EXTRACTION OF A "LIQUID-DROP" PART OF THE HF-ENERGY

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Once a reasonable effective nucleon-nucleon interaction v is found and has been fitted to reproduce nuclear masses, radii and deformations in the HF-approximation, one might try to extract from the HF-energy some smooth part which varies only slowly with deformation and with nucleon numbers, such that it can be fitted by some liquid-drop like expression. This procedure can then be used to extract the liquid-drop (LD) parameters like surface energy, volume and surface symmetry coefficients, etc. from that given effective interaction.

I report here about some work which is under progress in collaboration with Ph. Quentin. In a previous paper (1) we have presented in detail our method which is basically relying upon Strutinsky's method (2) of averaging the single particle energy spectrum. Without repeating any details, we summarize here the main steps to be taken.

1. We start from the HF-solution for any given nucleus at any deformation (obtained, if necessary, with a constrained HF-calculation). From the selfconsistent density matrix ρ, we extract a smooth part $\tilde{\rho}$ obtained by averaging the spectrum of HF-energies ε_i, thus writing

$$\rho = \tilde{\rho} + \delta\rho . \qquad \text{(A)}$$

2. The smooth density matrix $\tilde{\rho}$ defines some average ("shell model") potential $\tilde{U}$ through the relation

$$\tilde{U} = \mathrm{tr}(v\tilde{\rho}) \qquad \text{(B)}$$

(we write only the direct terms here; the exchange can easily be included in the method). The average potential $\tilde{U}$ has the eigenvalues $\hat{\varepsilon}_i$ which can be found by solving the corresponding Schrödinger equation.

3. The total HF-energy E_{HF} can then be written as

$$E_{HF} = \bar{E} + \delta E_1 + \delta E_2 , \qquad \text{(C)}$$

where $\bar{E}$ is only dependent on smooth quantities like $\tilde{\rho}$; δE_1 is the first order shell-correction extracted from the "shell model" spectrum $\hat{\varepsilon}_i$ (not ε_i !) in the usual way; δE_2 is a sum of terms containing only second and higher powers of $\delta\rho$. The quantities $\bar{E}$ and δE_1 can be calculated explicitly; δE_2 is then found by subtracting them from E_{HF} .

4. The energy $\bar{E}$ can now be fitted to a LD mass formula in order to gain LD-parameters. The fit can be done in two

dimensions: either as a function of proton and neutron numbers or as a function of deformation. The surface energy can then be determined in both ways independently.

In this method, the smooth part $\bar{E}$ and the shell-corrections $\delta E_1 + \delta E_2$ are defined in a consistent and unique way; no parameters are introduced in addition to those inherent in the effective force used. The only thing exceeding usual HF-theory is the use of the smoothed density $\tilde{\rho}$. Its definition using Strutinsky's averaging method is known to approximate closely the densities used in semiclassical theories like generalized Thomas-Fermi or statistical methods (3). By looking at the magnitude of δE_2, the convergence of the shell-correction series (C) can be checked. Comparing the values of δE_1 allows to test the quality of the shell-model potentials used in ordinary shell-correction calculations. In extracting LD-parameters, since we start from HF-calculations and not from experimental masses, we have the advantage that we can extrapolate to "fancy nuclei" with very large isospin asymmetry and therefore determine the asymmetry coefficients more accurately than in usual LD fits (e.g. ref. 4).

At present, we stay at the beginning of step 4 of the program outlined. We have calculated HF deformation energy curves and their decompositions (C) for the nuclei ^{168}Yb and ^{240}Pu; a constraint was put on the quadrupole moment Q (see ref.5). For ^{168}Yb we used both the Skyrme-force SIII (5) and Negele's force in the density matrix expansion (DME, see ref.6); results are shown in Fig.1. For ^{240}Pu we used the force SIII only, see Fig.2. The resulting curves $\bar{E}(Q)$ are indeed smooth as functions of Q. This in itself supports the way of defining $\tilde{\rho}$.

In fitting the curves $\bar{E}(Q)$ to LD deformation energy curves, one has to correct for the spurious rotational energy contained in E_{HF} and $\bar{E}$ which stems from the fact that the HF-wavefunctions are not exact eigenstates of the total spin J=0. Also, one has to consider that the solutions E_{HF} and $\bar{E}$ do not follow the lowest possible path in the LD energy surface; the deviations from it give rise to some oscillations of $\bar{E}$ of ca. ±1 MeV and to an increase of the LD fission barrier. Both effects can be seen in Fig.2.

