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The Quest for a Microscopic Nuclear Mass Formula ⋆

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Abstract. After stressing how well the purely macroscopic 1935 mass formula of von Weizsäcker works, we discuss the general problem of deriving nuclear masses from basic nucleonic interactions. We then describe the very recent Skyrme–Hartree–Fock–BCS mass formula of Goriely *et al.*, the first and only to be entirely microscopic. We conclude by stressing how much more work has to be done before reliable extrapolations can be made from the mass data out to the highly neutron-rich part of the nuclear chart where the r-process of nucleosynthesis takes place.

Key words: atomic mass, Hartree–Fock, nuclear binding energy.

1. Introduction

The interest of nuclear masses lies in the fact that the mass $M_{\rm nuc}(N, Z)$ of a nucleus with N neutrons (n) and Z protons (p) is measurably different from the sum of the masses of the free nucleons, whence a direct determination of the internal energy $E_{\rm nuc}$ (the negative of the binding energy) of the nucleus is possible,

$$E_{\rm nuc} = \left\{M_{\rm nuc}(N, Z) - NM_{\rm n} - ZM_{\rm p}\right\}c^2. \tag{1}$$

Attempts to develop formulas, or, more generally, algorithms, representing the variation in $E_{\rm nuc}$ from one nucleus to another go back to the 1935 'semi-empirical mass formula' of von Weizsäcker [1]. Being inspired by the liquid-drop model (DM) of the nucleus, this is the macroscopic mass formula *par excellence*, but we will see in Section 2 that it works remarkably well, accounting for all but a small part of the variation in the binding energy. The 65 years of effort that have already been devoted to accounting for the residual effects are characterized primarily by attempts to establish a coexistence between the DM on the one hand and microscopic effects such as shell-model (SM) and pairing corrections on the other.

On the face of it the macroscopic and microscopic features are mutually exclusive, and for many years the scene was dominated by the hybrid 'macroscopic–microscopic' (macro–micro) approach (see [2] for a guide to the literature), which simply decreed that the two aspects of nuclear structure must cohabit, with microscopic corrections grafted on to the DM. Like many arranged marriages, this

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worked very well, but there are serious ambiguities arising from the decision, dictated by computational limitations, to ignore the common origin that the two aspects must have in the basic nucleonic interactions.

Actually, the macro–micro approach is most easily understood in terms of the purely microscopic approach of having both DM and SM features emerge on an equal footing from the common starting point of nucleonic interactions, either realistic or effective. We shall thus violate the historical order of development and first outline, in Section 3, the latter approach; in the same section we also present the only mass formula developed so far that can be said to be purely microscopic, being based essentially on the Hartree–Fock (HF) method. Section 4 then describes the older macro–micro approach, including variants in which the macroscopic part is evaluated semi-classically rather than by the DM. Finally, in Section 5, we look to the future, showing how much work remains to be done.

It is appropriate at this point to recall just why this sort of work continues to be important. In the first place, measuring the masses of more and more nuclei further and further away from the stability line with ever increasing precision is surely one way of testing our theories of nuclear structure. But much of the interest in constructing theoretically sound mass formulas that give precision fits to the mass (and other) data lies in the possibility thereby offered of being able to make reliable extrapolations away from the data out to the highly n-rich nuclei that play a crucial role in the r-process of nucleosynthesis but which are so unstable that there is no prospect of being able to measure them in the laboratory [3]. Mass formulas also permit an even greater leap from the mass data: the extrapolation out to infinite nuclear matter (INM), which also is of astrophysical interest.

2. The semi-empirical mass formula

We modify this slightly from the original form of [1], writing it as

$$\frac{E_{\rm nuc}}{A} = a_{\rm vol} + a_{\rm sf}A^{-1/3} + \frac{3e^2}{5r_0}Z^2A^{-4/3} + \left(a_{\rm sym} + a_{\rm ss}A^{-1/3}\right)I^2, \tag{2}$$

where $A = N + Z$. This is just the simplified form given in 1936 by Bethe and Bacher [4], with the addition of the surface-symmetry term ($a_{\rm ss}$) introduced in 1966 by Myers and Swiatecki [5]. The two leading terms correspond to the DM, which was inspired in large part by the observation that the radius R of any nucleus (N, Z) is given by $R \simeq r_0A^{1/3}$, where r_0 is a constant. The roughly constant density thereby implied is what one would expect in view of the finite range of nuclear forces, along with their strong short-range repulsion, and is referred to as the saturation property. With this picture of nuclei consisting simply of differently sized pieces of nuclear matter we expect the energy per nucleon to be constant, whence the term $a_{\rm vol}$ in Equation (2); the term in $a_{\rm sf}$ is then simply a correction for surface tension. However, the Coulomb force, being of infinite range, is not saturated, and must be taken into account explicitly: this is the third term of

Equation (2). One must also allow the specifically nuclear terms, both volume and surface, to depend not only on the total number of nucleons but also on the n–p composition. To a good approximation this dependence can be expected to be an even function of $I = (N - Z)/A$, since $M_n \simeq M_p$ and nuclear forces are more or less charge-symmetric.

