SELF-CONSISTENT AVERAGE DENSITY MATRICES
AND THE STRUTINSKY ENERGY THEOREM

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For nuclei ranging from ^{16}O to ^{208}Pb and for the Skyrme III effective interaction, it is shown that the sum of the average energy plus the first order shell correction reproduces perfectly well the exact Hartree-Fock energy, if the average density matrices are calculated self-consistently.

In recent extended calculations [1, 2] we have investigated numerically the validity of the Strutinsky shell-correction method [3] within the framework of the Hartree-Fock (HF) approximation. We followed there the program outlined by Strutinsky [3] in deriving the shell-correction expansion of the total HF energy:

$$E_{HF}(\rho) = \bar{E}(\rho) + \delta E_1 + \delta E_2 . \qquad (1)$$

Here $\bar{E}(\bar\rho)$ is the average ("liquid drop") energy defined by the smooth part $\bar\rho$ of the self-consistent density matrix ρ; δE_1 is the first order shell-correction found in the usual way from the eigenvalues $\hat\epsilon_i$ of the *averaged* one body HF-Hamiltonian $\bar{H}(\bar\rho)$; and δE_2 collects all terms of second and higher orders in the fluctuating part $\delta\rho = \rho - \bar\rho$ of the density matrix. The term δE_2 is neglected in the usual shell-correction approach.

In the calculations of refs. [1, 2], performed with various effective interactions for many different nuclei, it was indeed found that δE_2 plays a relatively unimportant role for medium and heavy nuclei. There the quantity δE_2, as a function of both deformation and nucleon numbers, fluctuates not more than by $\pm \sim 1$ MeV around a constant value of ~ 1.5 MeV. Furthermore, the energy $\bar{E}(\bar\rho)$ was found to have all the typical features of a liquid drop model energy.

In this letter we want to present an *alternative* way of obtaining an expression of the form (1). As discussed in ref. [2], one can define the quantities $\bar{E}$ and δE_1 in slightly different ways which alter them

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only by terms of second and higher orders in $\delta\rho$. We choose here to introduce a *self-consistent* average density matrix $\tilde\rho$ which leads to a self-consistent smooth part of the total energy. We define $\tilde\rho$ by replacing the HF occupation numbers in the exact one body density matrix ρ by the *average occupation numbers* $\tilde{n}_i$ used in the Strutinsky energy smoothing procedure (see e.g. ref. [4]). This can indeed be done iteratively following the general variational method outlined by Vautherin [5]. In fact, such a procedure resembles formally to the variational inclusion of some pairing correlations, as currently practised [1, 2, 5, 6], or to the one used in HF calculations at finite temperatures [7]. The occupation numbers $\tilde{n}_i$ differ, however, from the pairing or temperature occupation probabilities in one important aspect: due to the inclusion of the curvature-corrections and the fulfilment of the plateau (or stationary) condition [4], the Strutinsky smoothing leads to a *cold average*, i.e. no excitation energy is brought into the nucleus by it (see e.g. ref. [8] for a discussion of this point).

The possibility of introducing a self-consistent *semiclassical* energy in connection with the Strutinsky method has also been considered theoretically by Tyapin [9]. In the droplet model calculations of Myeres [10], the self-consistency problem was solved within the Thomas-Fermi approximation. The Strutinsky energy averaging has been shown to be equivalent to an *extended Thomas-Fermi* approximation [11], thus including semiclassical corrections to the pure Thomas-Fermi model which are necessary to describe correctly the average surface properties of finite nuclei.

After solving the variational equations one finds

Table 1
Zero, first and higher order terms in the Strutinsky energy expansion for five nuclei calculated at their ground states with the Skyrme III force. All energies are expressed in MeV. The energy reference is the HF energy E_{HF} listed in column 2. In columns 3, 5 and 7 are reported the quantities corresponding to the expansion (3) of E_{HF}, whereas those associated with the usual expansion (1) are to be found in columns 4, 6 and 8. Pairing correlations are included using the uniform gap method [3]. The basis of expansion of the single particle HF states corresponds to 7 oscillator shells for the nuclei ^{16}O and ^{40}Ca, 9 for the nucleus ^{90}Zr, 11 for the nuclei ^{168}Yb and ^{208}Pb.

