HARTREE-FOCK CALCULATIONS OF NUCLEAR MASSES

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Abstract

Hartree-Fock calculations pertaining to the determination of nuclear binding energies throughout the whole chart of nuclides are reviewed. Such an approach is compared with other methods. Main techniques in use are shortly presented. Advantages and drawbacks of these calculations are also discussed with a special emphasis on the extrapolation towards nuclei far from the stability valley. Finally, a discussion of some selected results from light to superheavy nuclei, is given.

1. Introduction

The atomic nucleus viewed as a many body system, has constituted a long lasting intriguing problem. Having undoubtedly a rather smaller number of particles, it has however been successfully described in a classical or semi-classical way. For example in the liquid drop model, the binding energy of heavy nuclei is given with an accuracy of less than 1%. On the other hand a nuclear shell structure which appears as a quantum fluctuation, was necessary to explain a collection of experimental facts. The recognition of the existence of an average nuclear potential has been hindered for a long time by the repulsive character at short range of the nucleon-nucleon force untill the correct understanding of the role of the Pauli principle.

The Hartree-Fock (HF) approach discussed here belongs to the second alternative class of models : nuclear wave functions are assumed to be well described by Slater determinants built on eigenfunctions of a mean potential generated by all the nucleons through the nucleon-nucleon force. Short range correlations are approximately taken into account by the use of an effective force understood as a kind of a Brueckner G-matrix [1], [2]. Long range correlation are definitely absent. On the other hand pairing correlations can be handled in a consistent way known as the Hartree-Fock-Bogolyubov (HFB) method. A non consistent but still reasonable treatment of such pairing correlations consists in a BCS calculation following the HF calculation.

The present talk pertains only to a review of calculations leading, at least in principle, to a complete description of the whole chart of nuclides. This excludes a priori all calculations based on "regional" forces aiming at the description of a special bunch of nuclei. This will also more or less limit our discussion to calculations using phenomenological effective forces since the technical difficulties of more fundamental approaches have prevented their extensive use.

In section II we will present a general outlook on the HF method. The HF approach will be compared with other relevant methods in section III. We will especially discuss the link between HF and liquid drop model calculations within the frame of the Strutinsky method. Advantages and drawbacks of the HF determination of nuclear masses will be discussed in section IV. A special emphasis will be put on the problem of extrapolating such calculations to nuclei far from the stability valley. Section V will be devoted to a short survey of the HF technology. Finally in section VI we will give some selected examples of HF results.

2. General outlook on the HF method

2.1 Generalities

The determination of nuclear ground state wave functions from the free nucleon-nucleon interaction has given raise to an enormous amount of theoretical work. A first family of approaches is referred to as realistic calculations. This family itself can be split into two classes. In the first one a soft core interaction is used and the HF problem plus second and third order corrections is solved in the framework of the Goldstone expansion. As an example one may quote the works of Maire [3] using the Gogny-Pires-de Tourreil interaction [4] and of Strayer [38] using the Tabakin potential [39]. The other class deals with calculations performed along the lines of the Brueckner-Goldstone expansion. Results of such calculations for finite nuclei have been recently reported, see e.g. Ref. 5]. The two previous types of calculations are of great numerical complexity. Even though they have brought a lot of interesting theoretical informations they have not yet clearly met with success in providing precise values of nuclear binding energies and radii.

In the second family of approaches, one derives from realistic nucleon-nucleon forces, the effective interaction in the framework of the Brueckner theory within the local density approximation (LDA). Higher order corrections are then included phenomenologically into the force. As a consequence, one completely leaves out the problem of further corrections to HF. Such an "effective force approach" have been successfully used e.g. by Negele [1] and by Campi and Sprung [2].

For the sake of simplicity one has also considered purely phenomenological effective forces. The most important feature of the more fundamental LDA approach (e.g.

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the density dependence) are generally retained. In a special case (the Skyrme force) it has been even possible to establish the connexion with the LDA [30]. Such phenomenological effective forces may be classified by their analytical form. A first group refers to delta forces plus gradient corrective terms for the two body part supplemented by a density dependent delta force. This group includes the Skyrme force [6] and the modified delta interaction of Moskowski [7] The energy density formalism[8] proposed by Beiner and Lombard, clearly belongs also to this group. In the second group one rather considers finite range interactions for the two body interaction. Gaussians are used in the Gogny force [9]. Finite range and velocity dependence are included in the Köhler [40] and the Montreal force [10]. The latter adds an OBEP tail on a purely phenomenological part. In all cases one must consider a two body spin-orbit force which is approximated in most cases by a zero range one [41]. Tensor effective forces are generally left out.

2.2 HF equations

Given an effective interaction v, the HF approximation consists in assuming that the nuclear ground state may be described by an independ particle wave function $|\psi>$. The latter is fixed by the minimisation of $E=<\psi|H|\psi>$ (where H is the hamiltonian of the system) with respect to the variations of $|\psi>$. From now on, we will assume for brevity that the effective force is only a two body operator. Introducing the reduced (one body) density matrix ρ, the energy E can be written as :

$$E = \sum_{ij} \left[<i|\rho|j> \left(<j|K|i> + \frac{1}{2} \sum_{k\ell} <k|\rho|\ell> <j\ell|\hat{v}|ik> \right) \right] \qquad (1)$$

K being the kinetic energy operator and $\hat{v}$ the antisymmetrised two body operator. With obvious short hand notations E writes as :

$$E(\rho) = \mathrm{tr}\ K\rho + \frac{1}{2}\ \mathrm{tr}\ \mathrm{tr}\ \rho\ v\ \rho \qquad (2)$$

The variation of E with respect to $|\psi>$ or equivalently to its corresponding density matrix ρ, leads to the definition of a set of single particle states $|\lambda>$ satisfying the so called HF equations :

$$(K + v(\rho))\,|\lambda> = e_\lambda\,|\lambda> \qquad (3)$$

The HF potential $v(\rho)$ is the one body reduction of v defined as

$$<i|v(\rho)|j> = \frac{\partial}{\partial <j|\rho|i>} <\psi|v|\psi> \qquad (4)$$

or equivalently if v is independent of the density

$$v(\rho) = \mathrm{tr}\ v\rho \qquad (5)$$

Finally the density matrix ρ is defined as a sum of projectors on a set of N eigenstates of $K+v(\rho)$ namely

$$\rho = \sum_{\lambda} |\lambda><\lambda| \qquad (6)$$

In other words, the Slater determinant $|\psi>$ is built out of N single particle states eigenfunctions $|\lambda>$ of a mean one body hamiltonian $K+v(\rho)$.

The solutions of the HF eq.(3) is generally obtained by iterations. Given an ansatz $\rho^{(o)}$ of ρ leads to a potential $v(\rho^{(o)})$ and after diagonalisation to a new density matrix $\rho^{(1)}$ and so on. Starting from a density matrix $\rho^{(o)}$ obtained in a phenomenological mean potential and asking for a reasonable rate of convergence for E (say less than 10 keV) needs generally some 10 iterations.

If one projects the HF equation (3) on the $\vec{x}$ representation basis, one finds a set of coupled integro-differential equations. In the case of interactions of the Skyrme type, E can be expressed [11] as a spatial integral of an algebraic function of two density functions $\rho(\vec{x})$ and $\tau(\vec{x})$:

$$E = \int d^3\vec{x}\ \ \mathcal{H}(\rho,\tau) \qquad (7)$$

where

$$\rho(\vec{x}) = <\vec{x}|\rho|\vec{x}> = \sum_{\lambda=1}^{N} |\varphi_\lambda(\vec{x})|^2 \qquad (8)$$

and

$$\tau(\vec{x}) = \sum_{\lambda=1}^{N} |\vec{\nabla}\varphi_\lambda(\vec{x})|^2 \qquad (9)$$

The HF equations then reduce to a purely differential system of equations of the type

$$\left\{ -\vec{\nabla}\,\frac{\hbar^2}{2m^*(\vec{x})}\,\vec{\nabla} + v(\vec{x}) \right\} \varphi_\lambda(\vec{x}) = e_\lambda\ \varphi_\lambda(\vec{x}) \qquad (10)$$

where all the $\vec{x}$ dependence in the effective mass $m^*(\vec{x})$ and the potential $v(\vec{x})$ is expressed again algebraically from the densities (8) and (9). It can be noted that in the energy density formalism of Ref. 8], instead of starting from an effective force, one parametrises directly the hamiltonian density defined in (7) and therefore ends up with the same type of HF equations (10).