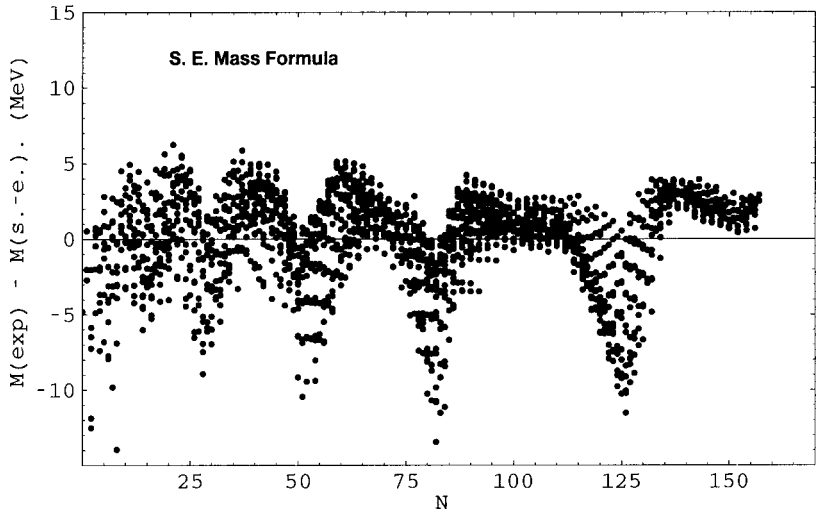
In the limit $A \to \infty$ the energy per nucleon becomes infinite and positive, because of the Coulomb term, unless we are dealing with a pure neutron system, $I = 1$. However, if we imagine the Coulomb force to be switched off we find a finite energy per nucleon, $a_{vol} + a_{sym} I^2$. This corresponds to the equilibrium energy of INM, which is, of course, a hypothetical medium, since the Coulomb force cannot be switched off. However, a similar situation is realized in neutron stars by the presence of electrons, which neutralize the small fraction of protons present.

We have fitted the mass formula (2) to the 1995 compilation of Audi and Wapstra [6], finding $a_{vol} = -15.65$ MeV, $a_{sym} = 27.72$ MeV, $a_{sf} = 17.63$ MeV, $a_{ss} = -25.60$ MeV, and $r_0 = 1.233$ fm, with an rms error of 3.02 MeV, which means that about 98% of the variation in the binding energy is being reproduced. This is remarkable, given that nearly 2000 data points are being fitted by 5 parameters. Nevertheless, the graphs of the residual errors (Figures 1a,b) show clearly the importance of the shell effects omitted in Equation (2); less apparent is the neglected even-odd pairing effect. Figure 2 shows how closely the drip lines predicted by the completely microscopic mass formula HFBCS-1 (Section 3D) are reproduced by the mass formula (2). In Figure 3 we see how well the limits of the zones of instability with respect to β-delayed nucleon emission lying just inside the drip lines are described by this same mass formula, while Figure 4 makes a similar comparison for the region of α-instability.

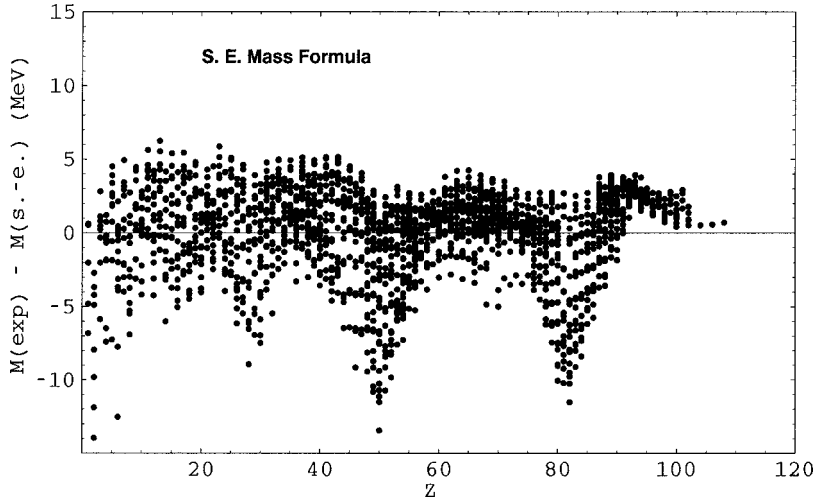
As a final example of what the semi-empirical formula can do, let us generalize it to include gravity. Since this has a non-saturating character formally identical to that of the Coulomb force, though with opposite sign, Equation (2) becomes

$$\frac{E_{nuc}}{A} = a_{vol} + a_{sf} A^{-1/3} + \frac{3}{5r_0}\left\{\frac{e^2}{4}(1 - I)^2 - GM^2\right\} A^{2/3} + \left(a_{sym} + a_{ss} A^{-1/3}\right) I^2. \tag{3}$$

For normal nuclei the gravitational correction will be utterly negligible, so let us consider very large values of A, and limit ourselves to systems consisting only of neutrons, $I = 1$, since otherwise the Coulomb repulsion would diverge. Using the above values of the parameters, we find that such a system will become gravitationally bound for $A > 3.4 \times 10^{56}$, i.e., for a mass in excess of 5.6×10^{29} kg, which is within an order of magnitude of the mass of a typical neutron star. Since furthermore the above value of r_0 implies that the density of a nucleus is within an order of magnitude that of a neutron star, we see that the semi-empirical formula can actually encompass the picture of a neutron star as consisting of an enormous gravitationally bound nucleus.



(a)



(b)

Figure 1. (a): Errors in mass fit to semi-empirical mass formula of Equation (2), as function of N. (b): Errors in mass fit to semi-empirical mass formula of Equation (2), as function of Z.