Nucleus	E_{HF}	$\widetilde{E}$	$\bar{E}$	$\delta E_1(\widetilde{\epsilon}_i)$	$\delta E_1(\hat{\epsilon}_i)$	$\delta E_2(\widetilde{\rho})$	$\delta E_2(\bar{\rho})$
^{16}O	−126.8	−122.1	−122.7	−4.7	−5.7	0.0	1.6
^{40}Ca	−339.6	−337.5	−338.1	−2.7	−4.8	0.5	3.3
^{90}Zr	−779.2	−774.3	−775.7	−5.5	−5.8	0.6	2.3
^{168}Yb	−1352.2	−1349.6	−1349.9	−3.0	−4.3	0.3	2.0
^{208}Pb	−1625.4	−1606.6	−1607.1	−19.2	−20.6	0.5	2.3

the average density matrix $\widetilde{\rho}$ and the self-consistent average energy

$$\widetilde{E} = E_{HF}(\widetilde{\rho}) = \mathrm{tr}\, \tau\widetilde{\rho} + \tfrac{1}{2}\, \mathrm{tr}\,\mathrm{tr}\, \widetilde{\rho}\, \mathcal{V}\, \widetilde{\rho} \qquad (2)$$

where τ is the matrix of the kinetic energy operator and $\mathcal{V}$ the antisymmetrized matrix of the effective nucleon interaction (which here for simplicity is assumed to be a two body interaction). We will denote the eigenvalues of the corresponding variational one body Hamiltonian $\widetilde{H}(\widetilde{\rho})$ by $\widetilde{\epsilon}_i$. Starting from the exact (i.e. not averaged) HF energy $E_{HF}(\rho)$, one can rewrite eq. (1) as

$$E_{HF} = E_{HF}(\rho) = E_{HF}(\widetilde{\rho}) + \delta E_1(\widetilde{\epsilon}_i) + \delta E_2(\widetilde{\rho}) \qquad (3)$$

where

$$\delta E_1(\widetilde{\epsilon}_i) = \sum_{i=1}^{N} \widetilde{\epsilon}_i - \sum_i \widetilde{\epsilon}_i \widetilde{n}_i \qquad (4)$$

is the usual shell correction and $\delta E_2(\widetilde{\rho})$ collects again all higher order terms. Eq. (3) assumes of course that the averaged and the exact HF solutions have been constrained to the same deformation.

In our numerical calculations we have used the effective interaction of Skyrme in the version S III [12]. Pairing correlations are included self-consistently in the exact HF energy E_{HF}, in the way proposed by Vautherin [5]. The constant pairing matrix elements G_p and G_n are determined using the average gap $\widetilde{\Delta}$ as a constant parameter [3]. A pairing correction is also added to the shell-correction $\delta E_1(\widetilde{\epsilon}_i)$ in the usual way [3]. Technical details of the constrained HF calculations as well as the modifications of eqs. (3) and
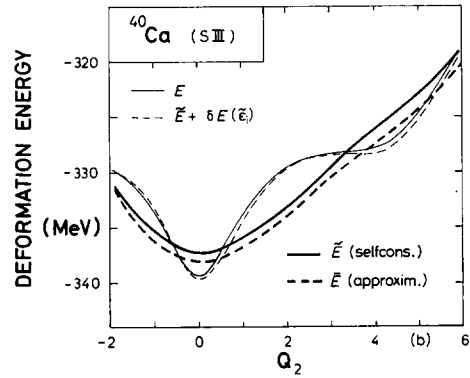

Fig. 1. Deformation energy curve for the ^{40}Ca nucleus, obtained with the Skyrme III force. Some pairing correlations have been included ($\widetilde{\Delta} = 1$ MeV). The basis of expansion of the single particle HF states corresponds for the spherical solution to 7 oscillator shells. The thin solid line is the HF energy E_{HF}, and the heavy dashed line the average energy $\bar{E}$ defined in (1). The heavy solid line is the self-consistent average energy $\widetilde{E}$ defined in (2) and the thin dashed line is the approximation $\widetilde{E} + \delta E_1(\widetilde{\epsilon}_i)$ to the HF energy.

