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SOME RECENT DEVELOPMENTS IN THE MEAN-FIELD DESCRIPTION OF LOW-ENERGY NUCLEAR PHYSICS#

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1. Introduction

In this talk I want to draw your attention to some progress which has recently been made in the Hartree-Fock or mean-field description of low-energy nuclear properties. I shall mainly concentrate on static nuclear properties such as binding energies, radii, charge distributions, deformation energies etc., but also briefly mention some calculations of giant resonances and sub-barrier fusion cross sections.

The theoretical description of the atomic nucleus represents (for $A \geq 4$) a doubly unsolvable problem because 1) of its nature as a many-fermion system and 2) we do not know the exact form of the basic nucleon-nucleon interaction. Therefore even the appearingly most simple extrapolation seen from the many-body point of view, namely that of infinite nuclear matter with constant density, is still not completely understood. For finite nuclei, a certain amount of modelling and parametrizing is unavoidable both on the more phenomenological level, e.g. when interpreting the exper-

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imental nuclear excitation spectra and data on various nuclear reactions, and also on a more microscopical level where one attempts to link nuclear properties with those of the basic nucleon-nucleon interaction.

On the microscopic level, the most successful and commonly used methods are based on the mean-field approach, i.e. on the assumption of an average (and in general nonlocal, spin and velocity dependent) potential in which the individual nucleons move independently. This potential can either be parametrized phenomenologically, as it was done when the shell model was invented, or it can be derived selfconsistently from an effective nucleon-nucleon interaction with the Hartree-Fock method. This interaction is not the one between the free nucleons, but that which is valid in the nuclear medium and thus incorporates many-body effects; it may be thought of as a re-parametrized G-matrix resulting from a Brückner-type calculation. In section 2 I shall review some of these effective interactions and present some selective results of recent Hartree-Fock calculations.

A second way to justify the mean-field approach from the many-body theory, which is perhaps less familiar to some nuclear physicists, is making use of the so-called Hohenberg-Kohn theorem. It tells us that, at least as far as ground-state energies and densities are concerned, the mean-field assumption is by no means limited to the Hartree-Fock approximation but allows in principle to incorporate any amount of exchange and many-body correlations in a (mainly) local potential. I shall discuss the Hohenberg-Kohn theorem and some of its consequences in section 3.

Section 4 is devoted to some semiclassical methods which recently have been successfully used for mean-field calculations with effective interactions. They constitute alternatives to the Hartree-Fock approach which are not only much more economical, but also in many ways more transparent, and allow to establish direct connections between the effective nuclear forces and the parameters of phenomenological models such as the liquid drop or the droplet model.

Whereas all the methods mentioned so far are starting

from the nonrelativistic Schrödinger equation, one may ask to which extent relativistic effects play any role in the description of low-energy nuclear phenomena. We shall see in section 5 that, indeed, recent relativistic Brückner-Hartree-Fock calculations have brought us one step closer to understanding the (extrapolated) infinite nuclear matter saturation properties. I shall also present in sect. 5 some recent relativistic mean-field calculations for finite nuclei.

The selection presented here is necessarily a personal one and is by no means thought to be exhaustive. I apologize with all those colleagues whose work I have not mentioned, either by lack of time and space, or by sheer ignorance. I am grateful to R. Brockmann, K. Goeke, P.G. Reinhard and their collaborators for making figures available to me prior to publication. Some of the newest results presented in sect. 4 have been obtained in agreeable collaboration with J. Bartel.

2. Hartree-Fock calculations with phenomenological effective forces

2.1. Effective nucleon-nucleon interactions

Due to the strong short-range repulsion of the free nucleon-nucleon interaction, its direct use in Hartree-Fock (HF) calculations is practically not possible. One way to solve this problem is to use Brückner theory to sum the repulsive short-range correlations into a G-matrix (see, e.g., refs. /1,2/). In terms of the G-matrix, a perturbation expansion is performed with the HF approximation as a starting point. This series can be brought to convergence for infinite nuclear matter (see sect. 5).

For finite nuclei, a number of simplifying approximations is necessary before a density-dependent effective nucleon-nucleon interaction (in short: effective force) can be extracted from the G-matrix and used in HF calculations /3/. Such calculations require very few adjustable parameters - beside those of the phenomenological nucleon-nucleon potential from which they usually start - but

rather large numerical efforts /4/. For large-scale systematical investigations and extensions like time-dependent HF(TDHF) or RPA calculations, one therefore often replaces these density-dependent effective G-matrices by phenomenological forces which are parametrized in a mathematically convenient form. From the large variety of effective forces used in HF calculations (see ref. /5/ for a review), we shall pick here only a few examples and present some recent results obtained with them.

The mathematically most simple and therefore also most popular type of effective interactions was originally proposed by SKYRME /6/ and used for the first time by VAUTHERIN and BRINK /7/ in HF calculations for finite nuclei. The Skyrme force has mathematically a zero range, but some velocity dependent terms simulate the finite range of the nuclear interaction. Due to this simple form, the nuclear part of the HF energy can be written as an integral over a local energy density

$$E_{HF} = \int d^3r\, \mathcal{E}_{Sky}(\vec{r}) = \int d^3r\, \mathcal{E}_{Sky}[\rho_q, \tau_q, \vec{J}_q], \tag{1}$$

where $\mathcal{E}_{Sky}(\vec{r})$ is a simple algebraic function of the nucleon densities $\rho_q(\vec{r})$ and their gradients, the kinetic energy densities $\tau_q(\vec{r})$ and the spin-orbit densities $\vec{J}_q(\vec{r})$, which are defined in terms of the single-particle wavefunctions $\varphi_i^q(\vec{r},s)$ and the occupation numbers n_i^q by

$$\rho_q(\vec{r}) = \sum_{i,s} |\varphi_i^q(\vec{r},s)|^2 n_i^q, \quad \tau_q(\vec{r}) = \sum_{i,s} |\vec{\nabla}\varphi_i^q(\vec{r},s)|^2 n_i^q,$$

$$\vec{J}_q(\vec{r}) = (-i)\sum_{i,s,s'} \varphi_i^*(\vec{r},s')(\vec{\nabla}\times\vec{\sigma})\varphi_i(\vec{r},s) n_i^q. \quad (q = n,p) \tag{2}$$

(The index q denotes neutrons or protons, s and i are the spin and spatial quantum numbers.) According to the number of exchange terms and the form of density dependence included (see ref. /8/ for a general formulation), a Skyrme force usually contains 6-10 free parameters. These are fixed once and for all by a fit to some observables (usually binding energies and radii of some spherical nuclei, sometimes also spectroscopical data) and then kept constant

in all applications and for all nuclei. Depending on the emphasis put on different observables in these fits, different parameter sets can of course be determined. The literature is unfortunately too abundant in such Skyrme force parameter sets; more efforts should go into broad-scale investigations, taking as many observables into account as possible (see e.g. ref. /9/), rather than into finding a new parameter set for each type of application.

Pairing correlations are usually included in the Skyrme-HF calculations in the BCS approach at each iteration (see ref. /10/), using one or two phenomenological constants G_q or Δ_q, although HF-Bogolyubov (HFB) calculations are in principle possible with Skyrme forces in a restricted space, if the exchange terms are suitably chosen /11/.

A finite-range effective force designed for HFB calculations was developed by GOGNY /12/. The technical difficulties connected with the nonlocal exchange terms were reduced here by choosing a Gaussian form of the interaction and by expanding the wavefunctions in a harmonic oscillator basis, so that most of the integrals can be done analytically. A density-dependent and a spin-orbit part with zero range are added like in the Skyrme force, leading to a total of 12 parameters for the Gogny force. No additional pairing parameters are needed since the pairing fields are obtained selfconsistently from the Gogny force in the HFB calculations.

A hybrid force with a direct finite-range part of Yukawa form and otherwise only zero-range terms was developed particularly for time-dependent HF (TDMF) calculations by BONCHE et al. /13/. It does not, however, allow for differences between neutrons and protons (except for the presence of the Coulomb interaction) and can therefore not be used for medium and heavy nuclei with $N \neq Z$.