The shell-corrections δE_1 and δE_2 obtained for ^{168}Yb are shown in Fig.3. The two curves for the forces SIII and DME agree in both cases within ca. 1.5 MeV. The shell-correction δE_1 found from a deformed Woods-Saxon potential (ref.2) along the same deformations is also shown; its agreement with the curves extracted from HF is very good. The higher-order corrections δE_2 are small; their oscillations around a constant mean value of ca. 1.5 MeV are not larger than ca. ± 1 MeV . (The same is true for ^{240}Pu.) Thus, the shell-correction series (C) is rapidly converging and omitting the higher-order terms δE_2 - which is done in all usual shell-correction calculations - does in most cases not affect the results considerably.

Summarizing the results obtained so far, we can state:

1. It is possible to extract a smooth "LD-part" from a given HF deformation energy curve which (by construction) is

smooth as function of particle numbers and (as a result) is smooth as function of deformation.

2. The surface energy coefficient of the force SIII is close to the value given by Myers and Swiatecki (4), probably some 0.5 to 1 MeV higher. The same coefficient of the DME-force seems to be much higher; but this result might change by including th starting energy corrections (see ref.6) omitted so far.

3. The shell-correction series (C) converges rapidly for both forces; the second and higher order corrections δE_2 are found to be sufficiently small to be neglected in most "normal" Strutinsky calculations (except probably for transition region nuclei, where δE_1 is of the same small order).

4. The deformed Woods-Saxon potential used in many Strutinsky calculations (ref.2) is very close to the average potential $\tilde{U}$ found from the Skyrme-HF solutions (see the close agreement of δE_1 in Fig.3).

5. An improvement of the fit of $\overline{E}(Q)$ to a LD curve can probably be reached by inclusion of a curvature-dependent term, corresponding to a term $\propto A^{1/3}$ in the mass formula.

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FIGURE CAPTIONS:

Fig.1: Deformation energies for the forces of Negele (DME) and Skyrme (SIII). The LD curve is taken along the same deformation path as $\overline{E}(Q)$; LD parameters from ref. (4). ^{168}Yb.

Fig.2: Deformation energies with force SIII for ^{240}Pu. Upper part: In the dashed-dotted curve, some estimate of the average spurious rotational energy is subtracted from $\overline{E}$. Lower part: E_{LD} is along same path in deformation space as $\overline{E}$; $E_{LD}^{(o)}$ is lowest possible path ("LD valley").

Fig.3: Shell-corrections for ^{168}Yb, forces SIII and DME. Upper part: sum of second and higher order corrections, δE_2. Lower part: First order shell-correction. The dashed-dotted curve is obtained from a deformed Woods-Saxon shell-model potential (2) as normally used; it is not fitted to this special case.

