THE VALIDITY OF THE STRUTINSKY METHOD FOR THE DETERMINATION OF NUCLEAR MASSES

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In theoretical estimates of nuclear masses of experimentally unknown isotopes, one has used two different kinds of methods. The first consists in deducing these masses from some known neighbouring ones with the help of a convenient extrapolation formula. This has been extensively discussed for instance in Ref. [1]. One of the problems of such an approach is that one cannot predict any sudden change (e.g. in deformation) in the unknown region if it has not shown up for any known nuclei in the vicinity. The other methods, on which we will concentrate here, are based on a detailed description of total binding energies within a given model. In the last two or three years, one has been able to parametrize phenomenological effective interactions and to give a very satisfactory systematic reproduction of nuclear masses on the whole chart of nuclides, using both the Hartree-Fock approximation [2-3] and the Hartree-Fock-Bogolyubov approximation [4]. But the oldest and still rather successful approach to nuclear masses is the liquid drop model [5]. For the description of fine details connected to the existence of magic nuclei one has been obliged to introduce some

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shell corrections as done in Ref. [6]. Strutinsky has given a consistent description of the nuclear binding energy in terms of a sum of a liquid drop energy plus first and higher order shell corrections [7]. Such an expansion relying on the validity of the Hartree-Fock description of the nuclear ground state is referred to as the Strutinsky energy theorem [8]. The energy averaging method widely used to extract the shell correction has been shown to be equivalent to many other possible prescriptions (such as the so-called temperature method or various semi-classical expansions) [9]. A consistent fit of the parameters of both the liquid drop model and the single particle potential needed in the Strutinsky method has been done by Seeger and co-workers (see e.g. Ref. [10]) for nuclei with $A \geq 40$. Such approaches to nuclear masses are met with two kinds of difficulties: i) how reliable is the extrapolation of single particle potential parameters? ii) What is the accuracy of the Strutinsky method itself?

The aim of this contribution is to provide an answer to the second question pertaining to the validity of the Strutinsky expansion of the energy when stopped after the first order terms. Starting from a microscopic hamiltonian with some effective nucleon-nucleon interaction, one can write [7] the total energy E in the Hartree-Fock approximation as:

$$E = \bar{E} + \delta E_1(\hat{\epsilon}_i) + \delta E_2 . \qquad (1)$$

In (1), $\bar{E}$ is a "liquid drop" energy which depends only on the average part of the density matrix. The quantity $\delta E_1(\hat{\epsilon}_i)$ is the usual shell correction energy evaluated for the spectrum $\hat{\epsilon}_i$ which will be defined below, whereas δE_2 is the sum of higher order shell corrections which is neglected in the usual shell correction approach. The single particle energies $\hat{\epsilon}_i$ are eigenvalues of the average part of the Hartree-Fock potential.

Using the effective interaction of Skyrme (in the parametrization SIII [2]) we have performed Hartree-Fock calculations leading to the knowledge of the energy E. From such self consistent solutions we have obtained the quantities $\bar{E}$ and $\delta E_1(\hat{\epsilon}_i)$, thus leading via Eq. (1) to the corrective term δE_2. Some results have already been discussed in Ref. [11]. Let us summarize the main conclusions.

i) The average energy $\bar{E}$ does behave like a liquid drop energy. This is illustrated in Fig. (1). The variation of $\bar{E}$ as a function the constrained quadrupole moment Q is smooth with the exception of some wiggles around the ground state and the first fission

barrier of the considered ^{240}Pu nucleus (Hartree-Fock solutions are taken from Ref. [12]). These wiggles are in fact due to a rapid variation (with respect to Q) of the hexadecapole moment h of the considered solutions. This is ascertained by the comparison of $\bar{E}$ with the energy of a liquid drop [6] having the same multipole moment Q and h, since the latter presents the same wiggles as $\bar{E}$. One could try to extract from such curves the liquid drop parameters associated with a given effective interaction. This is somewhat difficult [11] with a good accuracy, and a fit of $\bar{E}(A)$ for spherical solutions would be far better. Preliminary results are sufficiently realistic to confirm the relevance of the used interaction for testing the shell correction approach.