In the reminder of this section, we shall discuss a few illustrative results of HF (+ BCS) or HFB calculations obtained with these effective forces.

2.2 Static properties

Binding energies of stable spherical nuclei can be reproduced both with the Gogny and with Skyrme forces with an accuracy of ~ 1 MeV, i.e. the order of one part in a thousand for medium and heavy nuclei. This is perhaps not too surprising since the energies of nuclei like ^{40}Ca or ^{208}Pb are usually imposed when determining the force parameters. But it is still a surprisingly good achievement because, as we shall see, many other experimental data can be well reproduced with the same set of ~ 10 parameters. For deformed nuclei, the errors usually run up into several MeV; this is partially due to the presence of spurious rotational energies in the HF results (because deformed Slater determinants have no good total angular momentum), partially to truncation effects connected with the finite basis in which the deformed HF wavefunctions are expanded in most calculations (see refs. /5, 10, 12/).

For ß-unstable nuclei, the discrepancy between experimental and calculated binding energies increase for most standard Skyrme forces as one goes away from the ß-stability line. This shows that the asymmetry properties of these forces have not been well determined yet. There is, however, room for doing so by playing on the exchange parameters x_1 and x_2 which have been chosen to be zero in many cases. An improvement in this direction has been achieved by TONDEUR /14/.

The experimental charge r.m.s. radii can typically be reproduced within less than ~ 1 %, although the radial charge distributions are not always equally good. The Orsay family of Skyrme forces /15/, e.g., tends to give too steep surfaces, which is connected with the unrealistically large nuclear matter incompressibility coefficient K_∞ ~ 350 - 400 MeV of these forces. A particular problem with the charge distributions is that most HF results exhibit much stronger shell fluctuations in the nuclear interiour than the experimental ones. (We refer to CAMPI /16/ for an extensive discussion of HF charge densities.) This discrepancy has often been quoted as an evidence for correlations which go

beyond the HF approximation and should be included in the calculations before comparison is made to the experimental results.

As a counter-example we show in Fig. 1 the HF charge densities of four spherical nuclei, obtained with a recent Skyrme

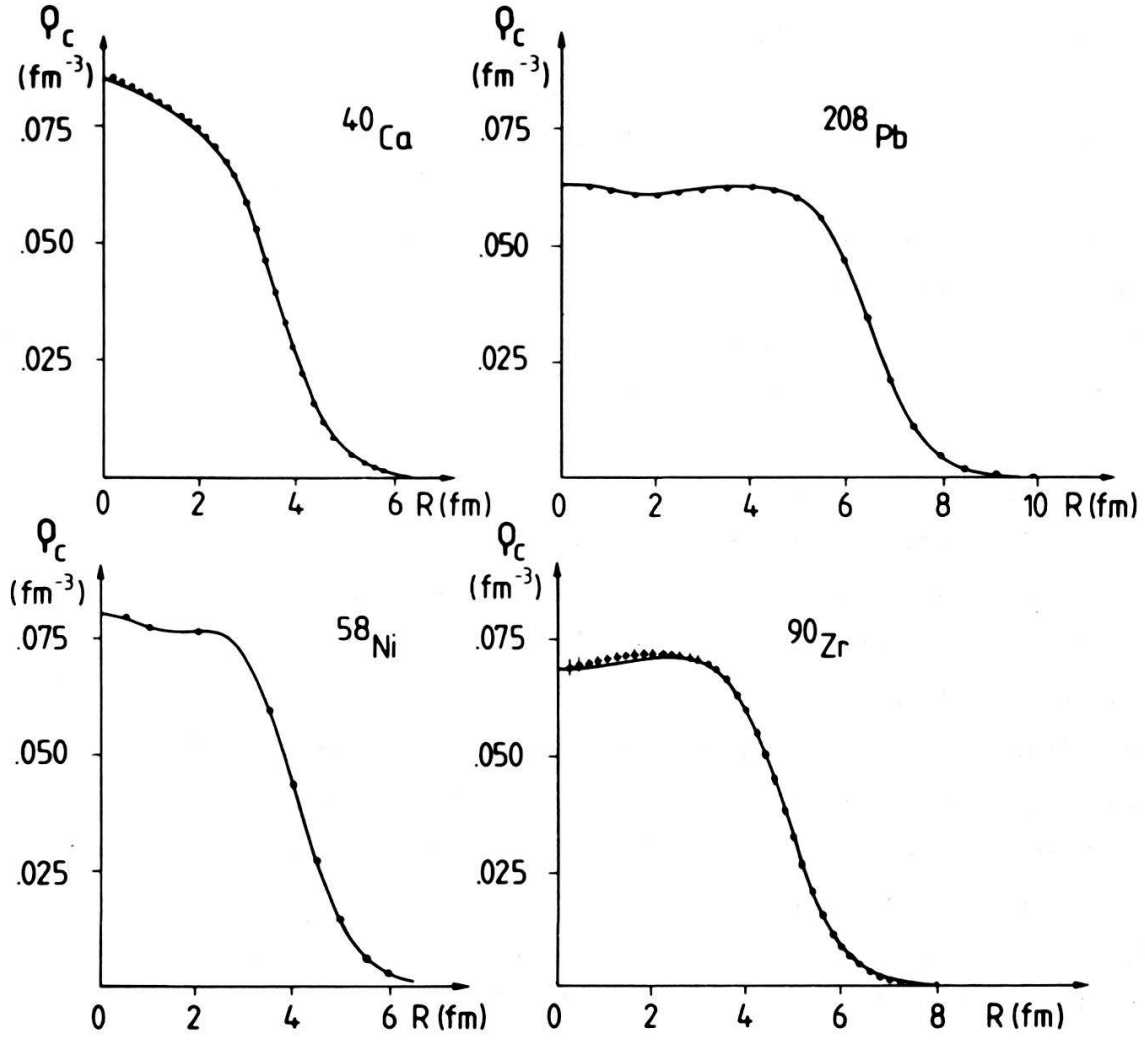

Fig. 1. HF charge distributions (full lines) compared with the experimental results (dots). From TONDEUR/14/.

force parametrization by TONDEUR /14/. (The same force gives very good binding energies and charge r.m.s. radii for a sample of 11 spherical nuclei including such ß-unstable isotopes as ^{48}Ca and ^{132}Sn.) The excellent agreement with the experimental charge

distributions should not be considered as accidental. In sect. 3 we shall see that all kinds of correlations can, indeed, be already included in the HF densities obtained from phenomenologica effective interactions. A recent systematic fit of Skyrme parameters to experimental binding energies and charge form factors, including a detailed discussion of χ^2 values and variances of the different parameters, can be found in ref. /17/.

The situation is different for the HF single-particle (s.p.) energies which only partially contain correlations. Particularly in magic spherical nuclei like ^{208}Pb, the coupling of the s.p. states to collective vibrations has been estimated to shift the s.p. energies quite appreciably (see, e.g., ref. /18/). Therefore the fact that some Skyrme-HF calculations give s.p. spectra of a quality comparable to that of Woods-Saxon or Nilsson shell-model potentials (see ref. /5/) should be taken with some care. (See also the discussion in sect. 3.)

The static HF method allows not only to calculate ground state properties but also deformation energies, if suitable constraints (i.e. external deformed fields) are applied /19/. An important application of the constrained HF (CHF) method is the calculation of fission barriers. These are until today still most efficiently and most accurately calculated with the well-known shell-correction method by STRUTINSKY /20/. (For a review on fissio barrier calculations until 1979, see ref. /21/.) Since the HF theory is the basic framework from which the Strutinsky method can be derived (see below), one should expect it also to be able to reproduce the experimental fission barriers. It was therefore quite a puzzle that the first fission barriers obtained in CHF calculations for ^{240}Pu, both with the Skyrme SIII force /22/ and with Gogny's force /23/, were appreciably higher than the experimental one (see also the discussion in ref. /21/).