3. Microscopic approaches

3.1. REALISTIC NUCLEONIC INTERACTIONS AND THE NUCLEAR MANY-BODY PROBLEM

The ideal mass formula would be one in which the binding energies of all nuclei were derived from the basic nucleonic interactions. Work on these lines was initiated in the fifties by Brueckner and co-workers, and since then a tremendous effort

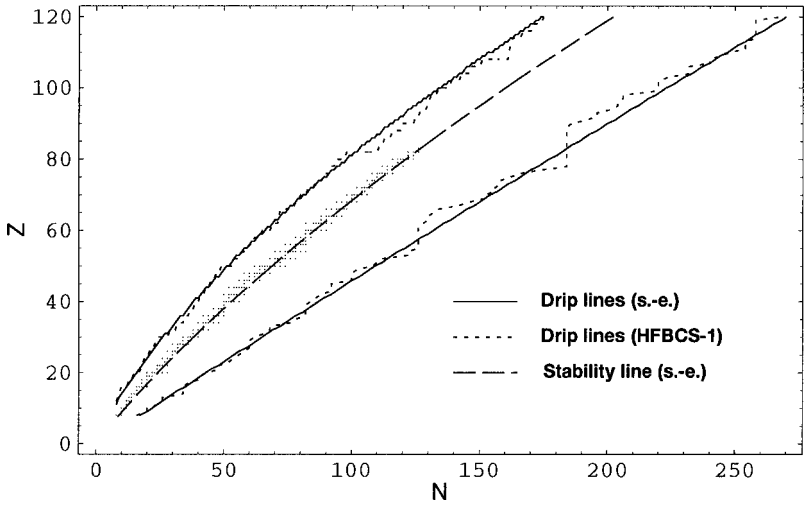


Figure 2. Drip lines according to semi-empirical mass formula of Equation (2) and mass formula HFBCS-1.

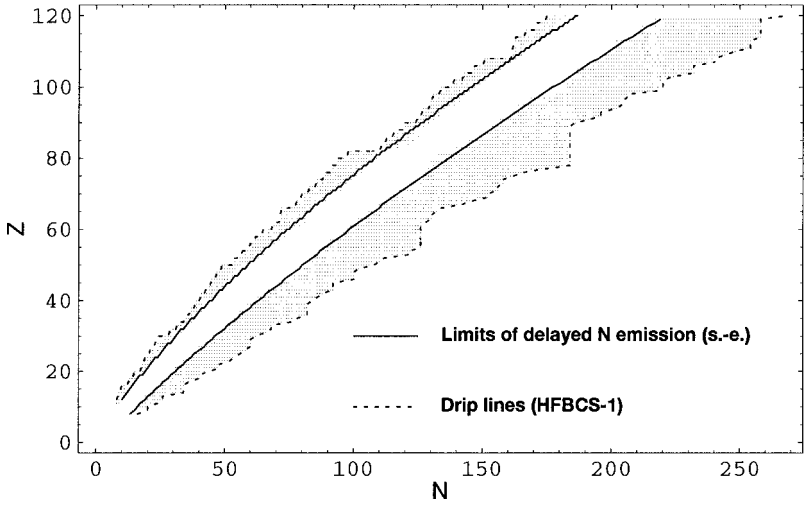


Figure 3. Dots represent nuclei that are unstable with respect to β-delayed nucleon emission according to mass formula HFBCS-1; solid lines represent inner limits of zones of such nuclei as given by semi-empirical mass formula of Equation (2).

has been expended in pursuing different possible approaches. Two main types of calculation can be discerned, as follows.

(a) *Non-relativistic methods.* These calculations assume that the nucleus is described by a non-relativistic Schrödinger equation

$$H\Psi = E_{\text{nuc}}\Psi, \tag{4}$$

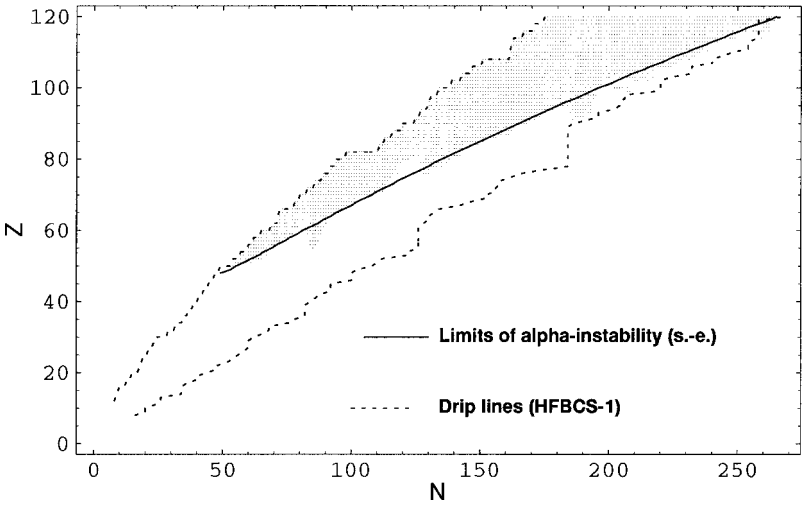


Figure 4. Dots represent nuclei that are unstable with respect to α-emission according to mass formula HFBCS-1; the solid line represents inner limit of zone of such nuclei as given by semi-empirical mass formula of Equation (2).

where

$$H = -\frac{\hbar^2}{2M}\sum_i \nabla_i^2 + \sum_{i>j} V_{ij} + \sum_{i>j>k} V_{ijk}. \tag{5}$$

Here V_{ij} and V_{ijk} are potentials representing the two-nucleon (N–N) and three-nucleon interactions, respectively, as determined by the scattering and bound-state properties of such systems, and by meson-exchange theories. To calculate the properties of complex nuclear systems in this non-relativistic framework both variational methods and Brueckner–Bethe–Goldstone theory have been used: guides to the literature can be found in [7] for the former, and [8, 9] for the latter.

(b) *Brueckner–Dirac methods.* Here the nucleons are treated fully relativistically, being represented by Dirac spinors. The degrees of freedom associated with the exchange of the mesons responsible for the nucleonic interactions are taken into account explicitly; moreover, the meson parameters are fitted to the N–N scattering data and measured meson properties. When fully developed this approach should be at least as reliable as the non-relativistic methods. (For a review see [10].)