ii) The obtained first order corrections $\delta E_1(\hat{\epsilon}_i)$ are close to those found in the usual calculations using

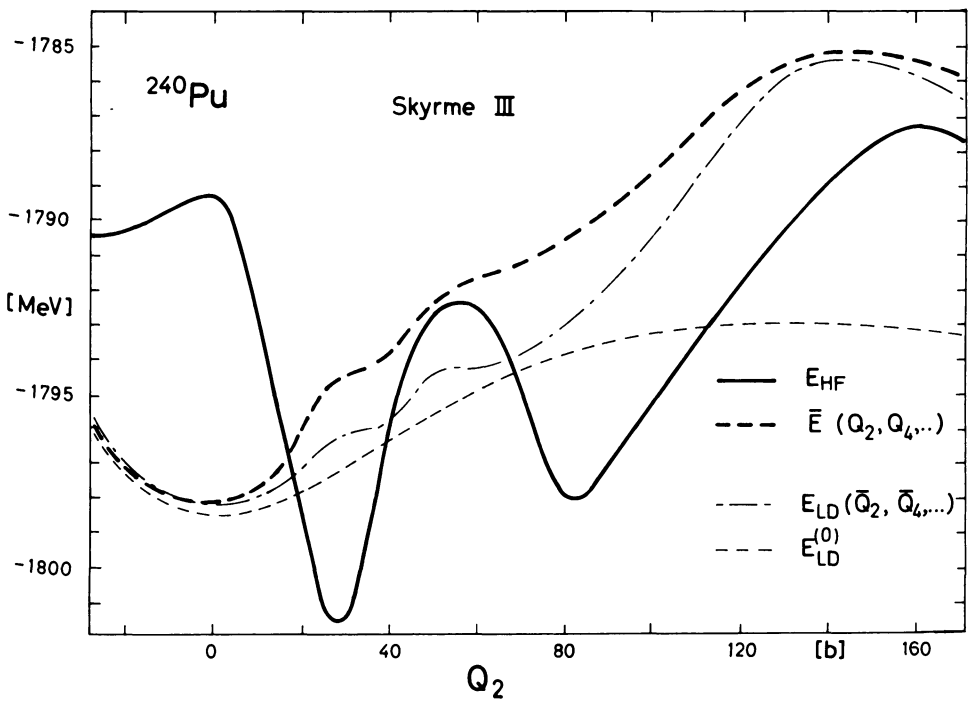

Figure 1: Deformation energy curves for the ^{240}Pu nucleus. Hartree-Fock (E_{HF}), Strutinsky smoothed ($\bar{E}$) and liquid drop model (E_{LD}) energies are shown. The curve $E_{LD}(\bar{Q}_2, \bar{Q}_4, \ldots)$ corresponds to a liquid drop having the same moments $\bar{Q}_2$ and $\bar{Q}_4$ as in $\bar{E}$, whereas the curve E_{LD} is obtained along the liquid drop fission valley. (Note that on the figure the argument in $\bar{E}$ must be read as $\bar{E}(\bar{Q}_2, \bar{Q}_4)$!).

phenomelogical single particle potentials. Some detailed differences may be due to small deficiencies in the parameters of one or the other approach (explaining e.g. the bad first fission barrier of ^{240}Pu as calculated with the interaction of Skyrme III).

iii) The sum of the higher order shell corrections δE_2 is found to be relatively small ($\sim$1-2 MeV) for medium and heavy nuclei. As expected, for light nuclei the convergence of the expansion (1) is less rapid than for heavier nuclei. Indeed in the ^{40}Ca nucleus, both $\delta E_1(\hat{\epsilon}_i)$ and δE_2 have the same order of magnitude, as can be seen on Fig. 2. (Pairing correlations with 3 different strengths have been included, corresponding to a constant average gap [7] of $\tilde{\Delta}$ = 0, 1 or 2 MeV). One should particularly note here the wrong value of the first order shell-correction of $\delta E_1 \sim$ -5 MeV for the ground state of ^{40}Ca. Inclusion of the higher order corrections brings the value of the shell-correction close to zero. This is in much better agreement with the small empirical value of $E=E_{exp}-E_{LD}$ deduced from the experimental mass E_{exp} of ^{40}Ca and its liquid-drop fit E_{LD} of Myers and Swiatecki [6]. However these last results have been found to be rather dependent on the way in which one defines the smoothed energy and the single particle spectrum entering the definition of δE_1. We have recently proposed [13] a slightly different version of the energy theorem (1) in which a selfconsistent