This problem was resolved when a new Skyrme force, labelled SkM*, was determined which reproduces the empirical average fission barrier of ^{240}Pu in a selfconsistent semiclassical calculation /24/ and at the same time gives excellent ground state

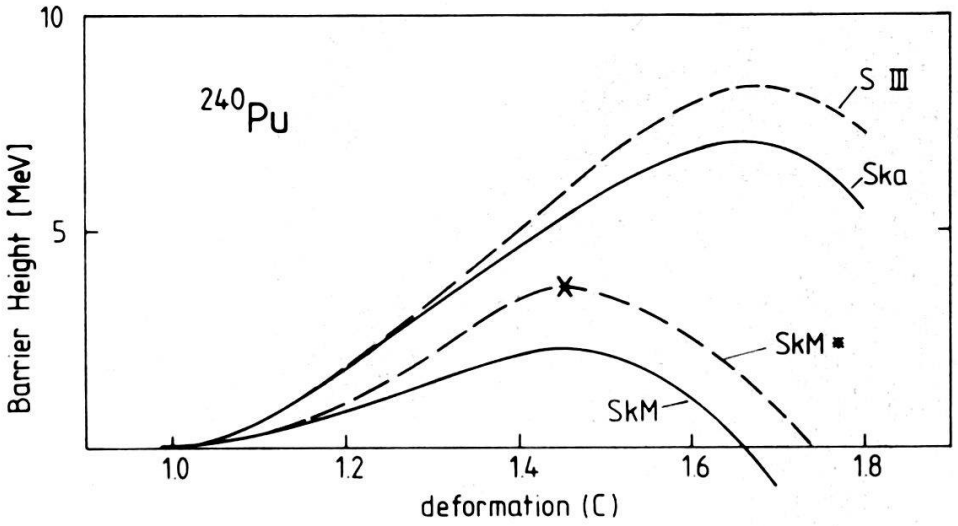

Fig. 2. Average fission barriers of ^{240}Pu calculated by the semiclassical density variational method with 4 Skyrme forces: SIII/15/, Ska /26/, SkM* /24, 25/ and SkM /27/. The cross indicates the empirical saddle point /28/. From BRACK et al /24/.

properties of stable spherical nuclei /25/. As an illustration, we show in Fig. 2 the average fission barriers of ^{240}Pu obtained in ref. /24/ with the density variational method, to be discussed in sect. 4.2, with four different Skyrme forces. (See ref. /28/ for the definition of the elongation parameter c; c = 1 corresponds to the spherical shape.) The SkM* force was adjusted to yield the empirical saddle point (shown by a cross). The fact that all the forces shown here except SkM give comparably good ground-state properties, yet barriers different by a factor ~ 2, shows that the ground-state properties of the known stable nuclei do not contain enough information for the extrapolation to the large deformations occurring in the fission process. Thus, similarly as it is practised in liquid drop /29/ or droplet model fits /30/, the large-deformation behaviour of effective forces must be imposed by including fission barriers along with the ground-state properties in the fitting of their parameters.

BERGER and collaborators /31/ have recently readjusted the parameters of the Gogny force such as to get a fission barrier of ^{240}Pu close to the experimental one. In Fig. 3 we show their

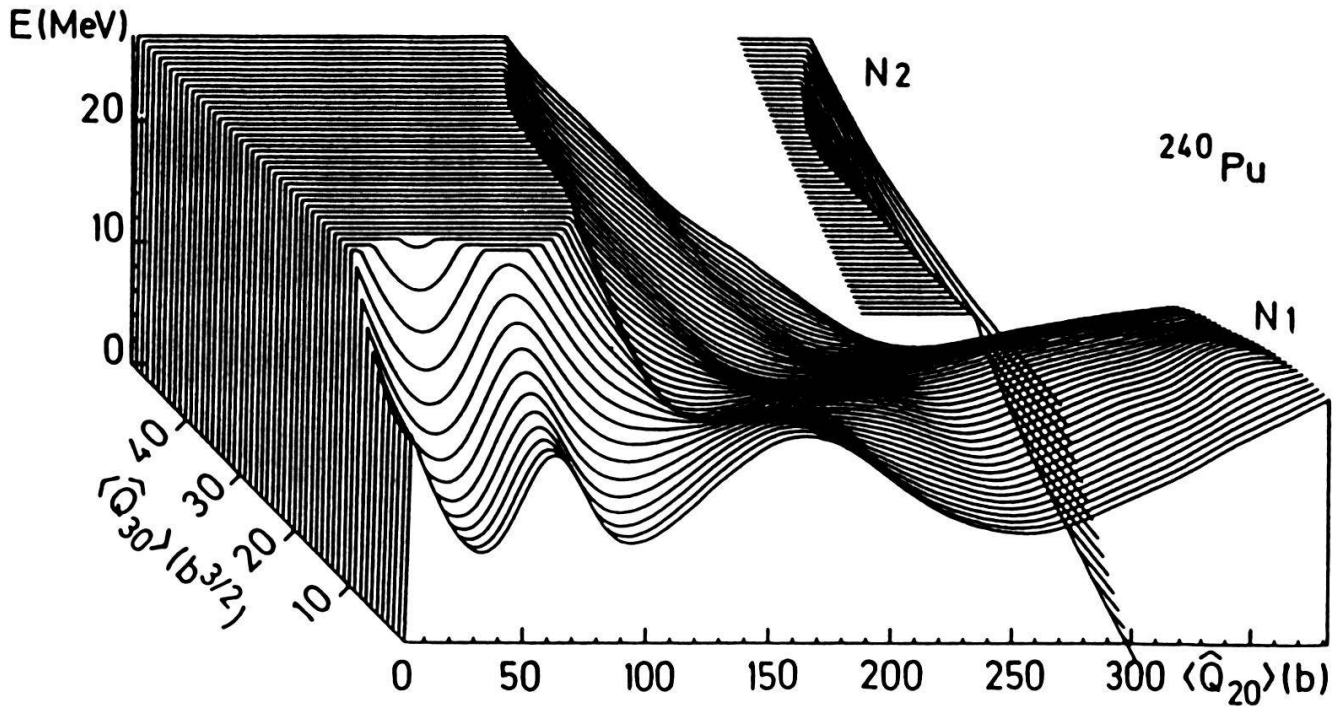

Fig. 3. Fission barrier of ^{240}Pu obtained in a HFB calculation with a modified Gogny force. $\langle Q_{20} \rangle$ and $\langle Q_{30} \rangle$ are the mass quadrupole and octopole moments. From BERGER et al. /31/.

result of a HFB calculation with simultaneous constraints on the quadrupole and the octopole moments. (For details, see ref. /31/.) The deformation energy surface seen in Fig. 3 has the topology known from Strutinsky calculations (see, e.g., ref. /28/). In particular, the octopole asymmetry of the second saddle point, which is the static origin of the mass asymmetry in the fission fragment distribution, is exhibited here for the first time in an HF calculation.

Before closing this section, we mention briefly that HF calculations with Skyrme forces have also allowed to test numerically the basic assumptions of the Strutinsky shell-correction method and to demonstrate that the latter is indeed an excellent approximation to HF theory, in particular if the shell model and the liquid drop model parameters are determined consistently from the same effective interaction /32/.

2.3 Some dynamic properties

The same or similar effective forces as mentioned above have also been used in numerous dynamical calculations. We cannot here discuss the multitude of dynamical nuclear processes which can be described by the TDHF method or approximations thereof We refer the interested reader to the proceedings of a recent conference about TDHF, its approximations and extensions /33/.