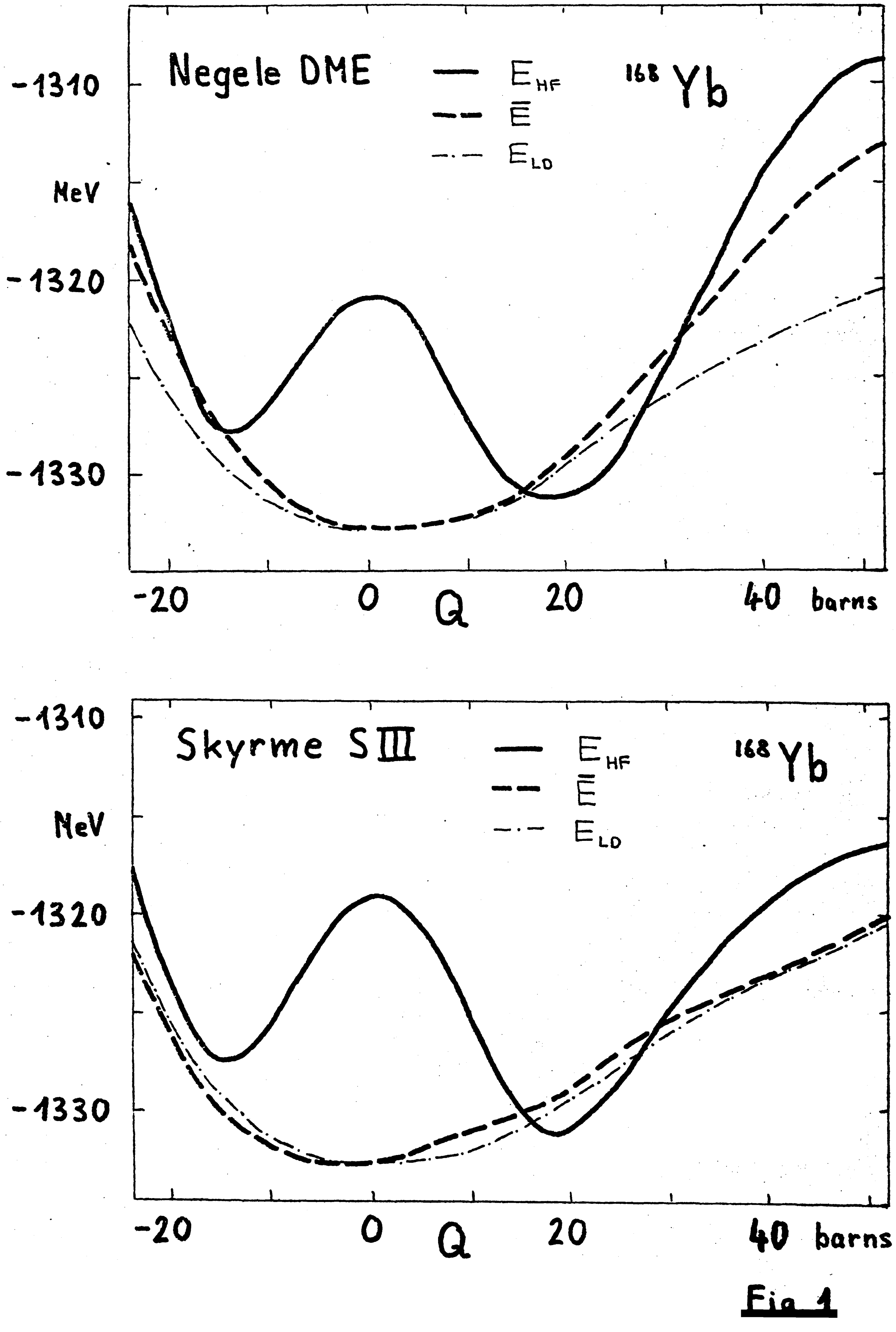
Negele DME
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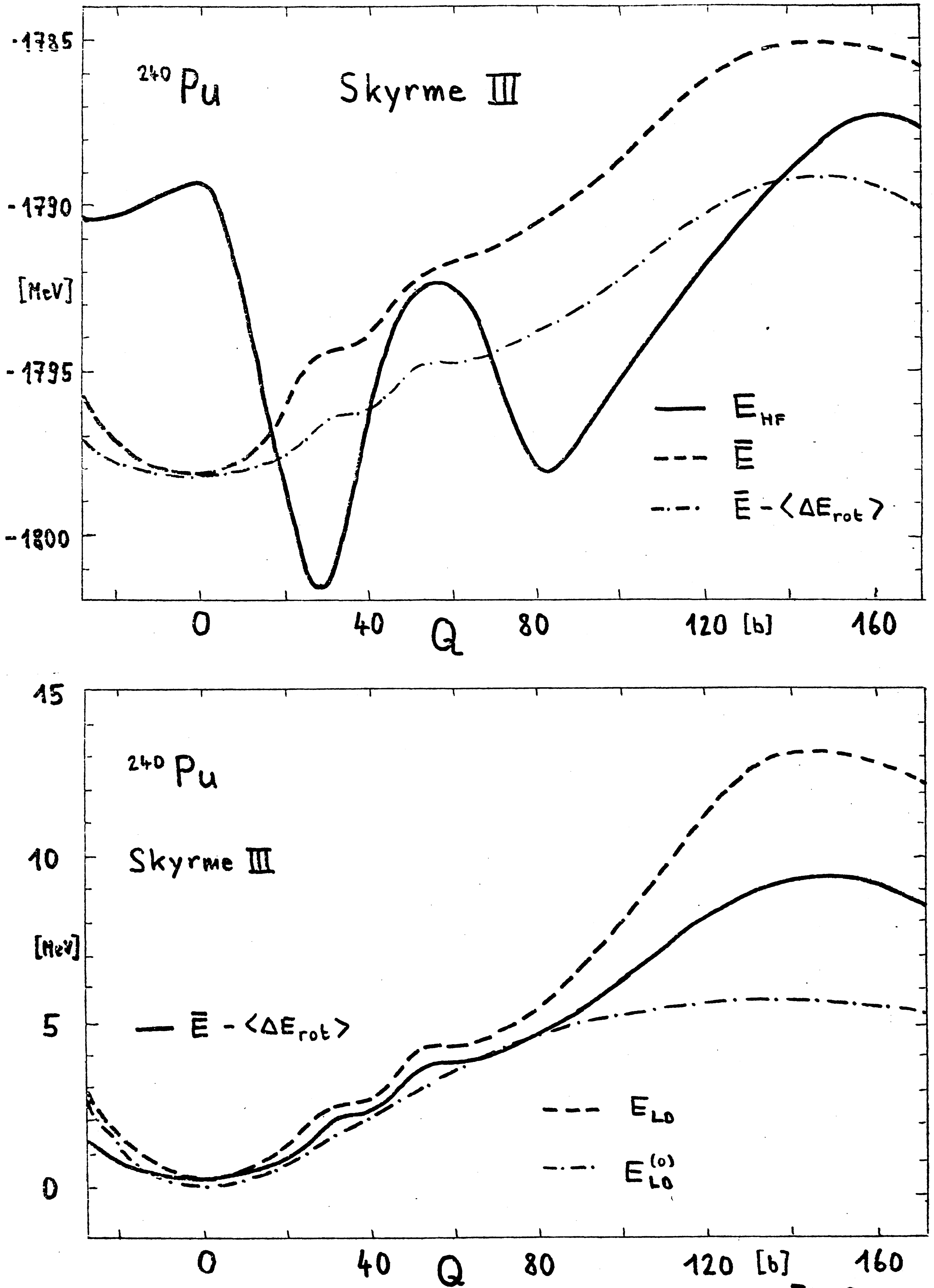
Fig 1