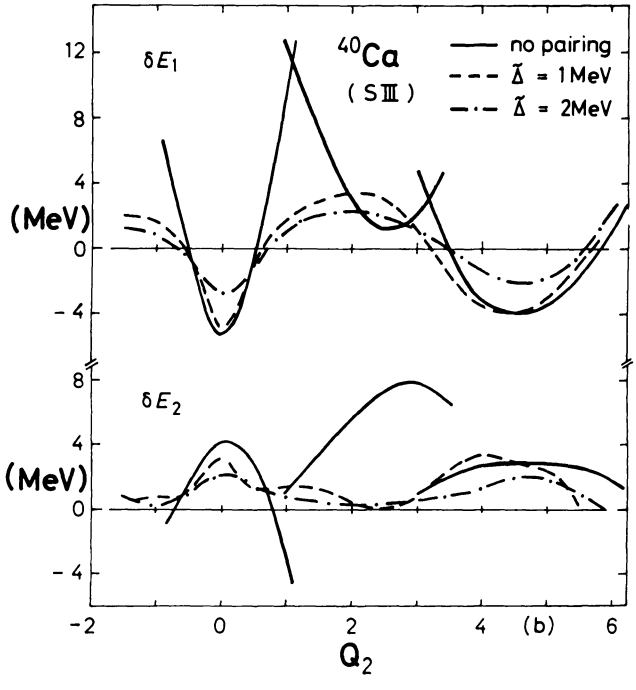

Figure 2: First order (δE_1) and second order (δE_2) shell corrections in the ^{40}Ca nucleus as a function of the mass quadrupole moment Q_2 (in barn). Three different values of the average (constant) pairing gap (see ref. [7]) have been used: $\tilde{\Delta}$ = 0, $\tilde{\Delta}$ = 1 MeV and $\tilde{\Delta}$ = 2 MeV.

average density matrix $\tilde{\rho}$ is introduced; the average energy $E(\tilde{\rho})$ and the eigenvalues $\tilde{\epsilon}_i$ of the average one body potential are then derived selfconsistently. It was found [13] that the alternative form

$$E = E(\tilde{\rho}) + \delta E_1 (\tilde{\epsilon}_i) + \delta E_2' \qquad (2)$$

for the expansion of the exact H.F. energy converges much more rapidly than eq. (1). For ground states of nuclei as light as ^{16}O or ^{40}Ca, as well as in heavy nuclei, the remaining corrections $\delta E_2'$ range from 0 to 0.6 MeV. On Fig. 3, the approximate deformation energy $E(\tilde{\rho}) + \delta E_1(\tilde{\epsilon}_i)$ for ^{40}Ca is compared to the exact energy E. The difference between the two energies is for all deformations as small as for the ground state.