As an example which fits into our above comparison of various Skyrme forces, we mention a recent calculation of the sub-barrier fission cross section for the system ^{16}O-^{16}O using the "quantised adiabatic TDHF" method by REINHARD et al. /34/. These authors have shown that this cross section is extremely sensitive to details of the effective force used. As one might expect for the fusion process, a good description of the nuclear surface is hereby crucial. In ref. /34/, a modified version of the BKN force /13/ was determined by fits in particular to the surface regions of the charge distributions in light nuclei and gave good agreement between the calculated and the experimental fission cross section. In a more recent calculation, different Skyrme forces were also used /35/. We show the results in Fig. 4. What is shown here is the so-called astrophysical S-factor, which is equal to the fusion cross section divided by a geometrical factor depending exponentially on the Coulomb barrier and thus the quantity mostly sensitive to the nuclear structure, as a function of the c.m. energy of the ^{16}O-^{16}O system. It is interesting to note the performance of the three Skyrme forces, which is very similar to that seen in Fig. 2 for the fission barriers of ^{240}Pu. In particular the fact that the force SkM*, which was adjusted to the fission barrier and thus to the surface property of a very heavy nucleus, gives the best results also for the fusion of very light nuclei, is gratifying.

Some dynamical quantities which are sometimes included in the fit of effective force parameters, are the energies of giant nuclear resonances. These are well described in the HF plus RPA approximation, but also with sum-rule or fluid-dynamical approaches. (See ref. /36/ for a recent review on the theoretical description

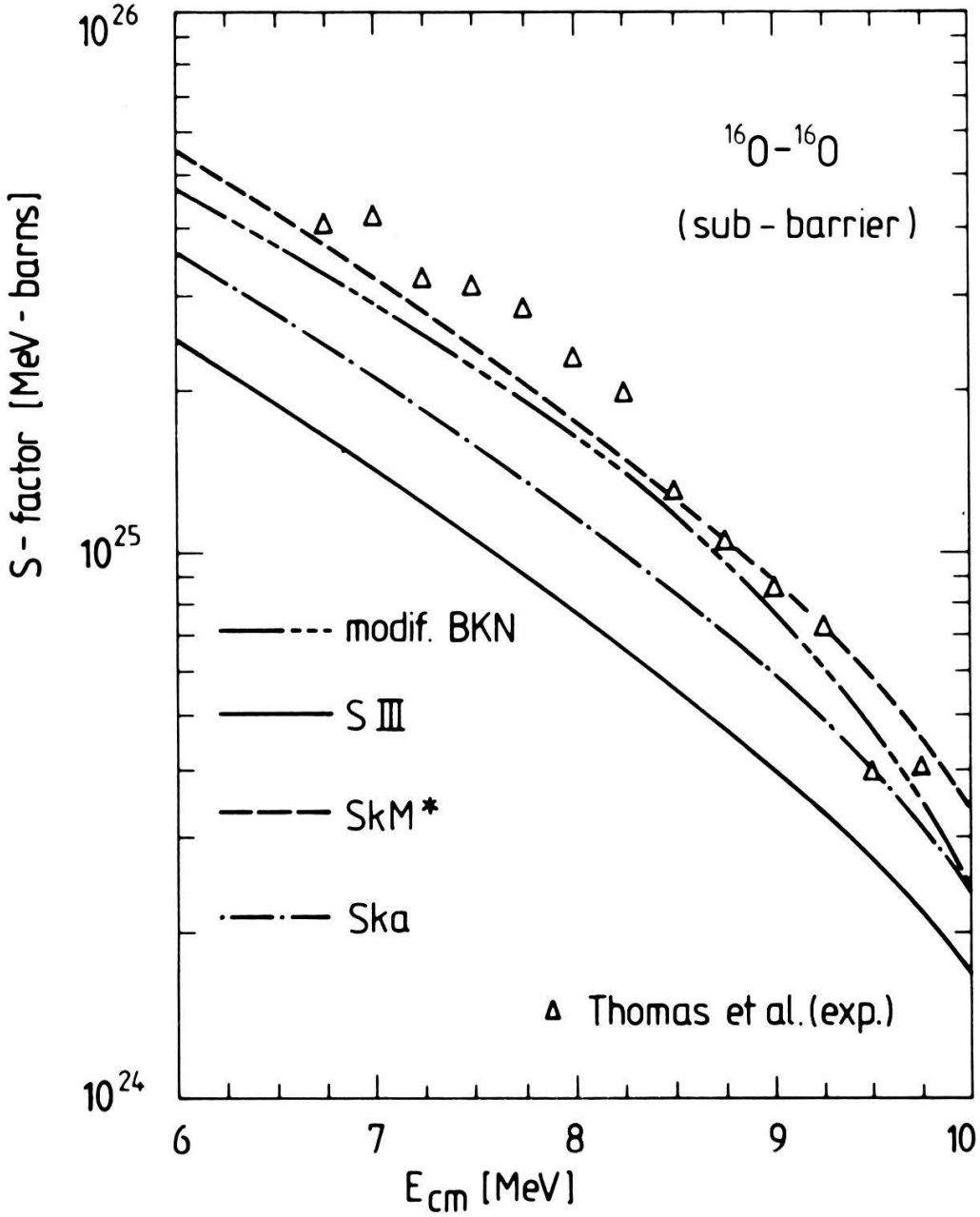

Fig. 4. S-factor for the sub-barrier fusion of ^{16}O on ^{16}O, obtained in a quantized ATDHF calculation with various effective forces. For the modified BKN force and the experimental results, see ref. /34/; the three Skyrme forces are as in Fig. 2. (Courtesy of K. GOEKE et al. /35/.)

of giant resonances.) The latter are particularly simple and allow systematical investigations with different forces. The energy of the breathing mode or giant monopole resonance (GMR) plays a special role because it depends sensitively on the incompressibi-

lity K_∞ which is easily determined from a given effective interaction. Detailed investigations /37, 38/ showed that forces with $K_\infty \gtrsim 300$ MeV can hardly give the correct GMR energies of finite nuclei; the most probable values are in the range 200 MeV $\lesssim K_\infty \lesssim$ $\lesssim$ 250 MeV. This rules out a series of older Skyrme forces with $K_\infty \gtrsim 350$ MeV /15/. (Note that SkM* has $K_\infty = 216$ MeV and the Gogny D1 force has $K_\infty = 228$ MeV.)

The fact that a certain amount of RPA-like correlations is most likely already contained in the HF ground states (see the discussions in sects. 2.2 and 3), raises a question of possible double-counting when calculating RPA excitation energies on top of HF results. This problem was discussed recently in ref. /39/, where the RPA-correlations were calculated in an approximate way and added to the HF energies before re-fitting the parameters of the Skyrme force (see also ref. /17/).

3. The Hohenberg-Kohn theorem and its relevance to nuclear physics

HOHENBERG and KOHN /40/ proved in 1964 the following theorem: Given N interacting electons in a local spin-independent external potential $V(\vec{r})$. The Hamiltonian is

$$\hat{H} = \hat{T} + \sum_{i=1}^{N} V(\vec{r}_i) + \frac{1}{2} \sum_{i<j}^{N} \frac{e^2}{|\vec{r}_i - \vec{r}_j|} \quad . \tag{3}$$

If the ground-state, given by the Schrödinger equation

$$\hat{H} \psi_0 = E_0 \psi_0 , \tag{4}$$

is non-degenerate, then the <u>exact</u> energy E_0 can be written as a universal functional of the local ground-state (g.s.) density

$$E_0 = \int d^3r \, \mathcal{E}[\rho_0(\vec{r})] = E[\rho_0] , \tag{5}$$

where the latter is defined by

$$\rho_0(\vec{r}) = \int d^3r_2 \int d^3r_3 \cdots \int d^3r_N \, |\psi_0(\vec{r}, \vec{r}_2, \vec{r}_3, \ldots \vec{r}_N)|^2 . \tag{6}$$

The functional $E[\rho]$ is independent of $V(\vec{r})$ and is such that it takes its variational minimum for ρ_0 with the value E_0.