(4) due to the pairing correlations and the density dependence of the interaction can be found in refs. [6] and [1].

The results for the average energy $\widetilde{E}$ are rather similar to the earlier results for $\bar{E}$ obtained when using the non-self-consistent average density matrix $\bar{\rho}$. The self-consistency of $\widetilde{\rho}$ has, generally, a more important influence on the shell-corrections: the first-order correction $\delta E_1(\widetilde{\epsilon}_i)$ is found to contain essentially all fluctuations of the total energy E_{HF}, the remaining term $\delta E_2(\widetilde{\rho})$ being very small and nearly constant.
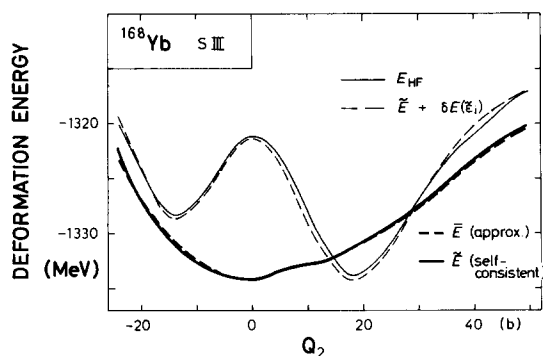
Fig. 2. The same as in fig. 1, but for the ^{168}Yb nucleus.

In table 1, the HF energies and the single terms of
the two expansions (1), (3) are lsietdd for 5 nuclei
ranging from ^{16}O to ^{208}Pb in their ground states. It
is seen that the values of $\delta E_2(\tilde{\rho})$ vary only from
~ 0.0 to 0.6 MeV, thus containing almost no oscilla-
tions, whereas the values $\delta E_2(\bar{\rho})$ vary more.

This effect is even more striking when the defor-
mation dependence is considered. Figs. 1 and 2 show
deformation energy curves obtained with a quadratic
constraint on the mass quadrupole moment Q_2 for
the nuclei ^{40}Ca and ^{168}Yb. Both the exact and the
averaged self-consistent energies, E_{HF} and $\tilde{E}$, are
shown. The non-self-consistent average energies $\bar{E}$,
obtained as in refs. [1, 2], are also plotted. The cur-
ves $\tilde{E} + \delta E_1(\tilde{\epsilon}_i)$ approximate the exact HF energy
curve E_{HF} very closely at all points, thus showing
the smallness of the term $\delta E_2(\tilde{\rho})$. Such a result is
particularly spectacular for the light nucleus ^{40}Ca.
For this nucleus indeed, in the usual expansion (1),
δE_2 was found [2] to be of the same order as δE_1,
namely oscillating between 0 and 3 MeV.

We have here presented some numerical evidence
that one can define the average density matrix in such
a way that the Strutinsky energy expansion (3) can
be truncated already after the first order term in a
very good approximation. Furthermore with the self-
consistent definition of the bulk part of ρ, the domain
of validity of the Strutinsky method has been extended
to nuclei as light as ^{40}Ca or ^{16}O.

It may also be stressed that we have provided here
a completely consistent calculation of the semiclassi-
cal solution associated with a given microscopic
Hamiltonian. The way it has been obtained here is

far from being cheap, since it needs as much computa-
tional time as complete microscopic calculation. How-
ever, the results presented above could have interesting
practical consequences. First of all, one could perform
usual Strutinsky calculations using the smoothed
single particle Hamiltonian $\tilde{H}(\tilde{\rho})$ and the correspond-
ing liquid drop energy $\tilde{E}$ as inexpensive substitutes of
HF calculations in the vicinity of some selected nuclei
(where complete HF calculations would be achieved).
Secondly, if one is able to realize the self-consistent
variation *only* for the semiclassical part of the solu-
tion (e.g. in the extended Thomas-Fermi approxima-
tion of ref. [11]) one would be able to produce
precise estimates of the total HF energy by simply
adding a standard shell-correction calculation.

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