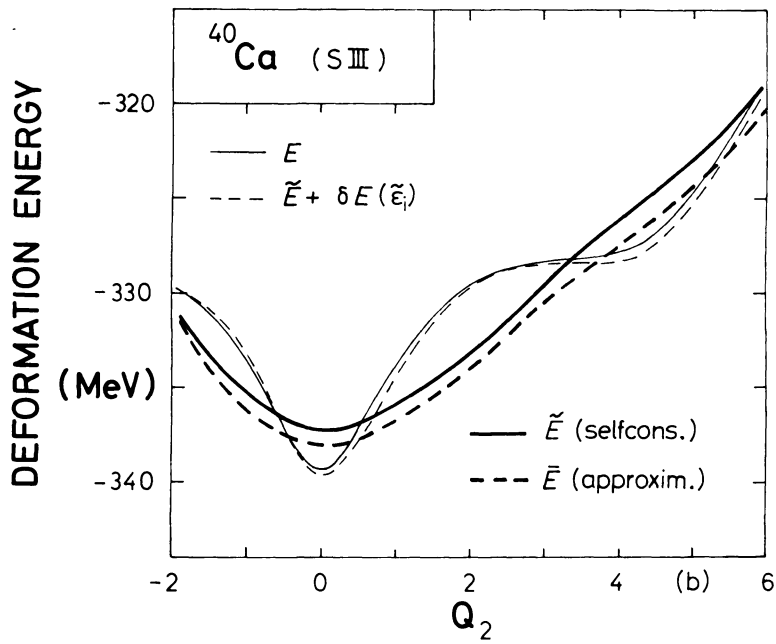

Figure 3: Deformation energies versus mass quadrupole moment Q_2 (in barn) for the ^{40}Ca nucleus. Hartree-Fock (E), normal smoothed ($\bar{E}$) and selfconsistently smoothed ($\tilde{E}$) energies are shown. The approximation $\tilde{E} + \delta E_1(\tilde{\epsilon}_i)$ to the energy E is also plotted. Pairing correlations are included ($\tilde{\Delta}$ = 1 MeV).

More stringent tests of theoretical calculations are provided by so-called transitional nuclei where ground state properties (among others) are crucially dependent on the difference in the binding energies of two distinct intrinsic states. Close to the isotopes where a change from one intrinsic state to another is to be expected, the binding energy differences are rather small, (i.e. $\sim$ 0-1 MeV). Therefore all possible sources of errors have to be investigated. Among others (related to e.g. pairing correlations, vibrational or rotational zero point. energies etc.) one should not forget possible fluctuations of higher order shell corrections. This is studied in the particular case of the neutron rich sodium isotopes where recent Hartree-Fock calculations [15] have provided a possible explanation for the experimentally observed raise in B_{2N} energy differences around A = 31 [16]. On Fig. 4 we present a comparison of Hartree-Fock [15] energies and approximate energies (smoothed energy plus first order shell corrections) in the version (2) of the energy theorem. For such neutron rich isotopes, the energy averaging procedure is less reliable due to the important contributions of neutron states in the continuum, which result only in an approximate fulfilment of the plateau condition. Such ambiguities could be in principle avoided by the use of some semi-classical expansion method [17]. Bearing these limitations in mind, it is however shown on Fig. 4, that the approximated

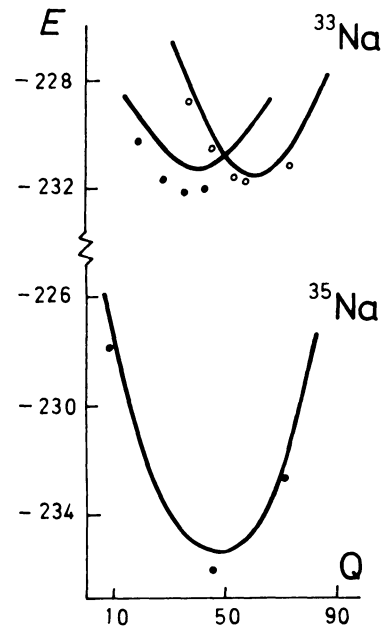

Figure 4: Deformation energy curves for two neutron-rich sodium isotopes, as functions of the charge quadrupole moments Q (in fm^2). Solid lines correspond to Hartree-Fock energies, dots to their approximation by $\tilde{E}+\delta E_1(\tilde{\epsilon}_i)$. Different branches of the curve are obtained for different neutron configurations.

energy differences reproduce the exact ones with a precision of $\sim$.5 MeV. Of course, in many cases a higher accuracy may be required.

In summarizing, it should be stressed that we have shown how the shell correction method in principle can be very accurate. As to its practical application with phenomenological liquid drop parameters and single particle potentials, the importance of the neglected higher order shell corrections depends on the region of nuclei. For light nuclei in the s-d shell we have demonstrated the importance of using selfconsistently obtained average potentials and liquid drop energies. On the other hand, in medium and heavy nuclei the higher order corrections were found not to contribute more than $\sim \pm$ 1 MeV in any case, which is an order of magnitude less than the amplitude of the first order shell corrections.

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