This theorem looks rather surprising since it allows in principle to calculate the exact g.s. energy, including exchange and correlation contributions, from the local density by a simple variational procedure. However, the exact functional $E[\rho]$ is not known and in practice one has to find approximate functionals with the help of soluble cases or model calculations. A very useful application of the Hohenberg-Kohn (HK) theorem has been formulated by KOHN and SHAM /41/: Assume that $\rho_0(\vec{r})$ is the g.s. density of a non-interacting electron system in some external potential $V(\vec{r})$ (i.e. so-called non-interacting V-representability). Then we can write $\rho_0(\vec{r})$ in terms of some s.p. wavefunctions $\varphi_i(\vec{r})$ as in eq. (2) (with occupation numbers 1 or 0), and the kinetic energy $T_s[\rho_0]$, which according to the HK theorem also is a unique functional, is just $\hbar^2/2m$ times the integral over the density $\tau(\vec{r})$ in eq. (2). We then rewrite the total energy of the interacting system as

$$E[\rho_0] = T_s[\rho_0] + F[\rho_0] , \tag{7}$$

where $F[\rho_0]$ now contains not only the total potential energy including exchange, but also the correlated part of the kinetic energy. Performing the variation of $E[\rho_0]$ not with respect to ρ_0, but with respect to the auxiliary functions φ_i, leads to a Hartree like equation:

$$\left\{ -\frac{\hbar^2}{2m} \Delta + V[\rho_0(\vec{r})] \right\} \varphi_i(\vec{r}) = \varepsilon_i \varphi_i(\vec{r}) . \tag{8}$$

The local potential $V(\vec{r}) = V[\rho_0(\vec{r})]$ is hereby the variational derivative of $F[\rho_0]$:

$$V[\rho_0] = \frac{\delta}{\delta \rho_0} F[\rho_0] . \tag{9}$$

If $\rho_o(\vec{r})$ is V-representable and if the exact functional $F[\rho_o]$ is used, one has mapped the exact N-body problem onto a simple Hartree-like 1-body equation which of course, must be solved selfconsistently. The φ_i's have hereby in general no physical significance; they are just auxiliary functions which allow to construct $\rho_o(\vec{r})$ and, via eq. (5), to calculate E_o.

This so-called Kohn-Sham theory has been widely used with approximate functionals in various domains of atomic, molecular and condensed matter physics. For the abundant literature we refer to the proceedings of a recent summer school on density functional methods /42/.

The HK theorem has repeatedly been subject to criticism. It was, however, recently proved under more general assumptions than in the original ref. /40/, in particular independently of V-representability (see the contributions of E. LIEB and of M.LEVY and J.P. PERDEW to ref. /42/). Also the Kohn-Sham theory has been generalized to a form which is independent of V-representability (LEVY and PERDEW in ref. /42/).

What is the relevance of the HK theorem and of Kohn-Sham theory to nuclear physics? The proofs of the HK theorem do not depend on the particular form of the two-body interaction; the theorem should therefore apply also to a system of interacting nucleons. The fact that there are two kinds of nucleons and the energy thus is a functional of two densities: $E[\rho_n, \rho_p]$, is a trivial extension. The presence of a spin-orbit interaction and, in the case of the Skyrme-type effective nuclear interactions, of further velocity-dependent terms which lead to a variable effective nucleon mass $m^*(\vec{r})$, can also easily be handled in an extended Kohn-Sham theory. We can therefore draw the following two important conclusions.

1. The HF theory with Skyrme-like forces is nothing but a Kohn-Sham theory, extended for spin-orbit and effective mass contributions. Seen in this light, we realize that all kinds of correlations <u>can</u> be included in what formally presents itself as the HF g.s. energies and densities. Which correlations exactly and how much of them is hard to say; certainly those long-range

correlations whose contributions to the energy functional take the form of powers and gradients of ρ, since several such terms are present in the Skyrme functional eq. (1) with adjustable parameters. When fitting these parameters to the experimental binding energies and densities, we cannot tell a priori how much comes from the HF part and how much from the correlations. The Gogny force /12/ leaves perhaps less room for such correlations since it contains only one density-dependent term with one adjustable parameter in the energy integral.

2. We can go one step further than the Kohn-Sham theory and try also to find local density functionals for the kinetic and the spin-orbit energies - they, too, must exist due to the HK theorem. The shell effects make it very difficult to determine the exact functional $T_s[\rho]$. However, if one is interested in the average kinetic energy of a nucleus - i.e. if one neglects the shell effects - the corresponding functional for the average kinetic energy $\bar{T}_s[\bar{\rho}]$ (and, similarly, the spin-orbit energy) can be determined rather accurately in a semiclassical model (see sect. 4.1). Thus, the HK theorem allows to calculate the average binding energies and densities of nuclei using the density variational method. We shall see examples of such calculations in sect. 4.2. The inclusion of the shell effects after the variation of the average energy by means of the Strutinsky method has been shown numerically /43/ to lead to an excellent approximation to a full HF calculation. A particularly interesting case is a system of Fermions at finite temperature. If the temperature is high enough (in the nuclear case, $kT \gtrsim 3$ MeV, which can be realized experimentally), the shell effects are washed out due to the broadening of the Fermi surface. In this case the semiclassical functional $T_s[\rho]$ - which depends explicitly on the temperature - becomes practically exact, as we shall see in the next section.

4. Semiclassical mean field calculations

Since the very first years of nuclear physics, density

variational calculations have been used to calculate the average energies of nuclei. BETHE and WEIZSÄCKER developed in this way the semi-empirical mass fomula /44/ using the Thomas-Fermi (TF) model /45/. More sophisticated energy density functionals were developed along with the Brückner theory /46/. A review of density variational calculations up to ~ 1972 is found in ref. /47/. In most of these calculations, the kinetic energy functional was approximated by the familiar TF relation

$$\tau_{TF}[\rho] = \mathcal{K}\rho^{5/3}\,, \qquad \mathcal{K} = \frac{3}{5}(3\pi^2)^{2/3}\,, \tag{10}$$

which is correct for an infinite Fermion system but does not take account of the density variation in the nuclear surface.

Over the last ~ 15 years, two main developments have allowed to refine appreciably the density variational calculations of static nuclear properties: 1. the development of the Skyrme type effective nuclear forces sketched in sect. 2.1, for which the energy is already a local functional of the densities ρ,τ and $\vec{J}$ eq. (2), and 2. the refinement of the so-called extended Thomas-Fermi (ETF) model, which we shall briefly discuss in the following section, and which allows to determine the functionals $\tau[\rho]$ and $\vec{J}[\rho]$ for the average densities.

4.1 The extended Thomas-Fermi (ETF) model

Systematic corrections to the TF functional $\tau_{TF}[\rho]$ eq. (10), which take variations of the density into account, can be obtained from a semiclassical expansion of the density matrix proposed originally by WIGNER and KIRKWOOD /48/, used in atomic physics e.g. for calculating virial coefficients /49/, and re-discovered in the context of nuclear physics only more recently /50/. (An independent alternative method was developed by KIRZHNITS /51/.) The resulting functional for the total kinetic energy for non-interacting Fermions in a local potential is /52, 53/

$$T_s[\rho] = \frac{\hbar^2}{2m}\int d^3r\Big\{\mathcal{K}\rho^{5/3} + \frac{1}{36}\frac{(\vec{\nabla}\rho)^2}{\rho} + \frac{1}{6480}(3\pi^2)^{-2/3}\rho^{1/3}\times \tag{11}$$

$$\times\left[8\left(\frac{\vec{\nabla}\rho}{\rho}\right)^4 - 27\left(\frac{\vec{\nabla}\rho}{\rho}\right)^2\frac{\Delta\rho}{\rho} + 24\left(\frac{\Delta\rho}{\rho}\right)^2\right]\Big\}. \qquad (11)$$

A phenomenological gradient correction of the same form as the second term in eq. (11) was proposed by WEIZSÄCKER /44/, although with a different coefficient which subsequently was discussed in the literature (see, e.g., ref. /54/). Corrections to $T_s[\rho]$ due to the spin-orbit potential and the variable effective mass in the Skyrme-HF-Hamiltonian, as well as a corresponding functional for the spin-orbit energy, have also been derived from the ETF model /53, 55/.

A formal difficulty of the ETF model was for a long time the fact that its expressions and thus also the functional eq. (11 could only be proved <u>inside</u> the classically allowed region defined for a given potential by $V(\vec{r}) < \lambda$, where λ is the Fermi energy. The functional eq. (11) was nevertheless used in the whole space, assuming that it could be analytically continued to the classically forbidden region. Only very recently, we have proved rigorously /56/ that it holds also outside the classical turning points, i.e. in the tail region of the density where the Fermions are tunnelling into the walls of the potential, by taking a suitable $T \to 0$ limit from the extension of the ETF model to finite temperatures T (see also sect. 6 of ref. 24 for a detailed discussion).