All of these different methods based on realistic nucleonic interactions are horrendously complicated, and the only system for which quantitatively satisfactory results have been obtained is the relatively simple case of INM. Even if this success shows that these theories are fundamentally correct, the fact remains that the few calculations that have been performed on finite nuclei give results whose accuracy is inacceptably poor. Nevertheless, many-body theories based on realistic nucleonic forces will be able to serve as a qualitative guide in tying down some of the

ambiguities in the more phenomenological approaches based on the shell model that we describe below. In fact, already by 1958 many-body theory had reconciled the validity of the shell model with the short-range character of nuclear forces [11], thereby underpinning these more phenomenological approaches.

3.2. MEAN-FIELD MODELS WITH PHENOMENOLOGICAL INTERACTIONS

Since one cannot solve the exact nuclear Schrödinger equation (4), or its relativistic counterpart, with the accuracy required for astrophysical purposes, the best that can be done is to be guided by the success of the shell model, and assume, at least at the outset, that all nucleons move in some single-particle (s.p.) field. We shall see how this renders both the non-relativistic and relativistic forms of nuclear many-body theory tractable. The appearance of SM features in such an approach is, of course, ensured; we will see that DM features can emerge as well.

Non-relativistic Hartree–Fock method. This is a variational method, with a trial wavefunction having the form of a Slater determinant $\Phi = \det\{\phi_i(x_i)\}$, this being a properly antisymmetrized product of s.p. wavefunctions $\phi_i(x_i)$. Since Φ cannot be identical to the exact wave function Ψ of Equation (4), whatever the choice of $\phi_i(x_i)$, it follows that the expectation value $\langle\Phi|H|\Phi\rangle$ can never give the exact eigenenergy $E_{\rm nuc}$ of Equation (4). We shall thus have to replace the exact Hamiltonian H by an effective Hamiltonian if the HF method is to give the exact energy $E_{\rm nuc}$. We thus write in place of Equation (5)

$$H^{\rm eff} = -\frac{\hbar^2}{2M}\sum_i \nabla_i^2 + \sum_{i>j} v_{ij}^{\rm eff}, \tag{6}$$

in which $v_{ij}^{\rm eff}$ is some effective N–N potential that does not have to fit the N–N data. One way in which this force could be determined, particularly appropriate to the present context of nuclear masses, would be to optimize the fit of the expectation values $E_{\rm HF} = \langle\Phi|H^{\rm eff}|\Phi\rangle$ to all the measured values of $E_{\rm nuc}$.

The method proceeds by minimizing $E_{\rm HF}$ with respect to arbitrary variations in the unknown s.p. functions $\phi_i(x_i)$, which are then given as eigensolutions to a s.p. Schrödinger equation

$$\left(-\frac{\hbar^2}{2M}\nabla^2 + U\right)\phi_i = \epsilon_i\phi_i, \tag{7}$$

where U is a s.p. field that in general is non-local and spin-dependent, but is determined uniquely by the force. Once the $\phi_i(x_i)$ are determined $E_{\rm HF}$ can be calculated.

Provided the effective force, unlike the Coulomb force, does not have an infinite range, and has a short-range repulsion, INM will be saturated, i.e., have a finite density and energy per nucleon. Thus both DM and SM aspects emerge automatically

and on an equal footing in this picture, so that a much more unified approach to the mass formula is offered than is possible with the hybrid macro–micro methods (Section 4).

A particularly suitable form of effective force is the Skyrme form [12]:

$$\begin{aligned} v_{ij} \;=\; & t_0(1+x_0P_\sigma)\delta(\mathbf{r}_{ij}) + t_1(1+x_1P_\sigma)\frac{1}{2\hbar^2}\left\{p_{ij}^2\delta(\mathbf{r}_{ij}) + h.c.\right\} \\ & + t_2(1+x_2P_\sigma)\frac{1}{\hbar^2}\mathbf{p}_{ij}.\delta(\mathbf{r}_{ij})\mathbf{p}_{ij} + \frac{1}{6}t_3(1+x_3P_\sigma)\rho^\gamma\delta(\mathbf{r}_{ij}) \\ & + \frac{i}{\hbar^2}W_0(\boldsymbol{\sigma}_i+\boldsymbol{\sigma}_j).\mathbf{p}_{ij}\times\delta(\mathbf{r}_{ij})\mathbf{p}_{ij}. \end{aligned} \tag{8}$$

All terms here are formally of zero range, although the momentum dependence of the t_1 and t_2 terms simulates a finite range.

With Skyrme forces the s.p. equation (7) takes the form

$$\left\{-\boldsymbol{\nabla}\cdot\frac{\hbar^2}{2M_q^*(\mathbf{r})}\boldsymbol{\nabla} + U_q(\mathbf{r}) + V_q^{\mathrm{coul}}(\mathbf{r}) - i\mathbf{W}_q(\mathbf{r})\cdot\boldsymbol{\nabla}\times\boldsymbol{\sigma}\right\}\phi_{i,q} = \epsilon_{i,q}\phi_{i,q}, \tag{9}$$

in which i labels all quantum numbers, and q denotes n or p. All the field terms are now local, essentially because one can introduce a position-dependent effective mass M_q^*. There are two such quantities, corresponding to the two types of charge, which can be expressed at the INM equilibrium density in terms of an isoscalar and an isovector effective mass, M_s^* and M_v^*, respectively; these are unique combinations of the Skyrme-force parameters. Expressions for all quantities appearing in this equation, and for E_{HF}, can be found in [13].