2.3 Pairing correlations

A consistent way to include pairing correlations is referred to as the Hartree-Fock-Bogolyubov (HFB) method. It consists in assuming that the ground state wave function is well represented as an independent quasi particle wave function $|\Phi\rangle$. The quasi particle states defined from particle states by a unitary Bogolyubov transformation, are determined through the minimisation of $\langle\Phi|H|\Phi\rangle$. This can be achieved by considering the reduced density matrix ρ :

$$\langle i|\rho|j\rangle = \langle\Phi|a_j^+ a_i|\Phi\rangle \qquad (11)$$

together with the so called pairing tensor $\mathcal{K}$:

$$\langle i|\mathcal{K}|j\rangle = \langle\Phi|a_i a_j|\Phi\rangle \qquad (12)$$

as new variational parameters.

Contrarily to the HF state $|\psi\rangle$, the state $|\Phi\rangle$ is not an eigenstate of the particle number operator N. Therefore in the variation, one must introduce a supplementary condition ensuring the conservation of the average particle number.

For a two body interaction, the expectation value of the hamiltonian can be written as

$$\langle\Phi|H|\Phi\rangle = \mathrm{tr}\ \rho K + \frac{1}{2}\ \mathrm{tr}\ [\rho\ v(\rho) + \mathcal{K}\ \Delta] \qquad (13)$$

where $v(\rho)$ is again the one body reduction of v :

$$\langle i|v(\rho)|j\rangle = \frac{\partial}{\partial\langle j|\rho|i\rangle}\langle\Phi|v|\Phi\rangle \qquad (14)$$

and the gap tensor Δ is defined as

$$\langle i|\Delta|j\rangle = 2\,\frac{\partial}{\partial\langle j|\mathcal{K}|i\rangle^*}\langle\Phi|v|\Phi\rangle \qquad (15)$$

Gogny has been the first to perform complete HFB calculations for both spherical and deformed as well as light and heavy nuclei [9].

A cheap way of including pairing correlations consists in doing a BCS calculation on the top of an HF calculation. The first difference with HFB lies in the quasi particle transformation used, the so-called Bogolyubov-Valatin transformation, which is less general than the Bogolyubov one. On the other hand, consistent variations of the occupation probabilities and of particle wave functions are not achieved at all.

An other level of approximation is reached when instead of using pairing type matrix elements (defined as $\langle i\bar{i}|v|j\bar{j}\rangle$) of the interaction v entering the microscopic hamiltonian, one utilises other matrix elements. For instance, in the HF+BCS calculations of Refs. 8] and 12], the pairing matrix elements are computed from HF particle states but with an other phenomenological two body interaction v' [13] specially adjusted to give correct pairing properties. In HF+BCS calculations of deformed nuclei using the Skyrme interaction, a further approximation(+) has been employed [14]. Pairing matrix elements $\langle i\bar{i}|v'|j\bar{j}\rangle$ are kept equal to $G, \forall i, j$, which clearly leaves out the dependence of G on the intrinsic configuration (e.g. on the deformation of the HF solution). This appears to be of some importance in shape transition region where one may hesitate between an oblate or a prolate solution for instance. Then the questions arises of the choice of the G constant in one and the other HF local minimum [43].

3. Relation with other approaches

3.1 Generalities

In this section we want to discuss the connexion between HF calculations of nuclear binding energies and liquid drop or Strutinsky approaches to them. We skip the discussion on extrapolation formulas (see e.g. Ref. 16]) mainly because for known nuclei they hardly go far beyond a simple parametrisation of experimental figures, whereas for unknown isotopes they are a priori unable to predict any sudden change in the nuclear structure if such a transition has not shown up for any known nuclei in the neighbourhood.

It has been soon realized that binding energies calculated within the liquid drop model exhibited clear deviations from experimental ones. Moreover, these discrepancies showed regularities connected with the location of magic numbers. Myers and Swiatecki [17] have been the first to systematically add to liquid drop masses a specific shell effect correction. Strutinsky [18] has settled down in the HF framework a proper microscopic deviation of these shell correction energies as well as a convenient technical procedure for their practical com-

(+) For brevity we skip the discussion of so called Δ constant calculations and refer to Refs. 14-15] for further details. In this connexion we would like to point out a mistake in Ref. 14], where the variational equation (7.7) writes as

$$\delta\left[E - \sum_i e_i \int |\varphi_i(\vec{R})|^2 d^3\vec{R} - \lambda_n \sum_i \delta_{q_i,-1/2} n_i - \lambda_p \sum_i \delta_{q_i,1/2} n_i\right] = 0 \qquad (16)$$

with

$$E = \int \mathcal{H}(\rho,\tau) d^3\vec{R} - \frac{G}{2}\left(\sum_i \sqrt{n_i(1-n_i)}\right)^2 \qquad (17)$$

If the variation in (16) with respect to $\delta\varphi_i^*$ leads to ordinary HF equations (7-8), the variation with respect to δn_i does not give the BCS equations (7-9). Should $\Sigma_i e_i$ in (16) be replaced by $\Sigma_i n_i e_i$, Eq.(7-9) would be fulfilled but not Eq. (7-8). Therefore the variational character of the determination of both occupation probabilities and wave functions is not ensured.

tation. The microscopic derivation will be referred to after Bethe [19] as the Strutinsky energy theorem whereas the technical recipe will be called the Strutinsky smoothing procedure. It should be emphasized that the later represents only one among other possible ways of achieving the smoothing procedure. Moreover its proper foundation in terms of a semi classical approximation has been further established as we will shortly discuss it. As a whole, the complete approach has received the name of the Strutinsky method and has been widely used, in particular for the determination of nuclear masses [20].

3.2 The Strutinsky energy theorem

The HF energy (2) can be considered as a functional $E(\rho)$ of the reduced density matrix ρ . The "theorem" consists in expanding such a functional around a semi-classical approximation $\bar{\rho}$ of ρ. So far we reserve the discussion of how $\bar{\rho}$ would be defined for sub-section 3.3 and take for granted that the Strutinsky smoothing procedure does it well for us. Namely we will define $\bar{\rho}$ as

$$\bar{\rho} = \sum_{\lambda} \bar{n}_{\lambda} |\lambda\rangle \langle\lambda| \qquad (18)$$

where the set of $\{\bar{n}_{\lambda}\}$ is the ordinary set of Strutinsky occupation probabilities [21] defined only through the HF single particle energy spectrum. The expansion of $E(\rho)$ writes :

$$E(\rho)=E(\bar{\rho})+\mathrm{tr}(K+\mathrm{tr}\rho v)(\rho-\bar{\rho})-\frac{1}{2}\mathrm{trtr}(\rho-\bar{\rho})v(\rho-\bar{\rho}) \qquad (19)$$

The first term is the semi-classical approximation to $E(\rho)$ and according to Strutinsky represents the liquid drop model energy. The second term is nothing else than the first order (ordinary) shell correction since

$$\mathrm{tr}(K + \mathrm{tr}\rho v)(\rho-\bar{\rho}) \equiv \Sigma e - \overline{\Sigma e} \qquad (20)$$

where Σe is the sum of HF occupied single particle energies and $\overline{\Sigma e}$ its Strutinsky smoothed value.

The last term of Eq.(19) has been assumed by Strutinsky sufficiently small to be neglected.

As a matter of fact Strutinsky [18] has not exactly proposed his theorem according to the previous lines, but in a slightly more involved way. Starting from the HF density ρ, he first defines $\bar{\rho}$ as in (18) and then diagonalising the mean hamiltonian $K+v(\bar{\rho})$, he gets a new density $\hat{\rho}$, the smooth value of which is $\bar{\hat{\rho}}$. Finally utilising the stationarity of $E(\rho)$ around ρ in the space of normalised Slater determinants he gets

$$E(\rho) = (\overline{\Sigma\hat{e}} - \frac{1}{2}\mathrm{tr}\ \bar{\rho}v\bar{\rho}) + (\Sigma\hat{e} - \overline{\Sigma\hat{e}}) + \frac{1}{2}\mathrm{tr}\ \mathrm{tr}\ \{[(\hat{\rho}-\bar{\rho})v(\hat{\rho}-\bar{\rho}) - (\rho-\hat{\rho})v(\rho-\hat{\rho})]\} \qquad (21)$$

where the set $\{\hat{e}\}$ corresponds now to the spectrum of $K+v(\bar{\rho})$. Assuming with Strutinsky that $(\rho-\bar{\rho})$ and $(\hat{\rho}-\bar{\hat{\rho}})$ are of the same order, assuming also that $(\bar{\rho}-\bar{\hat{\rho}})$ is one order less, leads in (21) to zero and first order terms identical (up to second order terms) to those obtained in (19). Indeed Strutinsky wanted to define the first order shell correction from a single particle energy spectrum obtained in a smooth mean potential $v(\bar{\rho})$ as the phenomenological potentials are, contrarily to the HF ones. That is why he has derived his theorem through auxiliary $\hat{\rho}$ and $\bar{\hat{\rho}}$ densities.