The functional eq. (11) has been tested with Strutinsky-averaged quantum-mechanical densities for various potentials in refs. /53, 57/. It was shown to reproduce the exact average kinetic energy to within less than one part in a thousand. The use of the numerical Strutinsky averaging method /20/ for the elimination of the shell effects is consistent with the semiclassical ETF model, as shown explicitly in several examples /50, 58/.

The ETF model has recently been generalized for Fermion systems at <u>finite temperature T</u> /56, 59/. (The corresponding generalization of the HK theorem also exists /60/.) The functional $T_s[\rho]$ looks more complicated for $T > 0$ than eq. (11) and depends explicitly on the temperature T; a corresponding functional $S_s[\rho]$

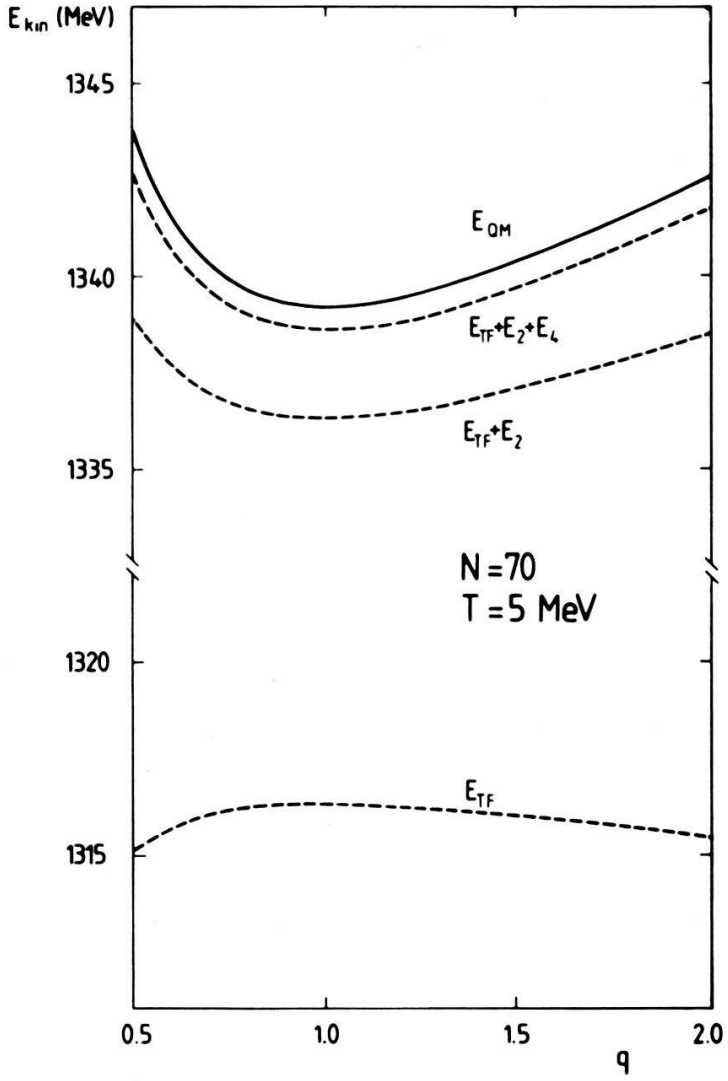

Fig. 5. Kinetic energy of 70 nucleons in an axially deformed harmonic oscillator potential at a temperature of kT = = 5 MeV. q = axis ratio. E_{QM} (solid line): exact quantum-mechanical result. Dashed lines: semiclassical results using the ETF functional $T_s[\rho]$ at various orders (see text). From BARTEL et al. /59/.

for the entropy with gradient corrections has also been derived. The knowledge of these functionals allows to extend the density variational calculations to systems at finite temperatures (see sect.4.2 for some results). These functionals have been tested in ref. /59/ with exact quantum-mechanical densities $\rho(\vec{r})$ defined as in eq. (2) with Fermi occupation numbers n_i. As an example, we show in Fig. 5 the kinetic energy of 70 nucleons at a temperature of 5 MeV in an axially deformed harmonic oscillator potential as a

function of the axis ratio q. The solid line shows the exact quantum-mechanical kinetic energy. The dashed lines are the results obtained via the ETF functional in terms of the exact density $\rho(\vec{r})$. Three approximations are shown: taking only the lowest order (TF) term in the functional $T_s[\rho]$, adding the Weizsäcker-type correction ($E_{TF} + E_2$), and adding all gradient corrections up to fourth order (as in eq. (11) for T=0). We see that in this latter case the ETF functional reproduces the exact kinetic energy with an accuracy of $\sim 10^{-3}$. Similar results were obtained in ref. /59/ for the entropy. This is perhaps the first time that the exact kinetic energy and entropy of a finite Fermion system have been calculated from the local density alone; it constitutes a nice - and by no means trivial! - example for the Hohenberg-Kohn theorem.

4.2. Results of density variational calculations

Many density variational calculations for average nuclear properties have been performed in the last years using Skyrme type forces and the ETF functionals. We refer the interested reader to a recent review article /24/ and the literature quoted therein. As an illustration we show in Fig. 6 a comparison of the nucleon densities obtained for two spherical nuclei, both microscopically by the HF method and semiclassically by the ETF variational method. Apart from the shell fluctuations in the HF densities, the agreement between the two approaches is excellent, in particular in the nuclear surface region. The higher-order gradient corrections in the functional eq. (11) were hereby essential to obtain the good agreement in the tail regions.

An example of a semiclassical fission barrier calculation has already been shown in Fig. 2. Needless to say that such a semiclassical calculation for a deformed nucleus is faster by 2 to 3 orders of magnitude than a constrained HF calculation. Thus, even if one HF iteration must be added at the end in order to recover the shell effects, the density variational method constitutes a very economical tool for systematical calculations of masses or deformation energies and for searches of new force parametrisations, in particular when including barriers.

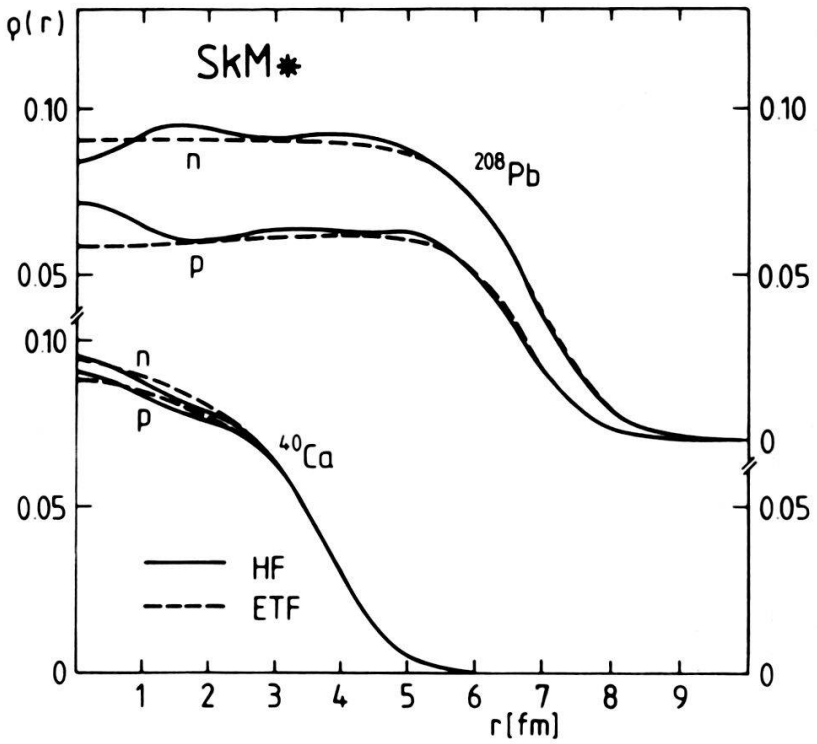

Fig. 6. Neutron and proton densities of ^{208}Pb and ^{40}Ca, obtained with the Skyrme force SkM* in HF (solid lines) and density variational ETF calculations (dashed lines). The corresponding r.m.s. radii agree within less than one permille. From BRACK et al. /24/.