Most nuclear HF calculations that have been performed use Skyrme forces, although the Gogny group uses forces that are explicitly finite-range [14]. While the latter may be regarded as more realistic, the essential non-locality of the s.p. fields complicates the calculations considerably. Until very recently no HF effective force had been fitted to more than ten or so nuclei, all spherical, presumably because of the computer-time limitations that arose in the past with deformed nuclei. However, it is now possible to fit to the masses of all nuclei (Section 3.4).

Relativistic Hartree method. As in the Dirac–Brueckner method, nucleons are represented by Dirac spinors, and the mesons mediating the nucleonic interactions are taken into account explicitly. However, their sole effect is to generate a mean field in which the nucleons move, and since no two-body forces appear explicitly there are no exchange terms, so we are dealing with a Hartree, rather than a HF, theory. Unlike the Dirac–Brueckner method, the meson parameters are determined by fitting directly to finite-nucleus properties, rather than to N–N scattering. In this sense the method, also known as the relativistic mean-field (RMF) method, is comparable to the non-relativistic HF method. A further similarity lies in the fact that here too INM will be saturated, so that again both DM and SM aspects emerge

automatically with equal status. However, the RMF method has the important merit of being Lorentz-invariant, a feature which allows the spontaneous appearance of a spin-orbit term in the field. Thus in the event of a contradiction between this method and the non-relativistic HF method, there would be good reasons for preferring the former, despite the highly phenomenological character of both methods.

So far the basic meson-parameter set of this method has not been fitted to the properties of more than ten nuclei. However, using a parameter set determined in this way, the masses (and other properties) of over a thousand nuclei have been calculated [15]. Unfortunately, the rms error of 2.6 MeV is unacceptable for astrophysical purposes; moreover, only even-even nuclei were calculated. But even if this means that no RMF mass formula can be said to be available at the present time, the tabulation [15] can still serve as a useful guide to the behaviour of the spin-orbit field far from stability.

3.3. CORRELATIONS

Even when the Slater determinant Φ satisfies the HF equations (7), it can never be identical to the exact nuclear wave function Ψ. Thus we must expect nuclear properties to show features that cannot be accounted for within the HF framework; such irreducible deviations from the mean-field picture are referred to as correlations.

Pairing correlations. These are the most conspicuous correlations in nuclear ground states, involving the tendency of like nucleons in time-reversed s.p. states to couple to zero total angular momentum. Their most obvious manifestation lies in the characteristic even-odd effect in binding energies, but they also account for the spherical shape of many open-shell nuclei: a nucleus with even one nucleon outside doubly-closed shells is deformed in the pure HF picture.

The simplest way to introduce pairing correlations into the HF framework is as follows. After each HF iteration, in the basis of s.p. states thereby generated, one applies the BCS method (borrowed from the theory of superconductivity) to the pairing interaction, which usually, but not invariably, is chosen to be distinct from the HF effective interaction: see, for example, [16, Chapter 8] or [17, Chapter 6]. This procedure neglects the fact that the scattering of nucleon pairs between different s.p. states under the influence of the pairing interaction will actually modify the s.p. states, a difficulty that becomes particularly serious close to the n-drip line, where nucleon pairs will be scattered into the continuum. This problem is avoided in the HF–Bogolyubov (HFB) method, which puts the pairing correlations into the variational function, so that the s.p. and pairing aspects are treated simultaneously and on the same footing (see [17, Chapter 7]).

Wigner correlations. Even when pairing correlations are correctly included, HF and other mean-field calculations systematically underbind nuclei with $N \simeq Z$ by about 2 MeV: see, for example, [18]. There seems to be a growing consensus that a

$T = 0$ pairing between neutrons and protons is responsible (see [19] and references quoted therein), but no systematic study has been made so far.

3.4. THE HFBCS-1 MASS FORMULA

Very recently [20] a complete mass table, labelled HFBCS-1, was constructed on the basis of HF calculations with a Skyrme force of the form (8), with pairing correlations taken into account in the BCS approach, using a δ-function pairing force. A Wigner correction term of the form [5, 21] $E_W = V_W \exp(-\lambda|N - Z|/A)$ was also included. With 16 parameters in all, a single constraint was applied before fitting: the isoscalar and isovector effective masses were set equal, $M_s^* = M_v^* (= M^*)$, there being no evidence to the contrary. The remaining 15 degrees of freedom were fitted (x_1 and γ only roughly) to the mass data [6]. The rms error for the 1888 measured nuclei with $Z, N \geqslant 8$ is 0.738 MeV.

Performing a HF calculation on a nucleus automatically yields a unique value for the charge radius, so that a comparison with the measured values provides an independent test of the validity of the calculations. For the 143 nuclei listed in the 1994 data compilation [22] the rms error is only 0.019 fm. It should be stressed that this good agreement has been achieved without any further parameter adjustment.

The Skyrme parameters of this force [20] imply an effective mass of $M^* = 1.05M$, which is consistent with the observation that unless $M^*/M \simeq 1.0$ the s.p. level density in the vicinity of the Fermi surface will be wrong [23], whence it would be impossible to fit the masses of open-shell nuclei, even if a fit to the masses of doubly magic nuclei were possible. On the other hand, all realistic estimates of M^*/M indicate a value of 0.7–0.8 (see [13, Section 1], where it will be seen that these values hold for both M_s^* and M_v^*): this is known as the 'k-mass' value. However, there is no contradiction between these two values of M^*/M, since Bernard and Giai [24] have shown that one can obtain reasonable s.p. level densities in finite nuclei with k-mass values of M^*/M, i.e., of 0.7–0.8, provided one takes into account the coupling between s.p. excitation modes and surface-vibration RPA modes. Since the good agreement with measured s.p. level densities found in [23] was obtained without making these corrections it must be supposed that the resulting error is being compensated by the higher value of M^*/M, i.e., $M^*/M \simeq 1.0$, which may thus be regarded as a phenomenological value, known as the 'ω-mass', that permits considerable success with straightforward HF, or other mean-field calculations, without any of the complications of [24]. Skyrme forces such as those of the Lyon group [25, 26] that are constrained to have a k-mass value of M^*/M, i.e., 0.7–0.8, cannot serve as the basis of a mass formula (unless one performed calculations of the Bernard–Giai type on all nuclei). This point is well illustrated in [26, Figures 1–4]. (In the same way, the poor agreement with the experimental masses of spherical open-shell nuclei given by the Gogny force, as displayed in [14, Figure 9], is presumably the result of the effective mass associated with the essentially non-local s.p. field being significantly smaller than unity.)