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Q
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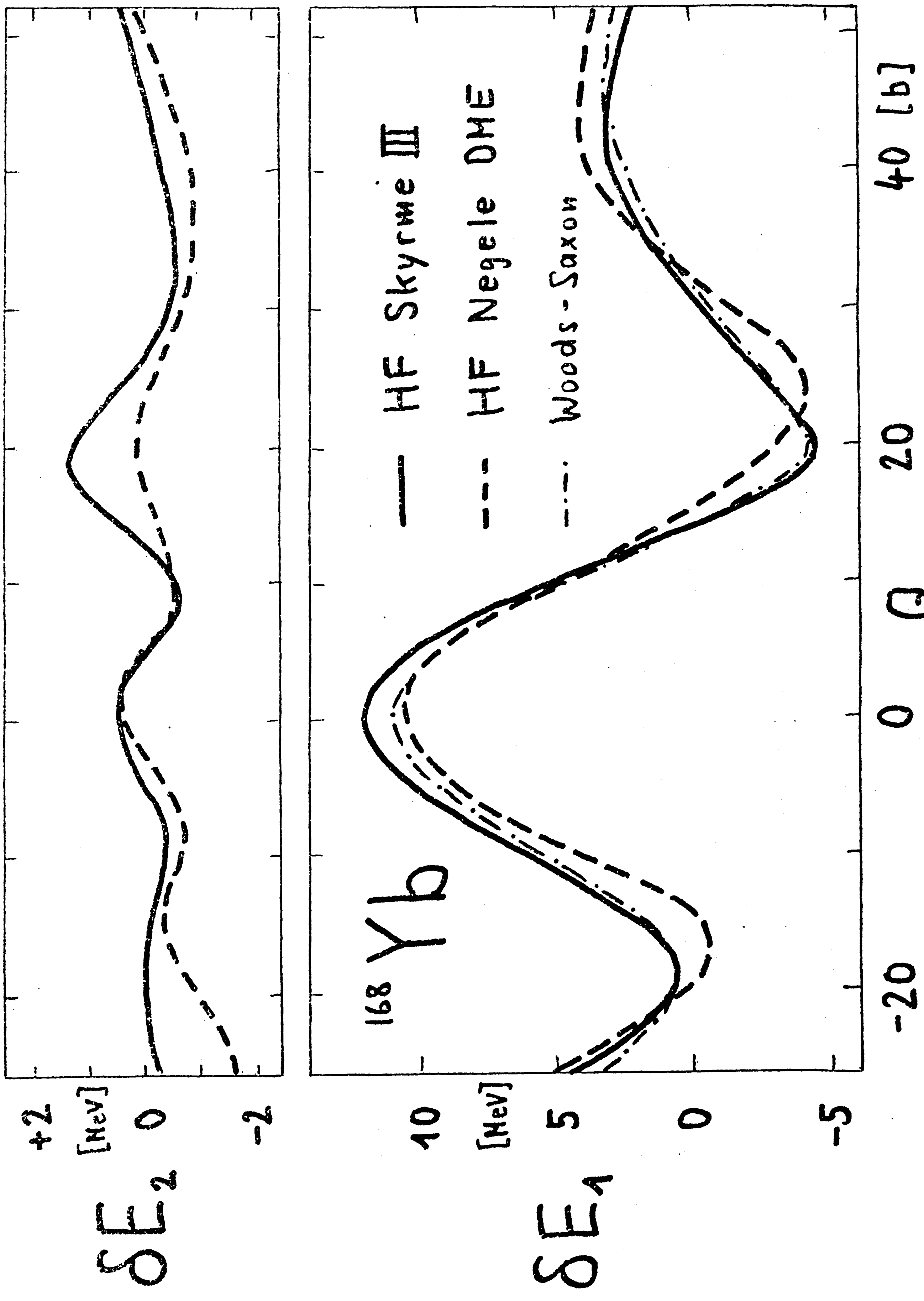
240 Pu
Skyrme III
Ē - ⟨ΔE rot⟩
E LD
E LD (0)
0
40
80
120 [b]
160
Q