The variational ETF method becomes particularly gratifying for systems at finite temperatures, where the shell effects disappear and the ETF functionals become exact, as demonstrated above. To demontrate this, we show in Fig. 7 the entropy of ^{208}Pb versus its excitation energy $E^* = E(T) - E(0)$, calculated with the Skyrme SIII force. The solid line is the result of an earlier HF calculation at T>0 /61/, the dashed line that of the semiclassical variational calculation with the T>0 (TETF) functionals /56/. Above an excitation energy E^* of ~ 100 MeV, which corresponds to $kT \simeq 2.5$ MeV, the shell effects are washed out and the two curves perfectly agree. In that region, the relations of the so-called shifted Fermi gas model /62/ are seen to be nicely fulfilled /56/:

$$S \sim 2\sqrt{a_0(E^*+\Delta E_0)}\,, \quad E^* \sim a_0 T^2 - \Delta E_0\,, \tag{12}$$

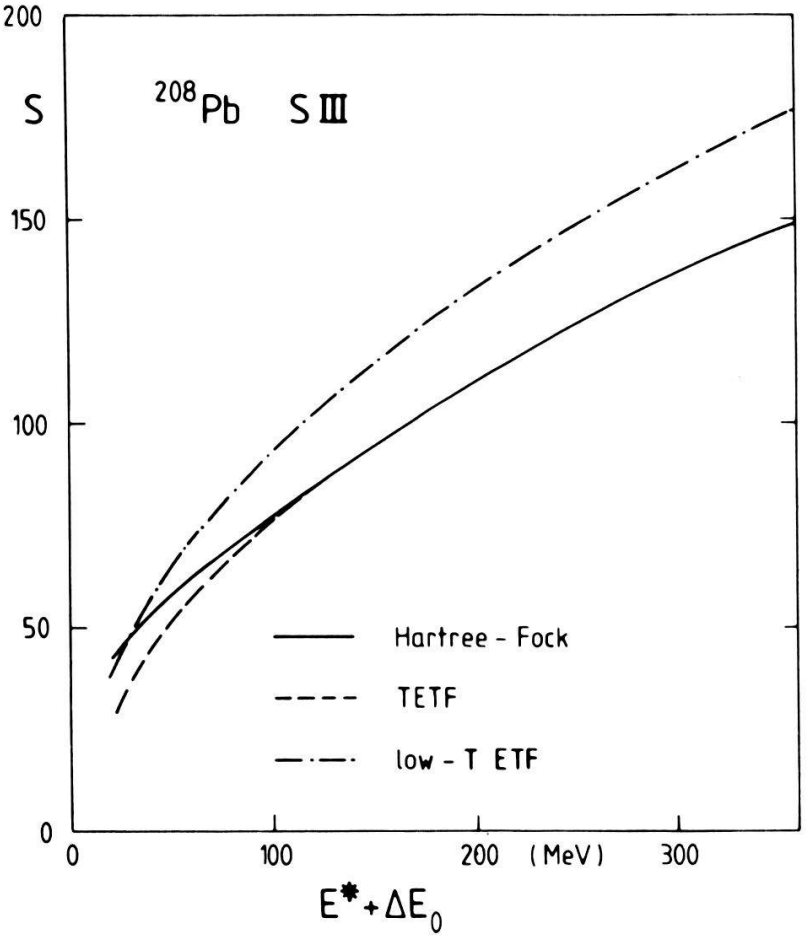

Fig. 7. Entropy versus excitation energy for ^{208}Pb, calculated with Skyrme SIII force in the HF (solid line), the variational TETF (dashed line) and the so-called low-temperature approximation (dashed-dotted line). (Results taken from refs. /56,61/.)

where a_o is the level density parameter and ΔE_o is the ground-state energy shell-correction (which is ~ -18 MeV for the HF and zero for the TETF case). Also shown in Fig. 7 is the (rather bad) result obtained in the so-called low-temperature expansion of the TETF functionals (see ref. /24/). In ref. /56/ we showed also that the proton and neutron r.m.s. radii of ^{208}Pb obtained in the HF and the TETF calculations agree within less than two permilles over the whole range of excitations energies $0 \leq E^* \lesssim 300$ MeV.

Such variational calculations of "hot" nuclear systems may be useful in the near future both in heavy-ion physics, where highly excited compound systems can be encountered, and in astrophysics, where the equation of state of hot nuclear matter can play

a crucial role in the evolution of supernovae (see e.g. ref./63/ and the literature quoted therein).

Another useful application of the density variational method consists in a so-called leptodermous expansion of the nuclear densities, which allows to establish direct relations between the effective nucleon-nucleon force and the liquid-drop /29/ or droplet model /30/. In particular, the droplet model relations can be tested and possible improvements can be derived (see esp. sect. 5 of ref. /24/). With this method it has also become possible to study the temperature dependence of liquid drop (or droplet model) parameters /64, 24/ which is of interest in the astrophysical context /65/ and allows to estimate the effect of the temperature on the fission barriers /66/. (The latter can, of course, also be calculated directly in finite-temperature variational calculations /24, 56/.) In ref. /59/, the surface and curvature energy coefficients have been calculated as functions of the temperature by solving exactly the (nonlinear, 4th order) Euler variational equation for the semi-infinite nuclear matter profile.

We finally mention that energies and sum rules for nuclear giant resonances have also been calculated using semiclassical (or "fluid-dynamical") methods, both for $T = 0$ /38, 67, 68/ and for $T > 0$ /69/, and lead practically to the same results as RPA calculations.

4.3 Partial resummation techniques

Another type of semiclassical mean-field calculation which does not make use of density functionals, but is closely related, has successfully been realized by BARTEL and VALLIERES /70/. It relies on a method originally proposed by BHADURI /71/ and then further developed in ref. /72/. Here the semiclassical Wigner-Kirkwood expansion /48/ is partially resummed to all orders in $\hbar$, neglecting only higher than first (or second) derivatives of the potential $V(\vec{r})$. In this way, semiclassical densities $\rho(\vec{r})$ and $\tau(\vec{r})$ can be obtained directly in terms of $V(\vec{r})$ and its lowest derivatives; no turning point problems are encountered, in contrast to the original $\hbar$-expansion /48-50/. Densities and potentials

can then be iterated like in a HF calculation, but without use of wave functions, until convergence is reached /70/. The results of this procedure /73/ are very similar to those of density variational calculations; in fact, the two methods confirm each other quantitatively.

A similar resummation procedure was also applied to the Coulomb case; it allows to calculate atomic binding energies and electron densities in a parameter-free way and yields results very close to HF results /74/.