4. Macroscopic–microscopic approaches

The way in which shell corrections are grafted on to the DM can be understood as an approximation to the HF method. If $\tilde{\rho}$ is any smooth diagonal approximation to the HF density matrix ρ_{HF} then an expansion of $E[\rho_{\mathrm{HF}}]$ in powers of $\delta\rho \equiv \rho_{\mathrm{HF}} - \tilde{\rho}$ leads to the Strutinsky theorem (see [17, p. 93]),

$$E_{\mathrm{HF}} \equiv E[\rho_{\mathrm{HF}}] \simeq E[\tilde{\rho}] + \sum_i \tilde{\epsilon}_i - \mathrm{tr}\,\tilde{h}\tilde{\rho}, \tag{10}$$

where we have neglected pairing and terms $O(\delta\rho)^2$. Also $\tilde{h} \equiv h[\tilde{\rho}]$ is the smoothed s.p. Hamiltonian approximating the exact s.p. Hamiltonian $h[\rho_{\mathrm{HF}}]$, and the $\tilde{\epsilon}_i$ are the corresponding eigenvalues, with the sum going over all occupied states: all the shell-model fluctuations arise in this sum.

The choice of $\tilde{\rho}$ is arbitrary, and this approach originally took it to correspond to the DM. As for the s.p. Hamiltonian $\tilde{h}$, this must have the same form as in Equation (7), whence a choice must be made for the field U. There is no unambiguous way of doing this for the DM choice of $\tilde{\rho}$, and in practice one has been guided by considerations of plausibility and convenience. Once this choice has been made the determination of the $\tilde{\epsilon}_i$ is straightforward, and there remains only the last term to calculate. Formally, this corresponds to a smoothed version of the sum in the preceding term, $\mathrm{tr}\,\tilde{h}\tilde{\rho} \equiv \widetilde{\sum_i}\tilde{\epsilon}_i$, and it is evaluated by the various 'Strutinsky smoothing procedures' that have been devised (see, for example, [16, Section 12.4]). We have here a second source of uncertainty, especially for nuclei close to the n-drip line [27].

As for pairing corrections, BCS calculations are straightforward in this approach, once the s.p. states have been calculated.

The most recent and elaborate mass formula of this type is the 'finite-range droplet model' (FRDM) of [2]. Here the simple DM of Equation (2) is replaced by the more sophisticated 'droplet' model, but otherwise the model conforms to the above scheme. The data fit has an rms error of 0.689 MeV for the above set of 1888 nuclei, which is somewhat better than for HFBCS-1. However, in addition to the usual uncertainty associated with Strutinsky smoothing, the inevitable uncertainty associated with the choice of s.p. field is exacerbated by the fact that the symmetry coefficient a_{sym} (J in their notation) corresponding to this field has the value of 35 MeV, while this same coefficient takes the value of 32.73 MeV in the macroscopic part. We do not know whether the quality of the fit would have deteriorated if it had been reiterated until a_{sym} took the same values in both parts. Moreover, it is difficult to assess the impact on the reliability of the extrapolations.

The ETFSI Approximation. A much closer approximation to the HF method than the above DM-based method is the so-called ETFSI method [18, 28–32]. It is based entirely on a Skyrme force of the form (8), with the constraint of $M^* = M$, and the starting point is to calculate the energy of any given nucleus in the extended

Thomas–Fermi (ETF) approximation. The resulting energy varies smoothly as a function of N, Z and deformation, so that it constitutes a purely macroscopic term, for which microscopic corrections still have to be added. However, there is a fundamental difference compared to the earlier macro–micro calculations: a unique s.p. field U can now be generated simply by folding the same Skyrme force over the nucleon distribution determined in the first part of the calculation. There is thus a much closer unity between the two parts of the calculation than in earlier macro-micro calculations, the same Skyrme force underlying both parts. Furthermore, in applying the Strutinsky theorem, all the ambiguities that we mentioned in relation to smoothing vanish, since the last term of Equation (10) reduces to an integral over quantities determined in the ETF calculation: this is the Strutinsky integral (SI).

It turns out that in its latest form, ETFSI-2 [32], this method approximates HF so well that the two methods give essentially equivalent results. The rms errors of the respective data fits are virtually identical, and the fitted forces give very similar extrapolations out to the drip lines (note, however, that the fitted forces are *not* identical). Nevertheless, the ETFSI approximation is very much faster, being feasible at a time when the HF method itself was not. As far as mass formulas are concerned, the ETFSI approximation has now in a way been made redundant by the HF calculations, but it is still extremely valuable for the far more complicated calculations of fission barriers: ETFSI calculations of some 2000 barriers were recently performed [33, 34].