All the preceding assumptions have been recently numerically checked [22-24] within the HF approach. The HF solution ρ and energy $E(\rho)$ being known, one defines $\bar{\rho}$ according to the Strutinsky procedure then computes zero and first order terms and therefore deduce higher order terms.

The $E(\bar{\rho})$ term has been shown to be qualitatively and quantitatively very similar to a liquid drop energy. This is seen for instance on fig.1 where the deformation energy curve $E(\bar{\rho})$ of the ^{168}Yb nucleus for the quadrupole mode, is reported. On the other hand the higher order terms in (19) or (21) have been found very small (see fig.2). A third version of the energy theorem has been also derived in Ref.24]. It corresponds to a self consistent calculation of the density matrix labelled $\tilde{\rho}$. Such a calculation is self consistent in the sense that $\tilde{\rho}$ is formally identical to the $\bar{\rho}$ defined in (18) but with single particle wave functions eigenstates of $K+v(\tilde{\rho})$. This self-consistently smooth HF solution is formally similar to an HF solution at finite temperature [25].

Within this last version of the energy theorem, the zero and first order terms exhaust almost all the HF energy, leaving only less than .6MeV for higher order terms. The latter is true for a sample of nuclei scattered on the whole chart of nuclides as shown on Table 1. It should be noticed that for nuclei as light as ^{16}O, or even ^{40}Ca, the smallness of the corrective term is also obtained, whereas for the ordinary versions (19) or (21) of the energy theorem, first and higher order terms are found to be of the same order of magnitude.

3.3 Strutinsky smoothing method and semi-classical approximations

We are left now with the problem of how the Strutinsky smoothing procedure is related to a semi-classical approximation, since such an assumption has been made before (e.g. when considering $E(\bar{\rho})$ as a liquid drop model energy). Such a relation has been extensively studied, but so far only for one-body hamiltonian. Among other approaches it is worthwhile to quote the partition function method developed by Bhaduri and collaborators [26-28]. Starting from the fact that the single particle level density is the inverse laplace transform of the single particle partition function Z, they expand this function Z in powers of $\hbar$ using a general formalism due to Wigner and Kirkwood [29]. Retaining only the first terms

of such an expansion constitutes a semi-classical approximation to Z. By inverse Laplace transformation one obtains a smooth level density to be directly compared with the Strutinsky one. These two smooth level densities have been shown to be analytically equivalent in some special cases [27]. In other cases, the two methods yields numerically the same classical energies within ∿1MeV [26], this is also true when the one body hamiltonian includes a spin orbit term [28].

3.4 Conclusion

The expansion of the HF energy in terms of the difference between the HF density matrix and its semi-classical approximation seems to be rapidly convergent. However so far the practical way this approximation is made is not yet completely proven to be correct (even though it is likely to be the case) for two body (or more) hamiltonian. Should it be correct, the validity of the Strutinsky method as an approximation to the HF approach would result from the preceding. Nevertheless, disregarding small possible inaccuracies in the technical smoothing procedure, it should be emphasized that this validity has been essentially proven for a liquid drop model and shell correction energies deriving consistently from the same nucleon-nucleon interaction. This a priori condition is of course impossible to establish in practical utilizations of the method.

4. Advantages and drawbacks of HF calculations of nuclear masses

Let us start our general discussion of HF results by summarizing some general remarks on the main drawbacks of these calculations.

The first source of systematical errors in such an approach is naturally to be found in the choice of the force itself. In the most fundamental effective forces of Refs. 1-2] it has already been quoted that phenomonelogy is not quite absent, as far as inclusion of higher order diagrams is concerned. Moreover in these calculations as in the purely phenomenological ones (i.e. using entirely phenomenological effective force) one must choose a priori an analytical form for each part of the force, in particular for the density dependence (see e.g. the discussion of Ref. 2]). The preceding brings clearly into the whole approach a touch of arbitrariness and sometimes considerable limitations. This obviously happens for forces as the Skyrme ones with a zero range for the main part of the attractive force. On the other hand, in the absence of explicit tensor forces, one must exert caution about some predicted properties of non spin-saturated nuclei and spin-orbit splittings. The latter restriction is of primary importance for the discussion of HF results obtained in the super heavy nuclei region. Finally, one should bear in mind that as soon as the analytical skeleton of the force has been choosen, one has to determine the actual values of the parameters through a fit which is always to be understood as a compromise within a selected sample of constraints.

Due to its range, the Coulomb interaction does not contribute to the total energy in an analytical form as simple as the Skyrme force does. Therefore in calculations using Skyrme forces one generally approximates the Coulomb exchange total energy $E_{c.exc.}$ within a Slater approximation proposed in Ref. 30] :

$$E_{c.exc.} = -\frac{3e^2}{4}\left(\frac{3}{\pi}\right)^{1/3} \int [\rho_p(\vec{r})]^{4/3}\, d^3\vec{r} \qquad (22)$$

The contribution of $E_{c.exc.}$ to the HF potential is local and writes

$$v_{c.exc.}(\vec{r}) = -e^2\left(\frac{3}{\pi}\right)^{1/3} [\rho_p(\vec{r})]^{1/3} \qquad (23)$$

Some HF calculations including such an approximation have been tested against exact calculations [31] for light nuclei (from ^{16}O to ^{56}Ni). Relative errors for $E_{c.exc.}$ ranges from 5% to 8% (let us recall that $E_{c.exc.}$ represents roughly $(-0.76/Z^{2/3})$% of the direct Coulomb energy).

Practical resolution of the HF equations may lead to a systematical lack of binding energy. This can be first caused by the choice of too restrictive symmetries, as spherical or axial symmetry. So far the breaking of other symmetries, as left-right reflexion symmetry is generally not believed to play any role in the static description of nuclear ground states. With the exception of some HF codes working within the spherical symmetry, HF equations are generally solved, as we will see in the next section, by diagonalisation of the HF hamiltonian in a truncated basis. A dependence of the binding energy on the parameters defining the basis is yielded by this practical way of resolution. Such a dependence is sometimes very important, for instance is the size of the basis is small (see the discussion of section 5). The resulting lack of binding energy will be called the truncation energy. The question then arises of how one can determine such an energy ? For the Skyrme force case one can proceed in the following way. First one assumes that for a given size of the basis the truncation energy is independent on the deformation. On the other hand the truncation energy is known for the spherical solution since a direct resolution of the HF equations in the $\vec{x}$ space is available [11]. Therefore one can in such a way estimate truncation energies, even for deformed nuclei. In the Skyrme case [11],[12] parameters have been fitted by a direct comparison between calculated (with truncation correction) and experimental [44] binding energies. This was not the case for instance in the case of the Gogny force [9], where no spherically symmetric solutions were available to establish the truncation error. The parameters in that case have been fitted in such a way that nuclear masses computed in a reasonnably sized basis (∿7 major shells for s-d

shell nuclei, ∿11 for rare earth nuclei, ∿13 for actinide nuclei) fits relatively well with experimental ones.

In sub-section 2.3, the limitation of HF+BCS calculations with respect to fully consistent HFB calculations have been already discussed. Let us simply reformulate that when pairing correlations are present in the way we have included them, our solutions, being not eigenstates of the number of particles operator, are mixtures of different nuclei. This might have some importance in regions where any kind of transitions occurs where the nucleon number is changed. This could be in principle remedied by a projection on states having a good number of particles but has not been done in the calculations reported here.

We will now turn the discussion on some limitations arising from the independent particle or quasi particle character of our ansatz (HF, HF+BCS or HFB) for the ground state wave functions. Such wave functions are eigenstates neither of the total angular momentum nor of the total linear momentum. Both approximations introduce spurious energies due to the rotation or to the center of mass motions. When the collective variables associated with one or the other mode can be easily decoupled from intrinsic ones (e.g. for the rotation in the perfect rotor case, for the translation in the harmonic oscillator case) one knows the exact amount of energy to substract to the calculated HF mass. In that case this energy is for rotation *) 33] :

$$E_{rot.} = \frac{\hbar^2}{2\mathcal{J}} \langle \vec{J}^2 \rangle \qquad (24)$$

and for translation

$$E_{transl.} = \frac{\hbar^2}{2M} \langle \vec{P}^2 \rangle \qquad (25)$$

where the expectation value are to be taken on the HF wave function, and where $\mathcal{J}$ and M are respectively the total moment of inertia and the total mass of the nucleus. Generally the correction (25) has been taken into account during the variation of the individual states, whereas the correction (24) has been included after variation. It could be added that in the calculations using the Skyrme force [12], only an approximate correction energy (25) has been used, precisely the two body part of $\vec{P}^2$ has been omitted. The latter approximation has been tested [34] and found to only result in a slight renormalisation of the parameters of the force.

