired effect on the fission barriers remains to be investigated.

We have seen that the lengthy HF iterations are not always needed if one only relaxes the required accuracy by a couple of MeV. If carefully deformed realistic potentials are used, one can already in the first step (i.e. by solving the Schrödinger equation once only) obtain deformation energies which locally deviate from the exact CHF results only by a few MeV. This approximate ("expectation value" EV) method should be useful for large scale investigations and rough first-order determinations of force parameters to be used in CHF calculations.

We next discussed several aspects of the shell-correction method (SCM). We have seen that numerical investigations have given an excellent overall verification of the basic assumptions of the SCM within the HF framework. But we also saw that the selfconsistency of nuclear potentials, densities and average (LD) deformation energies play an essential role for the Strutinsky theorem to be accurately fulfilled. Future improvements of the SCM should thus aim at selfconsistent determinations of shell model and droplet model parameters. We showed that this should remove the old Pb-anomaly and argued that it might also improve the inner barriers of the lighter actinides (Th-anomaly). Whether the overall uncertainties of the SCM ever can be brought significantly below a ~ 1 MeV limit, is doubtful even if the ingredients are determined more consistently. When it comes to investigating the "fine structures" of fission barriers [114], we may thus definitely have reached the limits of this method.

One uf our conclusions reached in Sect. 3.1 was that shell effects may be treated in perturbation (like in the EVM or the SCM), and that selfconsistency is important mainly for the average potentials and deformation energies. To obtain the latter, semiclassical methods can be applied. Let us briefly outline some recent progress and some plans for the near future along these lines. We have already mentioned in Sect. 3.3 the refinements made in the extended Thomas-Fermi (ETF) method, which was seen to be completely equivalent to the Strutinsky energy averaging and allowed a quantitative confirmation of the latter method also in finite depth potentials. The ETF method cannot be used directly to determine selfconsistent deformation energies, because it leads to densities $\rho(r)$ which diverge at the classical turning point and are not defined outside. It yields, however, a kinetic energy density functional $\tau[\rho]$ [122] which has been used quite successfully together with the Skyrme force in variational calculations of average binding energies for spherical nuclei [39,40,123]. The first application of this formalism to calculate average fission barriers will be presented by Bengtsson [124] at this conference.

An important step was reached when it was realized [125] that a partial resummation of the $\hbar$-power series (used to derive the ETF expressions, see eq. 3.21) solves the turning point problem, leading to semiclassical densities which are smooth everywhere and fall off exponentially in the tail. With this method, which is still being further developed and tested [126], it is now possible to obtain average densities $\tilde{\tau}(r)$ and $\tilde{\rho}(r)$ directly from a given potential $V(r)$ without the need to evaluate any wavefunctions. This is, however, the most "expensive" step in a HF iteration. The step from ρ and τ to a new (and more selfconsistent) potential is usually done by a simple integration;

in the case of the Skyrme force even by a few algebraic manipulations (including derivatives of ρ). Thus, it will shortly be possible to do "short cut" HF iterations semiclassically, which should lead to selfconsistent average potentials and deformation energies at a rather low cost. It remains to be seen numerically to which accuracy this method can be pushed. But we express here the definite hope that most of the calculated fission barriers presented at the next IAEA fission symposium will be evaluated using this method to obtain the average part of the deformation energy.

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DISCUSSION

K.W. GOEKE: At the beginning of your paper you discuss some of the shortcomings of the Hartree-Fock and constrained Hartree-Fock (CHF) methods at the present time. I would like to add two further problems which, in my view, have prevented CHF from being applied to heavy nuclei on a large scale. One of these shortcomings is conceptual in nature. In CHF one uses a given constraining operator, usually the quadrupole moment, which, although correct near the Hartree-Fock minimum, is not necessarily so, for example, at the second barrier. Another shortcoming is the fact that the Hartree-Fock method is basically an iterative one. Each point on the potential energy surface has to be evaluated separately on the basis of a large number of iterations. P.G. Reinhard and I have tried to find methods of evaluating the potential energy surface 'in one go'. Indeed, within the framework of time-dependent Hartree-Fock, and in particular the adiabatic time-dependent Hartree-Fock method, one can derive a differential equation for the potential energy surface that can be solved by simple step-by-step methods. It determines, in addition, the collective mass parameters. These techniques are currently under investigation and although not yet fully studied, they certainly seem likely to be able to evaluate potential energy surfaces and masses under fully microscopic conditions, and are also much faster than the Hartree-Fock method.

M. BRACK: I completely agree with your comments. As far as the quadrupole constraint is concerned, there is a great deal of support from Strutinsky's calculations showing that Q is certainly a reasonably good fission mode up to the second barrier.

A. FAESSLER: You have told us that by using the Hartree-Fock method one gets a value for the second barrier that is too high on account of the finite basis (1–2 MeV) and also because of spurious effects from rotations (2–3 MeV). You also showed that the second barriers agree, within the limits of this error, if the pairing is taken as proportional to the surface. But I heard recently from Kneissl at Giessen that photofission in the rare-earth nuclei indicates that the data can be explained in this way only if G is constant. In such a case there is a discrepancy of 15 MeV for the second barrier. How do you explain this large difference?

I would also like to make a comment. You have mentioned the dependence of the shell correction plateau on the order of the correction polynomial. At high angular momenta it is no longer possible to obtain such a good plateau. The value of γ depends, further, on the angular momentum. In addition, we have to distinguish between the optimal values for the protons and neutrons, as calculations made here in Jülich have shown.

M. BRACK: In reply to your question, if $G \approx$ const. is confirmed by the Hartree-Fock-Bogolyubov results, then I can only say there is something basically wrong with these effective forces (Skyrme forces and K-matrix model) at large deformations. It is even more contradictory in view of the fact that the surface energy coefficient $a_s^{(0)}$ determined for the force Skyrme III in spherical nuclei is *not* too large, as I have shown.