The TF-FRDM approximation. A different semi-classical approximation, using a force that is finite-range and both momentum- and density-dependent, gives an rms error of 0.673 MeV for the above data set of 1888 nuclei [35], which is better than either FRDM or HFBCS-1. However, besides the force there are two other significant differences with respect to the ETFSI method. (a) The semi-classical calculation is zeroth-order Thomas–Fermi, rather than fourth-order extended Thomas–Fermi, which means that the nuclear surface is not as well represented as in ETFSI. The effect of this on the quality of the fit to the data is presumably taken up by the parameters, but the compensation will not hold in the unknown regions far from stability to which one will want to extrapolate. (b) The shell corrections are not calculated self-consistently, as in the HF method (and the ETFSI approximation), but are taken directly from the FRDM calculation, along with the pairing corrections and the deformations, making this much closer to the DM-based macro–micro mass formulas. In principle, once the force parameters had been fitted to the data, the shell corrections could have been recalculated, exactly as with the ETFSI method, but it is not at all clear that the new ones would have been similar to the original ones. Indeed, there is no *a priori* guarantee that the value of M^* corresponding to the rather novel form of force adopted in this calculation will lie close to M, a necessary condition for a good fit to the masses of open-shell nuclei in self-consistent calculations (see Section 3.4).

5. Summary and outlook

We have presented here a new mass formula, HFBCS-1, the first that is fully microscopic. The fit to the data is not quite as good as with the two macro–micro formulas in current usage, with an rms error of 0.738 MeV for 1888 masses, as opposed to 0.689 MeV in the case of the FRDM and 0.673 MeV with the TF-FRDM. However, both of the latter two formulas are incomplete in that they contain serious inconsistencies between the macroscopic and microscopic parts; these inconsistencies could be removed in each case by performing more iterations, as described above, but it is not clear that the high quality of the respective fits could survive this operation.

Despite the rough similarity in the quality of the data fits of all three mass formulas, striking differences emerge on extrapolating far from the data. These are discussed in detail elsewhere in these proceedings [3], but two important features must be mentioned here. (a) The shell gap at $N = 184$ on the n-rich side of the stability line, i.e., for p-deficient nuclei, is stronger for HFBCS-1 than for the FRDM (the TF-FRDM results are essentially identical to the FRDM results in this respect). The isospin dependence of the spin-orbit field is crucial here, and significantly the RMF calculations of [15] discriminate in favour of HFBCS-1 (see Figure 5, and also [36, 37]). (b) Concerning INM, the symmetry coefficient $a_{\rm sym}$ is markedly lower for HFBCS-1 than for FRDM or TF-FRDM: 28 MeV rather than 32–35 MeV. This is a much more difficult question to resolve, which is unfortunate, since $a_{\rm sym}$ is a critical factor in determining the rate of neutrino cooling of neutron stars.

Since one of the main sources of motivation for all this work is to use mass formulas to extrapolate far from the data, the obvious question to ask is: which one

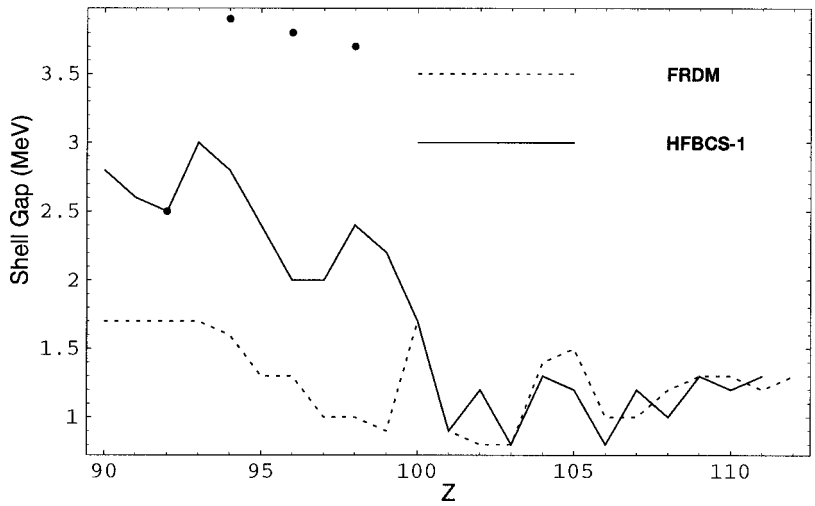


Figure 5. Shell gap at $N = 184$ as function of Z, defined in terms of $2n$-separation energy according to $S_{2n}(N = 186) - S_{2n}(N = 184)$. Dots correspond to RMF calculations [15].

of these mass formulas is to be believed? The ultimate mass formula, i.e., the one that gets everything right, *must* be microscopic, but one cannot pretend that with HFBCS-1 we have reached the end of history, as far as mass formulas go, with nothing more to do than refit the parameters every time Audi and Wapstra crank out another evaluation. On the contrary, I believe that the remaining uncertainties in the extrapolations of HFBCS-1 out to the n-drip line are at least as great as the differences between HFBCS-1 and the two modern macro–micro formulas. Here are some of the outstanding theoretical problems that must be addressed before we can really start to extrapolate out to the n-drip line with any confidence.

(1) Effective mass. Our data fits have confirmed the Bernard–Giai renormalization of M^* to take account of surface modes [24]. But their calculations were made only in the region of the stability line, so it is really only the isoscalar component M_s^*/M whose ω-mass value is well tied down to close to 1, and it is essential that they be extended towards the n-drip line in order to determine the ω-mass value of M_v^*/M. It should be stressed that there is no justification at the present time for our assumption that $M_s^* = M_v^*$ as far as ω-mass values are concerned; all that can be said is that there are no data against it.

