NUCLEAR BULK PROPERTIES CALCULATED FROM EFFECTIVE SKYRME INTERACTIONS: HOW FAR CAN THEY BE EXTRAPOLATED?

M. Brack, Institute for Theoretical Physics, University of Regensburg, D - 8400 Regensburg, W.-Germany

Abstract

The present status of Skyrme-Hartree-Fock calculations of nuclear bulk properties is briefly reviewed. Comparison is made to the liquid drop plus shell-correction approach and to semiclassical methods.

Preface

When I set up the title of this talk almost a year ago, it was my hope to give an extensive review about Hartree-Fock calculations of nuclear bulk properties with effective Skyrme interactions and to discuss their power of extrapolation to unknown regions. In particular, it was our hope - i.e. of my collaborators mentioned below and myself - to come up with a "new force" of the Skyrme type which would be free of all deficiencies known to us from older parametrizations and which could be used for extrapolations far off the stability line.

As it happens again and again, time went faster than our progress, and I will therefore not give any clear answer to the question put in the title of my talk. I shall nevertheless try to discuss a few merits and drawbacks of the Skyrme-HF method and compare it to the combined liquid-drop-plus-shell-correction approach, which still is the most popular method of calculating nuclear binding energies, as well as to some more recently developed semiclassical approaches.

More elaborate effective nuclear interactions with finite range have been derived and successfully used [1-4]. For simplicity I shall restrict the discussion to forces of the Skyrme type; most of the considerations can, however, also be applied to these other forces.

Many of the ideas put forward below are not of my own. I shall therefore at this place thank my colleagues, from whom I have been learning during our collaboration and exchange of ideas: P. Quentin and J. Bartel at Grenoble; J. Meyer at Lyon; H. Flocard, J. Treiner and H. Krivine at Orsay and, last but not least, C. Guet and H.-B. Håkansson at Regensburg.

1. Situation of Skyrme-HF calculations til 1980

The development of Skyrme type effective interactions [5-6] has made it possible to perform systematic Hartree-Fock calculations not only for many stable nuclei in their ground states [7], but also for fission barriers of heavy [8] and superheavy nuclei [9,10]. (For an extended review, comprising also other effective forces, see ref.[11].)

Let us briefly summarize the situation, as it presented itself at the end of the seventies for the HF-calculation of nuclear ground state properties and fission barriers. We hereby refer to calculations made with the traditional Orsay "family" of Skyrme forces SI - SVII [6,7], of which SIII is the favourite parametrization.

a) Binding energies: For spherical nuclei from O^{16} to Pb^{208}, the HF energies obtained with SIII agree up to $\sim$ 2 MeV with the experimental binding energies. For deformed nuclei, truncation errors and spurious rotational energies have to be estimated and subtracted, leading to an overall agreement within $\sim$ 2-4 MeV. Such a good agreement is quite amazing in view of the fact that only 7 parameters (including spin-orbit and a pairing strength) have been adjusted once for all. Concerning extrapolations away from stability, similarly good results have been obtained by Campi et al.[12] for the binding energies of neutron-rich sodium isotopes up to Na^{32}.

b) Densities, radii and quadrupole moments:

Apart from the notorious wiggles obtained in any independent-particle approach, the HF proton densities allow fairly good fits to elastic electron scattering cross sections, although they tend to be a little too steep in the surface region. Charge r.m.s. radii agree within about 2 % for light nuclei and $\sim$ 1 % for heavy nuclei with the experimental ones. It should be mentioned, though, that the Ca^{40} - Ca^{48} isotopic shift does not come out correctly. The intrinsic quadrupole moments of rare-earth and actinide nuclei agree with the experimental ones within $\sim$ 2-4 %, including the recently measured fission isomers (see the review ref. [13]).

c) Fission barriers:

The first really negative result of HF calculations is the by now established fact [14] that the Skyrme forces which lead to these nice groundstate properties seem to fail when extrapolated to large deformations such as encountered at the fission saddle point of Pu^{240}: The height of the outer barrier is larger than the experimental one by roughly a factor of 1.5 - 2. The same result was obtained in HFB calculations with the Gogny force [15].