More generally, long range correlations are known to play an important role in some nuclei (as the so-called vibrational nuclei). Their systematical inclusion which is presently far beyond the theoretical possibilities, would lead to a lowering of the calculated total energies. On the other hand it could be also said in other words that our approach is purely static. Choosing a set of collective variables, we assume that the ground state is defined as the absolute minimum in the energy surface obtained by the variation of all the collective variables. Since the inertial parameters may in principle (and do in many cases) vary strongly with the collective coordinates, a correct dynamical treatment could produce a displacement in the location of the ground state out of the statically defined one.

For symmetry reasons, one would expect a list of advantages to be found in HF calculations of nuclear masses, at least as long as the list of drawbacks. This will not be the case, mainly since advantages are only relative concepts. The related approaches to be compared with,are the extrapolation formulas and the liquid drop approach supplemented by the Strutinsky method. We have already recalled the limitations of the first approach, whereas we have previously insisted on the main problem of the second approach : the degree of consistency between parameters of its two ingredients (liquid drop model and shell model). On the other hand the Strutinsky method is faced with the problem of finding a correct parametrisation of the shell model for all region of nuclides [35] and of the liquid drop model especially for light nuclei [36]. Would such a fit be correct, again the above recalled inconsistency might lead to very bad results when the Strutinsky method is applied to light nuclei (e.g. ^{40}Ca [23-24]). Moreover the goodness of a fit does not imply the validity of extrapolation towards unknown region of nuclei if the correct concepts are not included in the theory.

Such a perspective is proper to understand the relative validity of the HF approach to nuclear masses. We do believe indeed, that even though drastically approximate, a solution of the many body problem out of a two body force provides an a priori correct scheme for extrapolation to unknown nuclear species. Such a confidence is substantiated by the fact that with the Skyrme force one is able to reproduce rather accurately a lot of nuclear properties on the whole chart of nuclides with only 6 constant parameters.

If it is apparent that HF calculations provides the more fundamental practical approach to nuclear masses, it remains to be shown that their results favourably or at least equally compare with those produced by more phenomenological methods. This will be the subject of section 6. However it is important to sketch rapidly at that point, some of the technical methods which have allowed the practical achievement of such calculations.

5. Short survey of main techniques in use

Two features dominate the technical problems raised by the practical resolution of the HF equations. The first is

*Clearly all calculated spherical nuclei correspond exactly to zero total angular momentum states as long as all magnetic substates of a subshell are equally filled, which is generally the case.

the analytical form of the interaction. For instance, as we have seen in section 2, the HF equations are considerably simplified in the case of Skyrme like forces. The second important feature consists in the symmetries imposed to the HF solution. In the case of the spherical symmetry, the angular variables are trivially taken into account and one is left simply with a one variable integro-differential (if not purely differential) system of equations. With axial symmetry one is left with a two variable problem.

For the practical resolution of HF equations two main possibilities are offered : either one projects these equations onto the $\vec{x}$ representation or one does it onto harmonic oscillator states. The first case is well suited for spherically symmetric solutions. Such integro-differential systems have been first solved by Brueckner et al. [42] and by Vautherin and Veneroni [37]. With Skyrme like forces the resolution of the HF differential system is quite easy to be achieved for spherical solutions [11]. For deformed nuclei, the resolution of the HF equations in the configuration space has not generally been adopted. On the contrary the projection onto a deformed harmonic oscillator basis has been widely used.

One of the main technical problem is the computation of the two body matrix elements v for such basis states labelled φ_i. Consider such a matrix element in the one dimensional case as

$$\langle ij|v|k\ell\rangle = \int \varphi_i^*(x_1)\varphi_j^*(x_2)v(x_1-x_2)\varphi_k(x_1)\varphi_\ell(x_2)dx_1dx_2 \qquad (26)$$

There are two methods to evaluate the integral (26). One consists in changing the product $\varphi_i(x_1)\varphi_j(x_2)$ by a Moshinsky transformation into states whose arguments are $(x_1+x_2)/\sqrt{2}$ and $(x_1-x_2)/\sqrt{2}$ [54-55]. The same is done for $\varphi_k(x_1)\varphi_\ell(x_2)$ and then the center of mass variable integration is readily done to yield a simple integral in the relative variable. This integral is given analytically if the force is e.g. gaussian or has a zero range character. For more complicated forces as the coulomb one one is lead back to the gaussian case by simple integral representations [55]. An alternative method to compute (26) has been proposed [56] and recently widely extended [57]. It consists in using the property of a product of two harmonic oscillator wave functions which can be written as the following restricted sum :

$$\varphi_i(x)\varphi_j(x) = \pi^{-1/4} \sum_k \sqrt{\frac{i!\,j!\,k!}{\left(\frac{i+j-k}{2}\right)!\left(\frac{i+k-j}{2}\right)!\left(\frac{j+k-i}{2}\right)!}}\, e^{-x^2/2}\varphi_k(x) \qquad (27)$$

$((i+j+k) = \text{even})$.

Furthermore if v is a gaussian, one uses an integral equation transforming $\int v(x_1-x_2)\varphi(x_1)dx_1$ into a harmonic oscillator wave function $\varphi(\alpha x_2)$, α being related to the width of the gaussian. The remaining integral for the x_2 variable is then trivial.

It should be emphasized that the method of projection onto an harmonic oscillator basis implies the use of truncated basis. As well known this introduces for a given size of the basis a dependence of the HF solution on the basis parameters, i.e. for the axial symmetry case the two frequencies $\omega_\perp$ and ω_z or equivalently $q=\omega_\perp/\omega_z$, $b=\sqrt{m\omega_0/\hbar}$ (with $\omega_0^3=\omega^2\omega_z$). In the spirit of the HF variational method, one searches for the lowest possible energy and therefore tries to minimize $E_{HF}(b,q)$ viewed as a function of b and q. The result of such a two dimensional minimization is reproduced in Fig.3 for the ^{248}Cm deformed nucleus [48], whereas in Fig.4 the variation of $E_{HF}(b,q=1)$ is given for the spherical nucleus ^{40}Ca [49]. The similar behaviour of $E_{HF}(b)$ for various effective interactions can be noticed.

6. Discussion of some selected HF results

Binding energies of some spherical nuclei obtained in the effective force calculations of Negele [1] and of Campi and Sprung [2] are displayed on Tables 2 and 3. Calculated values and experimental ones [44] are in reasonable qualitative agreement. In Table 2, the results of an approximation [30] to the calculations of Negele are also reported. Such an approximation is obtained by expanding the density matrix in order to produce a total HF energy given by an equation similar to Eq.(7), thus carrying most of the numerical simplicity of the Skyrme like forces. As seen on Table 2, the results obtained in this approximation (DME) are found in better agreement with experimental figures than those obtained in exact calculations (DDHF). However it should be mentionned that the effective force used in DME had not the same phenomenological correcting part than the one included in DDHF. On Fig.5 binding energies of even tin isotopes calculated [50] with the effective force of Campi and Sprung, are compared with experimental ones [44]. Pairing correlations are included in a HF+BCS way for neutrons. The reproduction of known masses is found excellent.

Gogny [9] has been the first to perform HFB calculations which are complete in the sense that no restricted (at least in principle) space is used for the variation of the quasi particle states and no kind of inert core is introduced. Such calculations have been extended in the whole chart of nuclides for spherical and axially symmetrical nuclei. Table 4 illustrates one of the main feature of such calculations. Splitting the HFB energy into two parts, one E_H stemming from the HF potential $v(\rho)$ and the other E_P from the pairing gap tensor Δ, one finds that the introduction of pairing correlations increases E_H and decreases E_P, resulting as expected in a lowering of the total energy. For all calculated nuclei the absolute value of the difference between calculated and experimental masses [44] lies within 0 and 5 Mev. Such a statement however is simply indicative since one should been in mind the problem encountered in that case with the truncation energy as recalled in section 4.

With simple phenomenological forces as the Skyrme force, one can rather cheaply perform a lot of HF calculations assuming the spherical symmetry for the solutions. The results for binding energies obtained with the Skyrme SIII force are summarized on Fig.6. The solid line corresponds to results obtained for nuclei located along a path in the N-Z plane, wiggling accross the stability valley. In region were nuclei are known to be deformed, the assumption of spherical symmetry leads to a lack of binding. For some nuclei, deformed ground states are available [48,51-52]. Estimating the truncation error as sketched in section 4,one yields agreement with experimental masses [44] better by far. As a result,calculated binding energies disagree by less than 5 MeV on the whole chart of nuclides. Rather similar results are obtained for spherical HF solutions obtained in the so-called energy density formalism [8]. Figure 7 shows the results of the latter calculations for the determination of the neutron and proton drip lines [53]. It should be stressed again that such calculations assume spherical symmetry and therefore might be corrected for specific deformation effects.