5. Relativistic calculations

5.1 The nuclear saturation problem

We have already in the introduction mentioned the problem of the saturation properties of infinite nuclear matter. Although this is a hypothetical system, we know from extrapolations of the experimentally known saturation properties of finite nuclei, that symmetric, uncharged infinite nuclear matter should have a binding energy per particle of $(E/A)_\infty \simeq -15.8$ MeV and a density of $\rho_o \simeq$ $\simeq 0.16$ fm^{-3} corresponding to a Fermi momentum $k_F \simeq 1.3$ fm^{-1}. These values could so far not be reproduced in conventional non-relativistic many-body calculations using realistic nucleon-nucleon (N-N) potentials. Brückner theory can be brought to convergence in the so-called hole-line expansion /75/, but it results either in too high densities or in too low binding energies. This is illustrated in Fig. 8, where $(E/A)_\infty$ is plotted versus k_F for symmetric infinite nuclear matter. The dashed lines are saturation curves obtained in a standard non-relativistic Brückner-HF calculation using three different N-N potentials (A,B,C) which give equally good fits to experimental phase shifts of N-N scattering /76/. The locus of the saturation points is roughly a straight line, often called the Coester line /75/, which clearly bypasses the empirical saturation point (lying in the squared area in Fig. 8). This line is found in all non-relativistic calculations: whether one includes higher-order diagrams in the hole-line expansion /75/ or internal

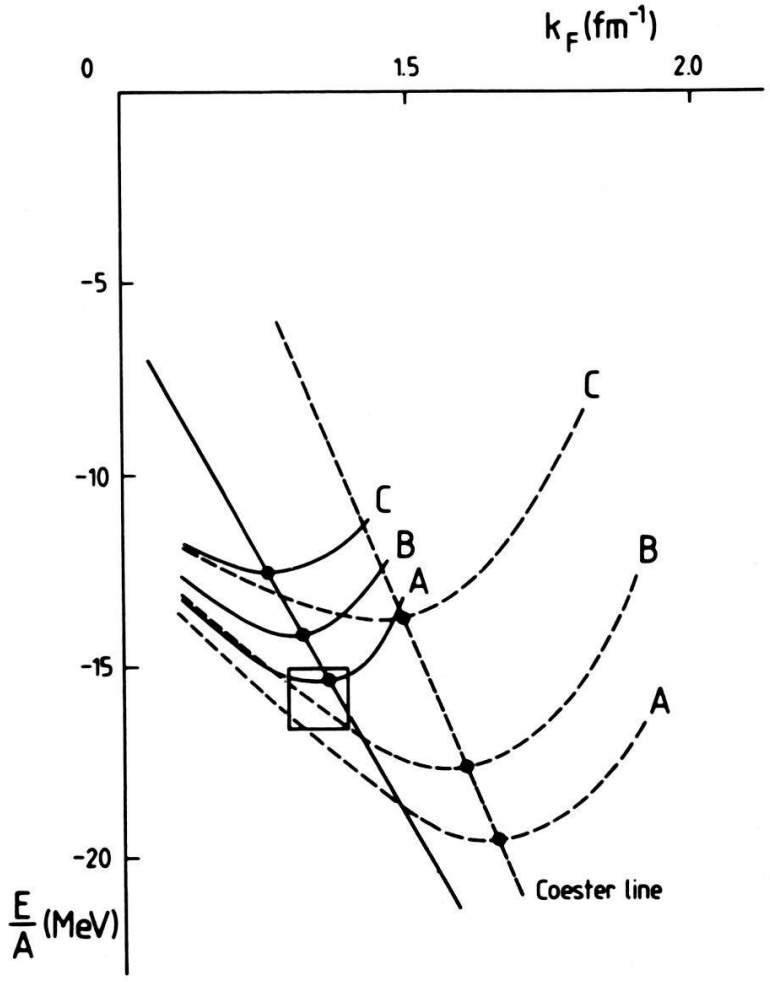

Fig. 8. Binding energy per nucleon (E/A) versus Fermi momentum k_F of symmetric infinite nuclear matter. Dashed lines: non-relativistic, solid lines: relativistic Brückner-HF calculations. A, B, C corresponds to different N-N potentials used. The empirical values lie in the squared area. (Courtesy of BROCKMANN /76/.)

degrees of freedom of the nucleons /77/, whether one uses phenomenological N-N potentials /78/ or these derived from meson-exchange theory /79/ - the results always lie more or less exactly on the same Coester line. Also more recent many-body theories (different from the Brückner approach) confirm these results /80/. (in finite nuclei, similar pictures as in Fig. 8 are found if one plots E/A versus the total r.m.s. radius.) Note that this problem does, of course, not exist in HF calculations with phenomenological effective N-N interactions which are adjusted to the experimental saturation properties.

Recent relativistic Brückner-HF calculations /81, 82/ have shown that the Coester line is moved in the right direction if the small components of the nucleon wavefunctions are taken into account. BROCKMANN and MACHLEIDT /82/ were the first to reproduce the empirical saturation point in a fully selfconsistent way using a N-N potential that fits the experimental phase shifts. Hereby the selfconsistent inclusion of the medium corrections (expressed in terms of the nucleon self-energy) in the small components of the Dirac spinors was crucial. It leads to an additional repulsion which shifts the Coester line to the empirical saturation point, as shown in Fig. 8. There remains to be shown that the higher-order diagrams (beyond HF) don't spoil this result. Still, it represents an important step forwards for the understanding of one of the most fundamental problems of the nuclear many-body theory.

5.2 Relativistic mean-field calculations for finite nuclei

In this final section, we shall very briefly mention some recent relativistic mean-field calculations for finite nuclei starting from phenomenological Lagrangians. One of their strongest motivations is the following. The above-mentioned relativistic effects are renormalized into the phenomenological effective forces discussed in sect. 2, which can successfully be used in non-relativistic HF calculations. However, these effective forces all contain one ingredient of clearly relativistic origin, namely the spin-orbit interaction which is, in fact, their least well-defined ingredient. This becomes a sincere handicap e.g. in the extrapolation to the so-called superheavy nuclei whose stability against fission depends most crucially on the strength of the spin-orbit interaction /83/.

In a relativistic mean-field calculation, the spin-orbit potential arises naturally along with the central potential and requires no extra free parameter. That such calculations are feasible /84/ with the present techniques and computers, is demonstrated in Fig. 9. Similar calculations have earlier been used to calculate the spin-orbit splitting in light hypernuclei /85/.

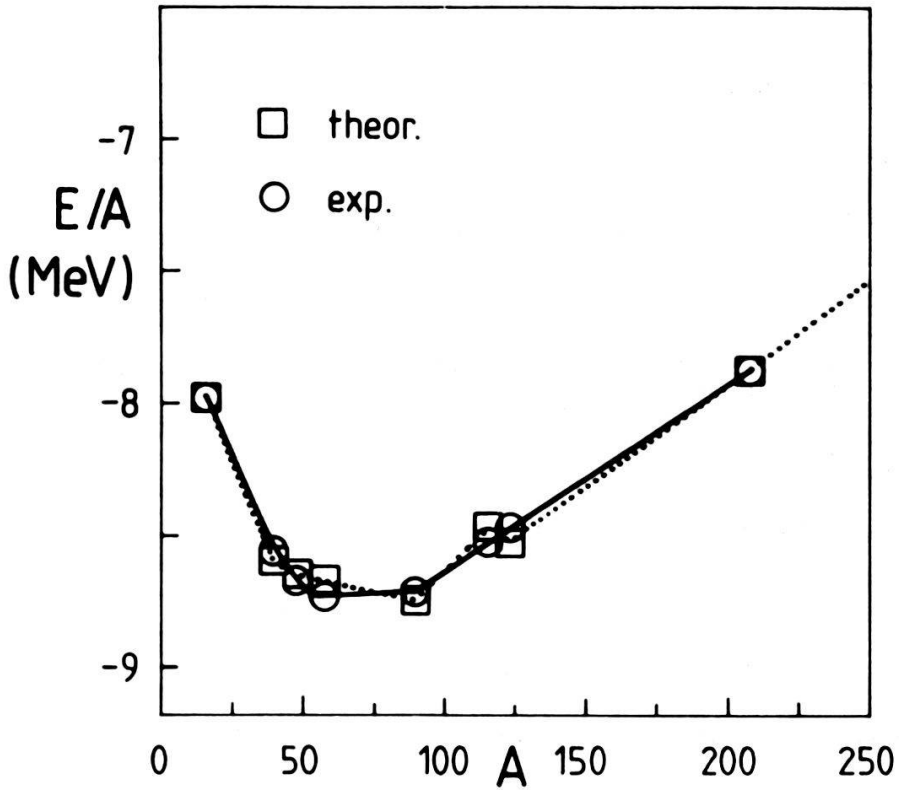

Fig. 9. Binding energy per nucleon for finite nuclei, obtained in a relativistic Hartree calculation with an effective Lagrangian (squares connected by dotted lines). The circles (connected by solid lines) show the experimental results. (Courtesy of P.G. REINHARD et al. /85/.)

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