The failure of HF calculations to reproduce fission barriers shed some doubts upon their power of extrapolation away from the nuclear ground states. The question arose whether something essential was wrong with constrained HF calculations, whether an ingredient of the force was missing which only showed up at large deformations, or whether one simply had not made the Skyrme-parametrization flexible enough. As it turned out (luckily), the latter case is true, as we shall see in sect. 4 below.

Another drawback of the Skyrme force baring upon the reliability of extrapolated HF calculations has been pointed out in ref.[10]: the sensitivity of the barrier heights of superheavy nuclei to the spin-orbit strength parameter W_0. As shown in ref.[10], a $\sim$ 10 % variation of W_0 can easily affect these barriers by several MeV and thus the fission life times by many orders of magnitude, or even turn a spherical nucleus into a deformed one. The spin-orbit term is thus the weakest part of the Skyrme forces, and great care should be taken in determining W_0 by fits to single-particle spectra.

2. Connection between HF and the shell-correction approach

Before turning to the most recent developments with Skyrme-HF calculations, let us briefly review their merit in testing the liquid-drop(let) plus shell-correction approach, which up to date still provides the most popular and refined tool for fitting mass tables. (For the most recent mass table using this method, see ref. [16].)

The shell-correction method need not be introduced here; it was presented by Strutinsky at the Lysekil Symposium which started this series of conferences 15 years ago[17]. (For a recent review concerning its application to fission, see ref.[14]). What concerns us here is how it can be related to the HF method, both in principle and numerically. Its theoretical derivation from the HF theory has been given by Strutinsky[18] and later discussed by many authors. Their references may be found in a recent publication[19] which contains both the formal developments, starting from the HFB framework, and the results of extended numerical tests based on HF calculations. The main results are the following:

a) The exact HF energy for any nucleon number at any deformation (obtained, if necessary, with an external constraint) is reproduced within less than $\sim$ 0.6 MeV by

$$E_{HF} = \tilde{E}_{HF} + \delta E, \qquad (1)$$

where $\tilde{E}$ is the selfconsistently averaged HF energy (kept at the same deformation as E_{HF}) and δE is the usual (first order) shell-correction calculated in terms of the eigenvalues $\hat{\varepsilon}_i$ of the corresponding selfconsistent average HF-potential $\tilde{V}_{HF}$. (This result is extendable to include pairing correlations and finite temperatures; see ref.[19].)

b) The energy $\tilde{E}_{HF}$ has all the properties of a liquid drop[20] or droplet model[21] energy. The quantity δE is very close (usually within $\sim$ 1-2 MeV) to the shell-correction obtained under the same conditions (same particle numbers, same deformation) from a phenomenological shell-model potential.

From this we can conclude that the shell-correction approach is in principle equivalent to the HF method. However, we have purposely underlined the word "selfconsistent" above: for the approximation eq. (1) to be good, it is essential that both the energy $\tilde{E}_{HF}$ and the potential $\tilde{V}_{HF}$ be derived selfconsistently from the same interaction. This is not guaranteed for the currently used phenomenological liquid drop and shell models. In fact, the so-called "Pb-anomaly" encountered in shell-correction calculations with a Woods-Saxon potential[22] can be traced back to a lack of selfconsistency[19].

Of course, a slight readjustment of one or several of the many parameters entering the liquid drop(let) and shell models might help to curve such a deficiency. But the quality of a mass fit obtained in this way is then not necessarily a guarantee for a successful extrapolation to unknown regions.

3. Semiclassical approaches

One obvious first attempt to cure the fission barrier problem mentioned in sect. 1 above would be a new fit of the Skyrme parameters, thereby imposing the correct barrier height. However, the rather large computation times of constrained HF calculations for heavy deformed nuclei prevent one to do this on a systematic scale. There is thus a need for more economical, but still selfconsistent methods for the calculation of fission barriers from a given effective interaction.