The determination of ground state properties needs sometimes a correct knowledge of the deformation energy curves. This is particularly the case of the so-called shape-transitional nuclei like the Cadmium isotopes calculated [45] with the Skyrme SIII force whose results are reported on Fig.8. Indeed one has to decide wether the ground state has an oblate or a prolate shape. No real choice is left in fact and one takes generally the solution yielding the lowest HF energy, but this is not free of all the questions raised in sections 2 and 4 (pairing treatment, dynamical effects, imposed symmetries, rotational spurious energies,...). However such calculations provide rather useful informations, in particular they ascertain the "soft" character of such nuclei.

In the HF calculations of neutron rich sodium isotopes of Ref.46], not only binding energy systematics has been fairly accounted for, but also a hint on the possible deformation behaviour of such isotopes has been proposed. The prolate side of deformation energy curves calculated with the Skyrme SIII effective force are displayed in Fig.9. Inspecting Fig.10, one clearly sees that for N=20 a negative shell effect should occur for a rather large ($\beta \sim .4, Q_p \sim 50$fm) deformation. Its origin is simply related to the crossings of 1f7/2 and 1d3/2 subshells. In fact one sees on Fig.9 the appearance at such a deformation of a secondary minimum for the ^{31}Na isotope. For this particular isotope the more deformed minimum lies higher in energy but correcting approximately (as written in (24)) for the spurious rotational energy makes the more deformed state more bound than the other minimum. This is summarized on Fig.11 together with other useful informations. The experimental results of Ref.58] have been displayed in the form of the two neutron separation energies B_{2n}. The most striking fact is the raise of the quantity B_{2n} for A=31. As in other nuclear regions, this could be related to a sudden change of deformation. Such an explanation is substantiated by the calculational results of Ref.46] as demonstrated in Part c) of Fig.11. Part a) displays quite a nice example of possibly misleading agreement between regional calculations and experimental results. Assuming spherical symmetry, HF results (with the Skyrme SIII force) just fit the B_{2n} systematics in the vicinity of the ^{31}Na nucleus. In fact it is purely coincidental as the bad results for lower value of N demonstrate. On the other hand it is interesting to notice the discrepancy between spherical solutions obtained with Skyrme SIII and SIV forces compared with their overall agreement when deformation is allowed. This example clearly indicates that one should exert caution before concluding from a too restricted sample of calculational evidence.

The stability of superheavy elements is known to be related to negative shell effects at sphericity producing a trap in the continuously decreasing liquid drop deformation energy. On Fig.12 the deformation energy of one possible candidate $^{298}114$ is displayed. It has been calculated [47] with the Skyrme SIII force and exhibits a first fission barrier which is lower than those obtained within the Strutinsky method [59-61]. Predictions of beta and alpha decay properties have been also derived from calculated HF masses with the help of some simple approximations. They are generally, as for the fission mode, more pessimistic than those calculated in more phenomenological approaches [59,32]. Finally an example of spherical single particle spectra near the Fermi level for some superheavy nuclei is displayed in Fig.13. The proton number Z=114 and to a lesser extent Z=120 and 138 together with the neutron numbers N=184 and 228 are found to be possible candidates for a sufficiently negative shell effect. One interesting detail lies in the fact that the gaps are self-consistently dependent on the filling of levels. For instance, in $^{292}114$ the gap at N=184 is 2.2 MeV and only 1.6 MeV in $^{298}114$, or in $^{348}120$ the gap at Z=120 is 1.4 MeV and only .7 MeV in $^{304}120$. This is of course of some importance to our problem and it is to be considered when appreciating the results obtained from phenomenological mean potentials. However as previously said, in that case the predicting power of all calculations (including HF) is greatly diminished a priori by the absence of an explicit tensor force.

7. Conclusion

It was the aim of this review to show how far HF determinations of nuclear masses have reached both in the technological aspects and in the precision of results. It is fair to conclude that for known nuclei they produce results which are in general as good as those obtained by more phenomenological approaches, whereas for unknown nuclei they provide a convenient tool for extrapolation.

Calculations within the HF appro-

ximation constitutes therefore a convenient tool for the study of nuclei far from stability, nothing more than a tool but quite an effective one which has already provided promising results.

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Nucleus	E_{HF}	$\tilde{E}$	$\bar{E}$	$\delta E_1(\tilde{\varepsilon})$	$\delta E_1(\hat{\varepsilon})$	$\delta E_2(\tilde{\varepsilon})$	$\delta E_2(\hat{\varepsilon})$
^{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
^{56}Ni	- 479.9	- 473.7	- 473.5	- 6.9	- 5.5	0.6	5.1
^{90}Zr	- 779.2	- 774.3	- 775.7	- 5.5	- 5.8	0.6	2.3
^{114}Sn	- 960.4	- 961.1	- 961.3	0.5	0.1	0.2	0.8
^{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

Table 1 : First order δE_1 and higher order δE_2 shell corrections calculated from HF solutions obtained with the Skyrme force (set of parameters SIII). The labels $\hat{\varepsilon}$ and $\tilde{\varepsilon}$ refer respectively to the version (21) of the Strutinsky energy theorem and to the one derived in Ref. 24]. For comparison, the two smooth energies $\bar{E}$ and $\tilde{E}$ (corresponding in that order to the two previous cases) are also reported along with the HF reference energy E_{HF}. Calculations were performed at the ground state deformations. Energies are given in MeV.

Nucleus	^{16}O	^{40}Ca	^{90}Zr	^{208}Pb
Exp	7.98	8.55	8.71	7.87
DDHF	7.59	7.99	8.33	7.83
DME	7.99	8.82	8.97	8.08

Table 2 : Comparison of experimental 44] and theoretical binding energies per particle expressed in MeV. The Negele force was used for DDHF results 1] and its approximation by Negele and Vautherin for DME results 30].

Nucleus	^{16}O	^{40}Ca	^{48}Ca	^{90}Zr	^{208}Pb
Exp	7.98	8.55	8.67	8.71	7.87
DDHF	7.68	8.33	8.40	8.63	7.87

Table 3 : Same table as table 2 but with the Campi and Sprung force 2].

Nucleus	^{70}Ge	^{114}Sn	^{118}Sn	^{122}Sn
$-E_{HF}$	601.7	968.4	1001.8	1017.9
$-E_P$	17.0	11.1	11.4	11.9
$-E_H$	590.4	959.1	993.2	1023.6
$-E_{HFB}$	607.4	970.2	1004.6	1035.5

Table 4 : Calculated binding energies in HFB calculations of Gogny 9]. Energies are given in MeV. The subscript HF refers to HF calculations and HFB to HFB calculations. The HFB energy is split into two pieces : E_H where enters the HF potential $v(\rho)$, E_P where enters the pairing gap tensor Δ (see formula (13) of the text).