Fig. 2



δE2
+2
[MeV]
0
-2
δE1
10
[MeV]
5
0
-5
168 Yb
HF Skyrme III
HF Negele DME
Woods-Saxon
-20
0
20
40 [b]
Q

Fig.3

R-Process Nucleosynthesis and Nuclei far from the Region of Beta-Stability*

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Summary

The slow-(s-) and rapid-(r-) neutron capture processes with intervening beta-decays have been known to be responsible for the synthesis of heavy elements.[1] In contrast to the case of the s-process, theoretical calculations on the r-process need large extrapolations of nuclear systematics as this process is expected to occur in the very-neutron rich region far from the beta-stability line. In 1965, Seeger et al. proposed the quasi-static model of the r-process.[2] Recently, several authors have attempted to treat its dynamics assuming the time-dependent neutron-density and temperature, claiming the more realistic astrophysical cite for the r-process.[3] Moving back onto the nuclear systematics' view-point, however, there seems to be little progress since Seeger et al.

The r-process calculation requires two gross properties of unknown nuclei concerned: nuclear masses and beta-decay half-lives. Many authors have made extensive investigations on the former variable, but not on the latter. Now that one wishes to treat the dynamic r-process, the improved estimates of the beta-decay half-lives are indispensable as they determine the absolute

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time-scale of the synthesis.

In this work, we use the gross theory of beta-decay[4] to get more reliable predictions of the beta-decay half-lives and related variables. In the abundance calculation, the quasi-static model is adopted for simplicity.

The results show that thcetime-scale of the synthesis is very likely much longer than those required in the recent dynamic-r-process calculation. This suggests the necessity of taking into account the energy releases due to beta-decays or fissions.[5] Another special attention is paid to the nuclear phenomena expected to occur after the shut-down (freezing) of the neutron-flux and temperature. Among them, the effect of delayed neutron emissions is very important and much enough to smooth out the even-odd fluctuation in the frozen abundance curve.[6] The effect of delayed fission seems to be very small. A comparison of the calculated abundance curve with the "experimental" one has been made in the hope for making a forward step to clarifying the "true" cite for the r-process. Meanwhile, the theoretical beta-strength functions are compared with the recent experimental data.

In conclusion, the authors wish to appreciate all the participants to this work-shop for their great interests in the present work.

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