The use of semiclassical approximations, giving up temporarily the shell effects, can be justified from eq. (1) and the corresponding numerical results [19]: selfconsistency is important only for the average energy $\tilde{E}_{HF}$, potentials $\tilde{V}_{HF}$ and densities $\tilde{\rho}$; the shell-corrections can be added perturbatively after this average selfconsistency has been reached. Now, it has been shown[23] that the Strutinsky averaging procedure used to obtain $\tilde{E}_{HF}$ in ref.[19], is completely equivalent to a semiclassical approximation to the energy based upon an expansion of the partition function (or, equivalently, the Bloch density) in powers ot $\hbar$. Therefore the microscopical calculation of $\tilde{E}_{HF}$ can be replaced by a variational calculation with the energy density method, using a semiclassical local density expansion of the kinetic energy.

Such calculations have recently become rather popular, using Skyrme interactions which lend themselves ideally to the energy density method [24-31]. We should, however, emphasize that the use of an incomplete kinetic energy functional with adjustable parameters, as it has been used by several authors [27-29,32], is a priori not justified and fails when applied to fission barriers. As pointed out in ref.[33], this functional is uniquely given and contains gradient terms of fourth order which are important for the calculation of deformation energies and for the correct description of the nuclear surface. All fourth order terms, as derived in ref.[34] including effective mass and spin-orbit contributions which are indispensible with realistic Skyrme forces, have been used in a parameter free way by Guet et al.[26,30,31], who calculated for the first time fission barriers with the semiclassical energy density method. The present status of these calculations, which soon will be published in detail[35], can be summarized as follows:

a) Deformation energies and in particular, fission barrier heights agree within $\sim$ 1-2 MeV with those of averaged HF calculations; the time saving factor is > 100. As in the exact HF calculations, the semiclassical barrier obtained for Pu^{240} with the SIII force is too high: about 10 MeV compared to the empirical liquid drop barrier of $\sim$ 4 MeV (see, e.g., ref. 22). In fact, for all of the Orsay Skyrme parameter sets SII-SVI[7] the average barrier heights are around $\sim$ 8-12 MeV.

b) Proton and neutron r.m.s. radii agree within less than 1 % with the HF radii. The surfaces and tails of densities follow very closely the HF ones.

c) The binding energies of spherical nuclei are lower by $\sim$ 1-2 % than the averaged HF energies. This defect is expected to be cured at the same time with the inclusion of the shell effects using a single HF iteration on top of the semiclassical results.

It is thus seen, that such calculations can, besides their interest per se, be used as very economical but accurate first estimates of nuclear bulk properties and are thus a helpful tool for refitting the parameters of Skyrme forces (see also sect. 4 below). Besides, the average energies and potentials thus obtained provide the ideal, selfconsistent input in Strutinsky type calculations (see eq. 1). Another application of the semiclassical energies is that they can serve to a very accurate determination of liquid drop or droplet model parameters for a given effective interaction. This will be discussed in detail in a separate contribution to this conference[36].

We shall not discuss an alternative approach running under the name "energy density formalism" in which single particle wavefunctions are used to calculate binding energies through some parametrized energy density, since this approach is not of semiclassical nature as we discussed it above, but, indeed, comes very close to a Hartree-Fock calculation. This method has been rather successful in producing mass tables[37,38] and will be represented by F. Tondeur at this Conference[39].

Another, purely semiclassical approach makes use of a partial resummation of the $\hbar$ expansion of the Bloch density[40], hereby leading to average densities which are well defined everywhere and thus free of the turning point divergences as they occur in the original $\hbar$ expansion[23]. In this way, the HF potential can be iterated directly without use of either wave-functions or kinetic energy density functionals.

Some first encouraging results for realistic Skyrme forces will soon be available[41].

4. New developments with Skyrme forces

In recent years, the improved experimental data on giant resonances have, together with their theoretical description with HF + RPA calculations[42], allowed to put new constraints on the parametrization of effective interactions. In particular, the observation of the breathing mode (see, e.g., ref.[43]) allows to pin down the infinite nuclear matter incompressibility K to be of the order of $\sim$ 220 MeV[44], rather than its old value of $\sim$ 350 - 400 MeV assumed in the SII-SVI Skyrme forces [7]. Similarly, the giant quadrupole (isoscalar) resonances give information about the effective nuclear mass[45] and the giant isovector dipole resonances about the isospin symmetry properties[27]. This combined information should be used in refitting Skyrme parameters in the future. Instead of the time consuming microscopical RPA calculations, sum rule relations[45] or dynamical semiclassical methods[46] may be helpful.