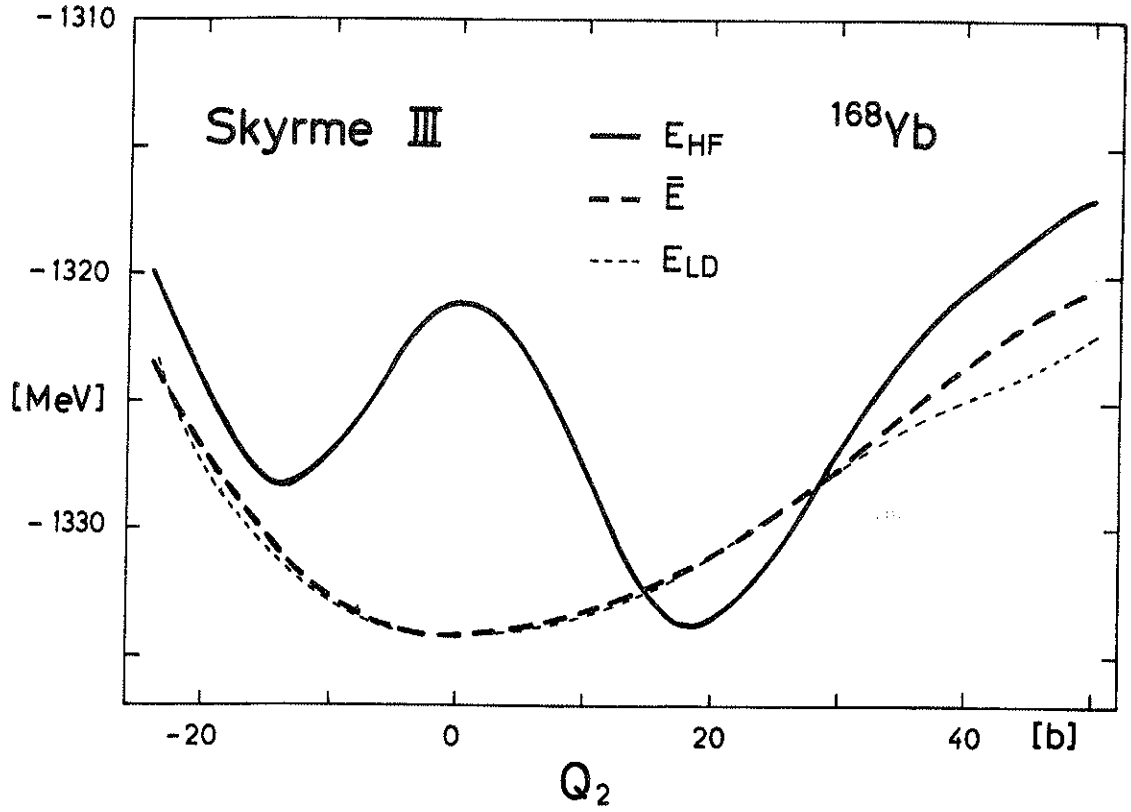

Figure 1 : Comparison of various deformation energy curves for the ^{168}Yb nucleus. The E_{HF} energy is obtained with the Skyrme SIII force, whereas $\bar{E}$ is the corresponding zero order part defined in the formula (21) of the text. The energy E_{LD} is obtained with the Myers and Swiatecki liquid drop parameters [17] . The energies E are plotted versus the mass quadrupole moment Q expressed in barn.

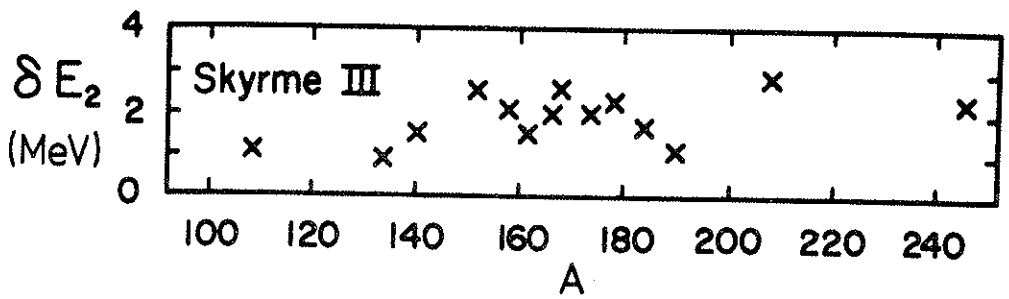

Figure 2 : Variation of the sum of higher order terms δE_2 defined in the formula (21) of the text as a function of the nucleon number A. Calculations [22] have been performed with the Skyrme SIII force.

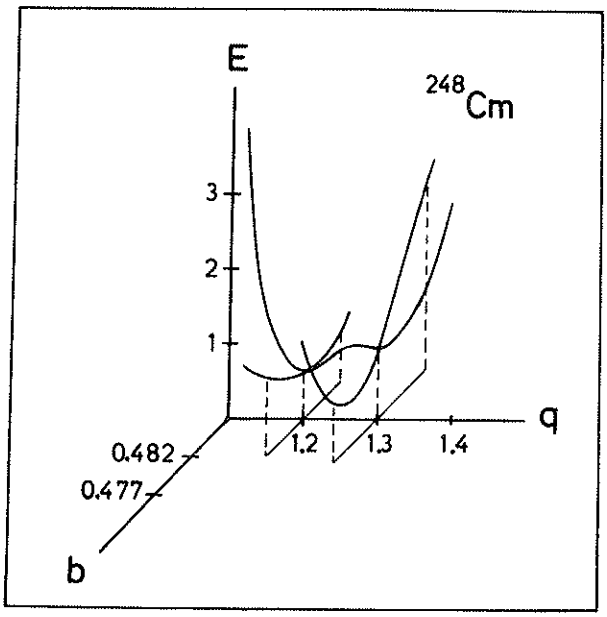

Figure 3 : Example of a two parameters optimization of the HF energy E, for a typical deformed nucleus [48]. Basis parameters b and q are defined in the text and energies E are expressed in MeV. The Skyrme SIII force has been used.

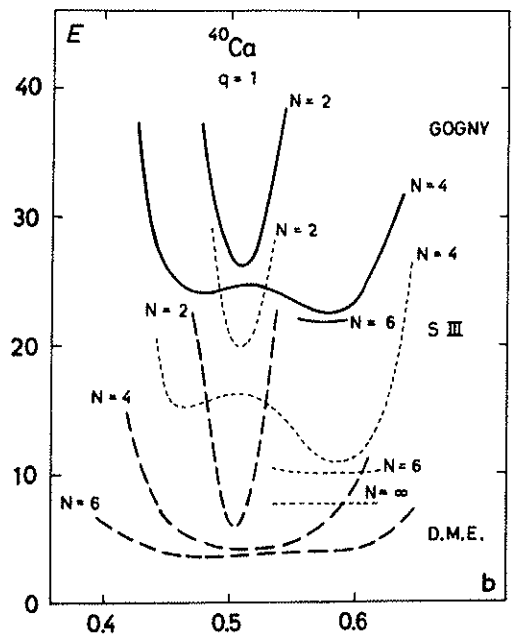

Figure 4 : Example of a one parameter optimization of the HF energy E for the ^{40}Ca nucleus [49]. The solid lines correspond to the Gogny force [9], the dotted line to the Skyrme SIII force [12] and the dashed one to the DME approximation [30] of the Negele force [1]. The numbers N refer to the size of the spherical harmonic oscillator basis (N=n means n+1 major shells included in the basis). The line N=∞ refers to a calculation in the x space [11]. Energies computed with different forces have arbitrary origins and are expressed in MeV. The parameter b is defined in the text.

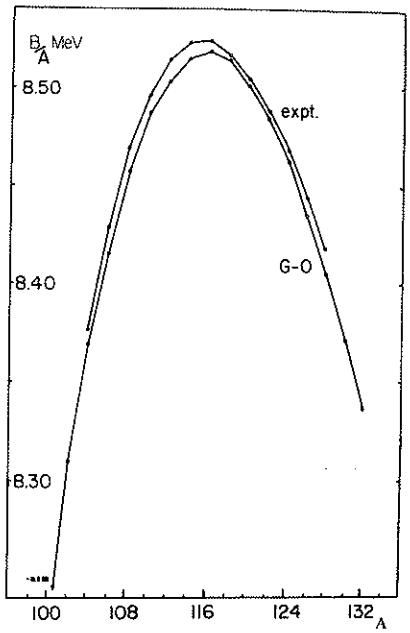

Figure 5 : Comparison of experimental [44] and calculated [50] binding energies per particle for tin isotopes. Spherical symmetry has been assumed. The GO force of Campi and Sprung [2] has been used. Energies are plotted against the nucleon number A.

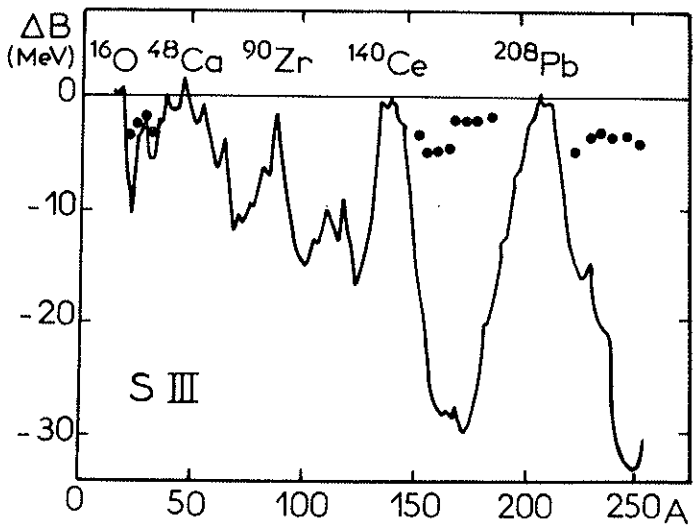

Figure 6 : Comparison of energy differences between calculated[12] and experimental [44] binding energies. The Skyrme SIII force has been used. The solid line has been obtained along some paths accross the stability valley and with spherical symmetry assumed. Dots correspond to energy differences corrected for the deformation energy (s.d. shell nuclei : 51], rare-earth nuclei : 52], actinide nuclei 48]). Energy differences defined as $\Delta B = B_{calc} - B_{exp}$, are plotted against the nucleon number A.