A systematic redetermination of the Skyrme force, incorporating both static and dynamical information and using microscopical and semiclassical techniques, is now in progress[47]. In fact, the force SkM obtained by Krivine et al.[27] from fits to giant isovector dipole resonances, has turned out surprisingly to solve the fission barrier problem: as first shown in the semiclassical energy density calculations of ref.[30,31] the average barrier height obtained for Pu^{240} with the SkM force is rather close to the empirical liquid drop barrier. Succeeding microscopic calculations[48] showed that the HF barrier indeed is slightly lower than the experimental one, in agreement with the most recent semiclassical results[35]. This tells us that the failure of the HF method in predicting the right fission barriers was only due to a lack in the Skyrme force parametrization. As it seems to come out of systematic investigations[35], the barrier heigth decreases with decreasing power α of the density dependent part $\sim t_3\rho^{\alpha}\delta^{(3)}(\vec{r}-\vec{r}')$ of the Skyrme force. (The forces SII-SVI have α = 1, whereas SkM has α = 1/6.) Parallel to this goes a decrease of the incompressibility modulus K (K $\approx$ 220 MeV for SkM). There is thus definite hope that new Skyrme forces soon will be available which allow extrapolations to large deformations and to excited states of the giant resonance type.

References

1) J.W. Negele, Phys. Rev. C 1 (1970) 1260
2) X. Campi, D.W.L. Sprung, Nucl. Phys. A194(1972)401
3) D. Gogny, "Nuclear Selfconsistent Fields", Eds. G. Ripka, M. Porneuf, (North-Holland, 1975) p. 333
4) for more references, see ref. 11) below.
5) T.H.R. Skyrme, Phil. Mag. 1 (1956) 1043; Nucl. Phys. 9 (1959) 615
6) D. Vautherin, D.M. Brink, Phys. Rev. C5(1972)626; D. Vautherin, Phys. Rev. C7(1973)296
7) M. Beiner et al., Nucl. Phys. A 238 (1975) 29
8) H. Flocard et al., "Physics and Chemistry of Fission 1973", Rochester (IAEA Vienna, 1974) Vol.I, p. 221; Nucl. Phys. A 231 (1974) 176
9) M. Beiner et al., "Nobel Symposium on Super-Heavy Elements", Ronneby, Physica Scripta 10A(1974)84
10) M. Brack, P. Quentin, D. Vautherin, "Int. Symp. on Super-Heavy Elements", Lubbock (Pergamon, New York 1978) p. 309
11) P. Quentin, H. Flocard, Ann. Rev. Nucl. Part. Sci. 28 (1978) 523
12) X. Campi et al., Nucl. Phys. A 251 (1975) 193
13) V. Metag, "Physics and Chemistry of Fission 1979" Jülich, (IAEA Vienna, 1980) Vol. I, p. 153
14) M. Brack, as ref. 13, p. 227
15) J.F. Berger, M. Girod, as ref. 13, p. 265
16) P. Möller, J.R. Nix, Nucl. Phys. A361(1981)117
17) V.M. Strutinsky, International Symp. "Why and how ... ", Lysekil, (Almquist and Wiksell, Stockholm, 1966) p. 629
18) V.M.Strutinsky, Nucl. Phys. A 95 (1967) 420; A 122 (1968) 1.
19) M. Brack, P. Quentin, Nucl. Phys. A361(1981)35
20) W.D. Myers, W.J. Swiatecki, Nucl. Phys.81(1974)186
21) W.D. Myers, W.J. Swiatecki, Ann. of Phys. 55 (1970) 395; 84 (1974) 186
22) M. Brack et al., Rev. Mod. Phys. 44 (1972) 320
23) B.K. Jennings, R.K. Bhaduri, M. Brack, Nucl. Phys. A 253 (1975) 29 and references quoted therein
24) O. Bohigas et al., Phys. Lett. 64 B (1976) 381
25) Y.H. Chu, B.K. Jennings, M. Brack, Phys. Lett. 68 B (1977) 407
26) C. Guet, R.Bengtsson, M. Brack, as ref. 13, Vol. II, p. 411
27) H. Krivine, J. Treiner, O. Bohigas, Nucl. Phys. A 336 (1980) 155
28) H. Krivine, J. Treiner, Phys. Lett. 88B(1979)212
29) X. Campi, S. Stringari, Nucl. Phys. A337(1980)313
30) C. Guet, H.-B. Håkansson, M. Brack, Phys. Lett. 97 B (1980) 7
31) J. Bartel et al., Contribution to Int. Workshop IX on Gross Properties of Nuclei, Hirschegg 1981 (TH Darmstadt) in print
32) for a review of earlier energy density calculations, see R. Lombard, Ann. of Phys. 77(1973)380
33) C. Guet, M. Brack, Z. Phys. A 297 (1980) 247
34) B. Grammaticos, A. Voros, Ann. of Phys. 123 (1979) 359; 129 (1980) 153
35) C. Guet, H.-B. Håkansson, M. Brack, to be publ.
36) M. Brack, C. Guet, H.-B. Håkansson, A. Magner, V.M. Strutinsky, this conference
37) M. Beiner, R. Lombard, D. Mas, At.Data Nucl. Data Tables 17 (1976) 450
38) F. Tondeur, Nucl. Phys. A 303 (1978) 185
39) F. Tondeur, this conference
40) R.K. Badhuri, Phys. Rev. Lett. 39 (1977) 329; M. Durand, P. Schuck, M. Brack, Z. Physik A 286 (1978) 381; A 296 (1980) 87
41) J. Bartel, to be published (see also ref. 31)
42) G.F. Bertsch, S.F. Tsai, Phys. Rep. 18C(1975)125; S. Krewald et al., Nucl. Phys. A 281 (1977) 166; J.P. Blaizot, D. Gogny, Nucl. Phys. A284(1977)429;
43) M. Buenerd et al., Phys. Lett. 84 B (1980) 305 and older experiments quoted there
44) J.P. Blaizot, D. Gogny, B. Grammaticos, Nucl. Phys. A 265 (1976) 315; B.K. Jennings, A.D. Jackson, Phys. Rep. 66 C (1980) 141
45) O. Bohigas, A.M. Lane, J. Martorell, Phys. Rep. 51 C (1979) 267
46) G. Holzwarth, G. Eckart, Nucl. Phys. A 325(1979)1 and references quoted therein
47) J. Meyer et al., to be published
48) J. Bartel, P. Quentin, C. Guet, H.-B. Håkansson, M. Brack, Preprint ILL (Grenoble)-Regensburg 1981