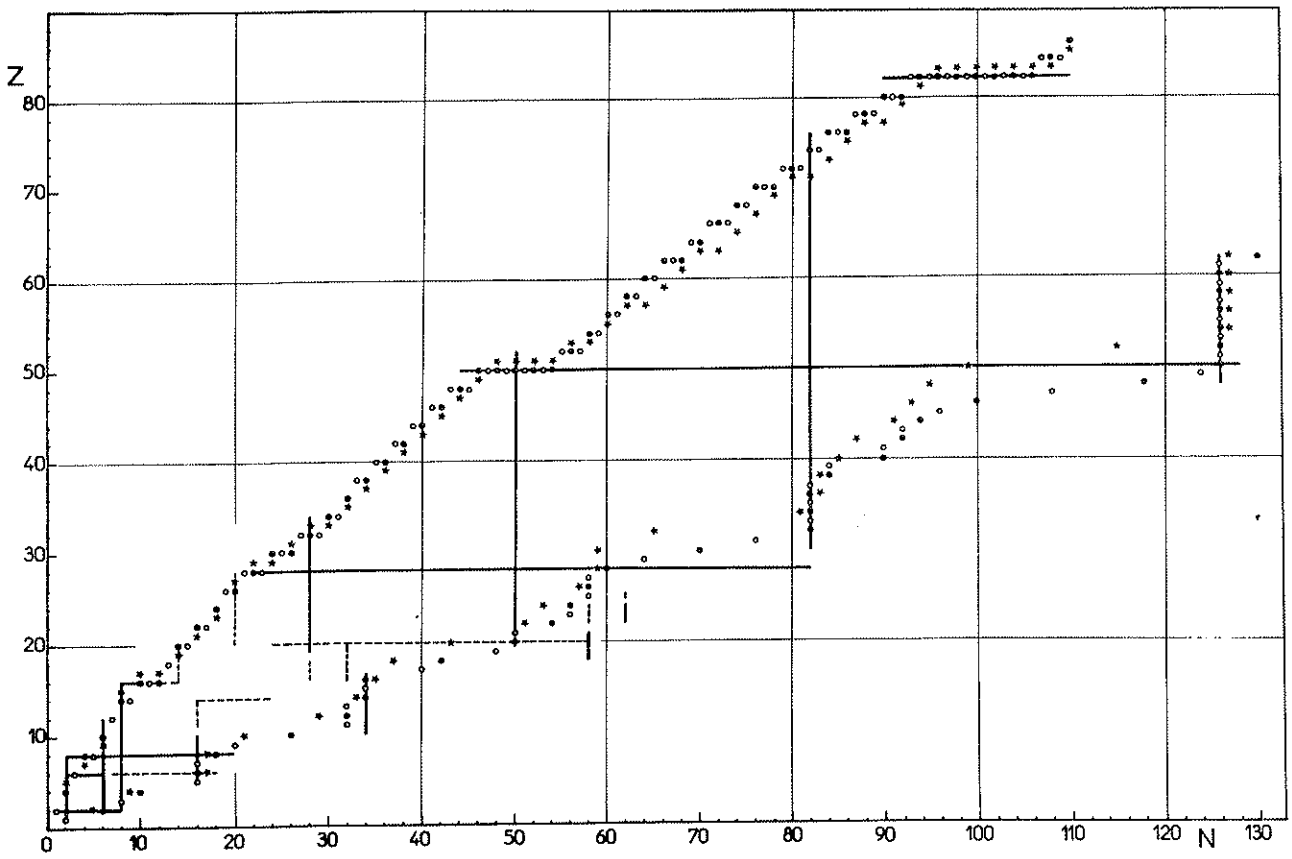

Figure 7 : Structure of the nucleon drip lines for light and medium spherical nuclei [53]. Full circles indicate the last doubly even stable nuclei. Open circles denote the last even-Z odd-N stable nuclei on the proton side and the last even N odd-Z stable nuclei on the neutron side. Stars indicate the first unstable nuclei for odd-Z on the proton side and for odd-N on the neutron side. The thick lines indicate the position of the magic numbers ; the dotted lines show the semi-magic numbers.

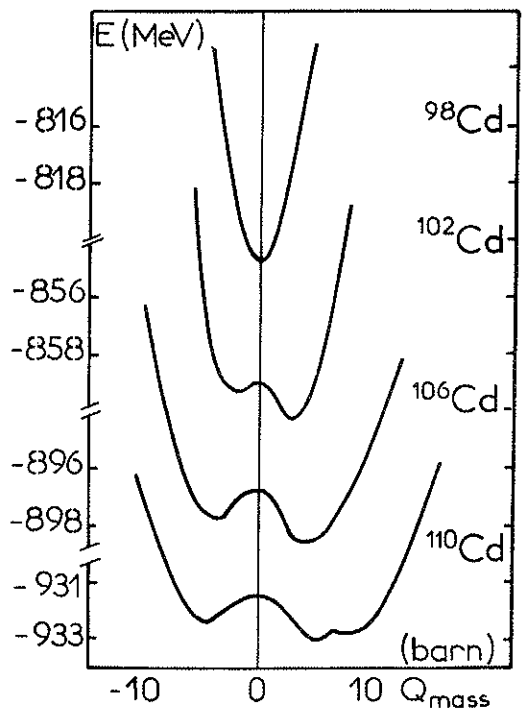

Figure 8 : Deformation energy curves as a function of mass quadrupole moment for some Cadmium isotopes. Calculations [45] have been performed with the Skyrme SIII force.

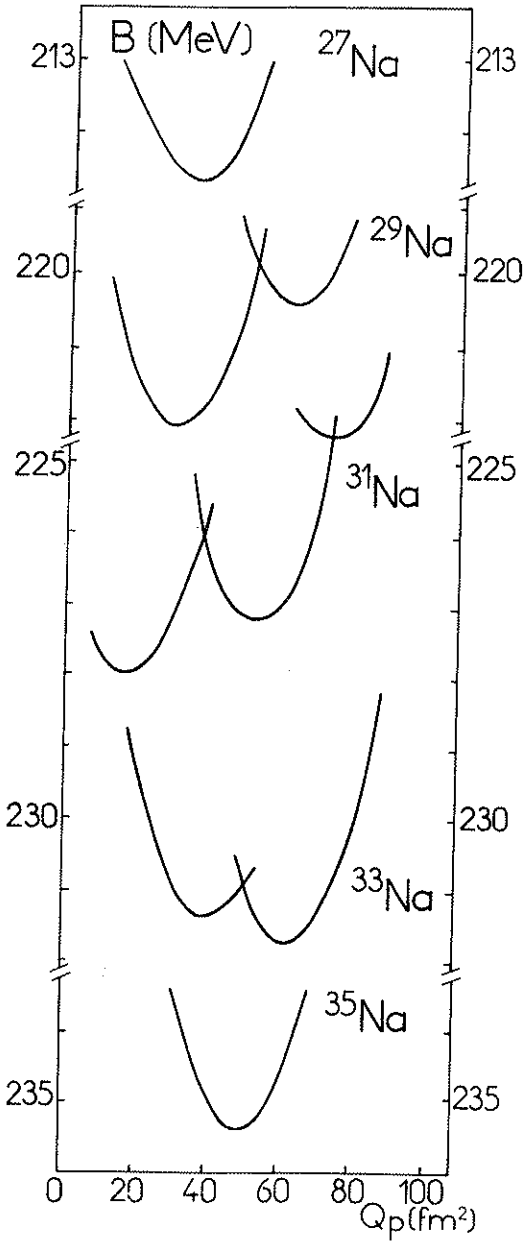

Figure 9 : Deformation energy curves as a function of proton quadrupole moment for some odd sodium isotopes. Calculations [46] have been performed with the Skyrme SIII force.

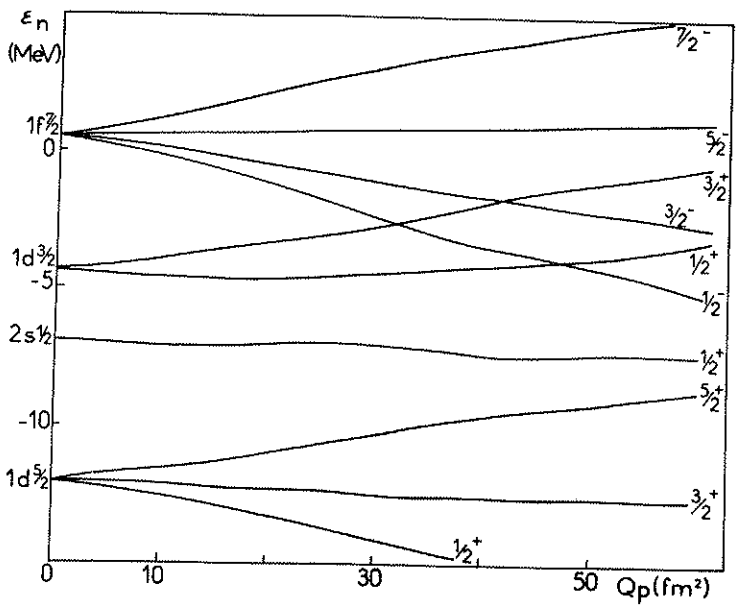

Figure 10 : Single particle neutron spectrum of ^{31}Na as a function of the proton quadrupole moment (prolate part only). For the spherical symmetry case, levels are labelled by nℓj whereas for deformed states they are referred to by Ω^{π}. Calculations [46] have been performed with the Skyrme SIII force.