DISCUSSION

J. Theobald: HF-calculations provide for known nuclei in the actinide region fission barriers with the second lump (much) larger than the first one in contradiction to experimental data but in agreement with your examples (^{240}Pu). In the transparency, in which you explain the influence of the spin-orbit term on the fission-barrier height, the second potential maximum is smaller than the first. What is the reason or did you compare barriers of different nuclei?

M. Brack: The example shown in the transparency was a hypothetical superheavy nucleus with Z=126 and N=228, for which the average (liquid drop) deformation energy decreases as soon as one goes away from sphericity. This explains the lower second barriers which are also known in the heavier actinides.

K. Bleuler: Realistic potentials (like Reid) which are in agreement with nucleon-nucleon scattering yield relatively reasonable values for binding and density through a Brueckner approximation scheme. It is amazing to see that the various Skyrme-forces which have very different properties (attractive core instead of a repulsive one) and disagree strongly with scattering, yield nearly the same results for binding and density.

M. Brack: Skyrme-forces are phenomenologically parametrized, density-dependent G-matrices. They can therefore not be compared to the free nucleon-nucleon potentials and have nothing to do with N-N scattering data. (They do, however, have an overall repulsive core and thus yield saturation.) A semi-quantitative derivation of Skyrme-type effective forces from a Brueckner-LDA-HF calculation using the Reid potential has been given by Negele and Vantherin (Phys.Rev. C, 1972).

J.R. Nix: What would you expect your extended Thomas-Fermi method to yield for the fission-barrier heights of very light nuclei?

M. Brack: We have not yet looked at them, mainly because of the failure of the Skyrme forces to give the right actinide barriers. As soon as we have fixed a reasonably good force, we shall calculate light nuclei.