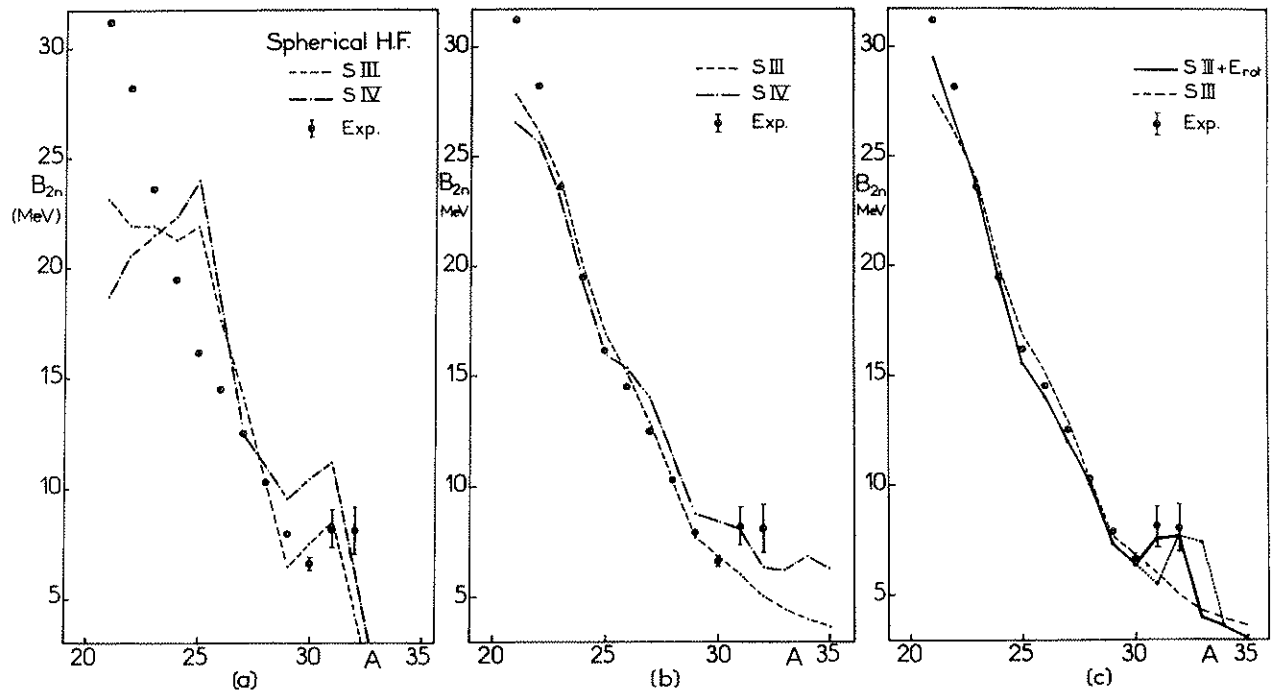

Figure 11 : Comparison of calculated [46] and experimental [58] two neutrons separation energies B_{2n}, as a function of the nucleon number A. Calculations have been performed with SIII and SIV effective forces. Part a) of the figure is obtained when the spherical symmetry is imposed, Part b) when deformation is allowed. In Part c) the solid line represents the calculated B_{2n} after rotation energy correction as defined in the formula (24) of the text. The dashed line is the same as in Part b). The dotted line corresponds to B_{2n} energies not corrected for rotation energy but obtained when the more deformed minimum is used in the computation of B_{2n} in the ^{31}Na region (see text).

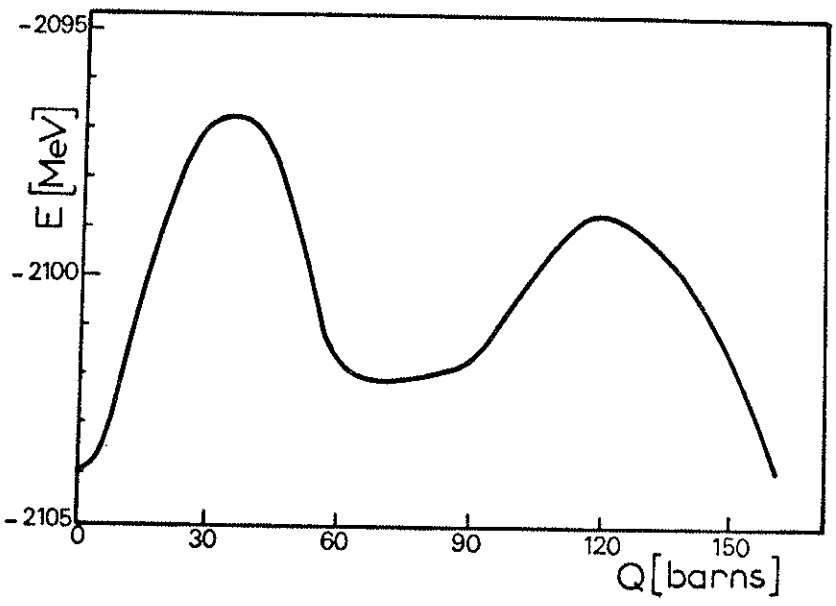

Figure 12 : Fission barrier of the ^{298}114 nucleus expressed as a function of the mass quadrupole moment. Calculations [47] have been performed with the Skyrme SIII force.

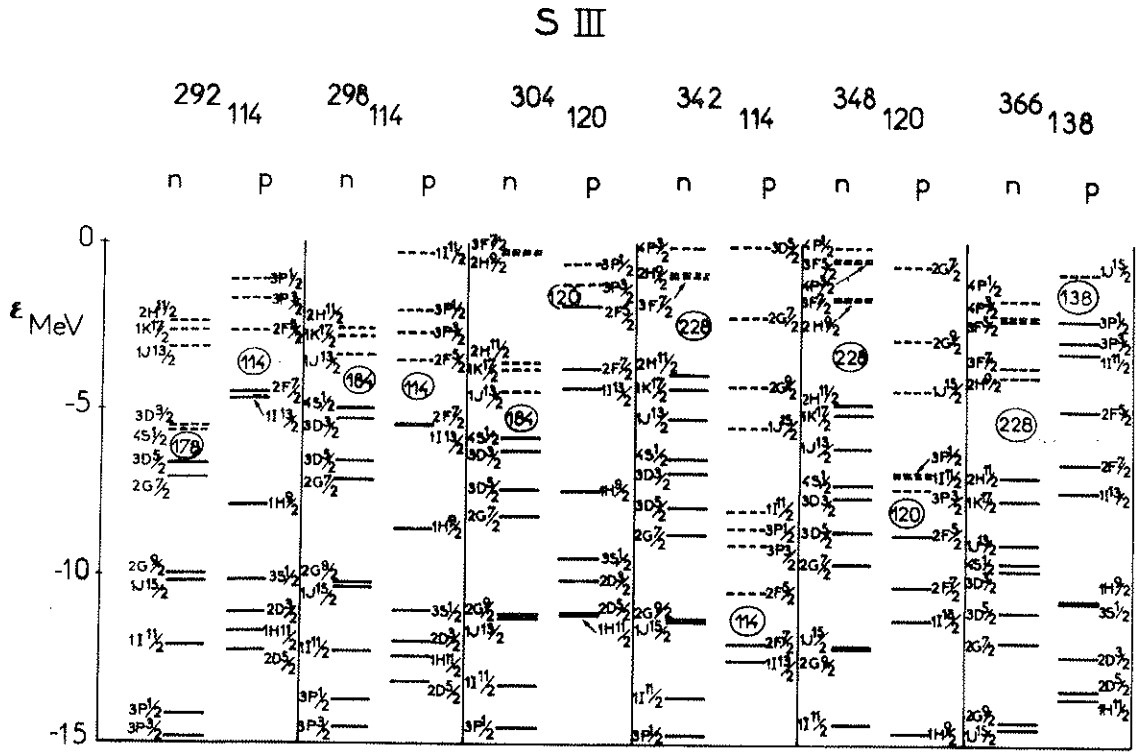

Figure 13 : Calculated single particle spectra near the fermi level of some super heavy nuclei. Calculations [47] have been performed with the Skyrme SIII force.