(2) Pairing. Firstly, if we are to have any confidence in the extrapolations out to the n-drip line, it is essential that the HF-BCS method used here be replaced by HFB. Calculations performed with the Skyrme force SkP [38, 39] on spherical nuclei indicate that the effect of replacing HF-BCS by HFB will be to quench shell effects at the n-drip line, but there have been no extensive HFB calculations for arbitrary deformations. Actually, a somewhat improvised attempt to modify the original ETFSI calculations [18] for Bogolyubov quenching has already been made [40], but a complete HFB calculation would be preferable. However, the extent of the quenching depends on the s.p. spectra, and thus on the value of M^*/M assumed for highly n-rich nuclei, and it must be stressed that there is as yet no firm support for the value of 1 taken for the force SkP. Thus before undertaking any extensive HFB calculations it will be necessary to resolve the problem of M_v^*/M.

Beyond that, attention has to be paid to the choice of the pairing interaction, noting that it does not have to be identical to the HF force. Should it be density-dependent? Should it depend on the gradient of the density in order to confine it to the surface? These are all open questions, and one welcomes the recent efforts to relate the pairing force, hitherto treated on a purely phenomenological basis, to more basic nuclear processes, as in [41–43].

Experiment. There will always be a need for more and more data further and further from the stability line, not only to tie down the parameters of the various theories, but also to weed out the weakest of them. Of particular importance here is the need to shed light on the M_v^*/M problem, and to find firm evidence for the existence of shell quenching. In both these connections I would stress the importance not only of mass data, but particularly of s.p. spectra. And again, while the n-rich side of the stability line is the one of most direct interest for the r-process, data on the p-rich side can be just as invaluable in tying down theories. Finally, to conclude

on a completely different note, let me point out that it would be very useful indeed if one could measure neutron-skin thicknesses, since these provide an independent determination of the symmetry coefficient $a_{\rm sym}$.

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References

1. v. Weizsäcker, C. F., *Zeit. f. Phys.* **96** (1935), 431.
2. Möller, P., Nix, J. R., Myers, W. D. and Swiatecki, W. J., *At. Data Nucl. Data Tables* **59** (1995), 185.
3. Goriely, S., this issue, 105.
4. Bethe, H. A. and Bacher, R. F., *Rev. Mod. Phys.* **8** (1936), 82.
5. Myers, W. D. and Swiatecki, W. D., *Nucl. Phys.* **81** (1966), 1.
6. Audi, G. and Wapstra, A. H., *Nucl. Phys. A* **595** (1995), 409.
7. Akmal, A., Pandharipande, V. R. and Ravenhall, D. G., *Phys. Rev. C* **58** (1998), 1804.
8. Baldo, M., Giansiracusa, G., Lombardo, U. and Song, H. Q., *Phys. Lett. B* **473** (2000), 1.
9. Lejeune, A., Lombardo, U. and Zuo, W., *Phys. Lett. B* **477** (2000), 45.
10. Machleidt, R., *Adv. Nucl. Phys.* **19** (1989), 189.
11. Gomes, L. C., Walecka, J. D. and Weisskopf, V. F., *Ann. Phys*. **3** (1958), 241.
12. Vautherin, D. and Brink, D. M., *Phys. Rev. C* **5** (1972) 626.
13. Tondeur, F., Goriely, S., Pearson, J. M. and Onsi, M., *Phys. Rev. C* **62** (2000), 024308.
14. Dechargé, J. and Gogny, D., *Phys. Rev. C* **21** (1980), 1568.
15. Lalazissis, G. A., Raman, S. and Ring, P., *At. Data Nucl. Data Tables* **71** (1999), 1.
16. Preston, M. A. and Bhaduri, R. K., *Structure of the Nucleus*, Addison-Wesley, Reading, MA, 1975.
17. Ring, P. and Schuck, P., *The Nuclear Many-Body Problem*, Springer, New York, 1980.
18. Aboussir, Y., Pearson, J. M., Dutta, A. K. and Tondeur, F., *At. Data Nucl. Data Tables* **61** (1995), 127.
19. Satula, W., Dean, D. J., Gary, J., Mizutori, S. and Nazarewicz, W., *Phys. Lett. B* **407** (1997), 103.
20. Goriely, S., Tondeur, F. and Pearson, J. M., *At. Data Nucl. Data Tables* **77** (2001), 311.
21. Myers, W. D. and Swiatecki, W. J., *Nucl. Phys. A* **612** (1997), 249.
22. Nadjakov, E. G., Marinova, K. P. and Gangrsky, Yu. P., *At. Data Nucl. Data Tables* **56** (1994), 134.
23. Barranco, M. and Treiner, J., *Nucl. Phys. A* **351** (1981), 269.
24. Bernard, V. and Van Giai, Nguyen: *Nucl. Phys. A* **348** (1980), 75.
25. Chabanat, E., Bonche, P., Haensel, P., Meyer, J. and Schaeffer, R., *Nucl. Phys. A* **627** (1997), 710.
26. Chabanat, E., Bonche, P., Haensel, P., Meyer, J. and Schaeffer, R., *Nucl. Phys. A* **635** (1998), 231.
27. Nazarewicz, W., Werner, T. R. and Dobaczewski, J., *Phys. Rev. C* **50** (1994), 2860.
28. Dutta, A. K., Arcoragi, J.-P., Pearson, J. M., Behrman, R. and Tondeur, F., *Nucl. Phys. A* **458** (1986), 77.
29. Tondeur, F., Dutta, A. K., Pearson, J. M. and Behrman, R., *Nucl. Phys. A* **470** (1987), 93.

30. Pearson, J. M., Aboussir, Y., Dutta, A. K., Nayak, R. C., Farine, M. and Tondeur, F., *Nucl. Phys. A* **528** (1991), 1.
31. Aboussir, Y., Pearson, J. M., Dutta, A. K. and Tondeur, F., *Nucl. Phys. A* **549** (1992), 155.
32. Goriely, S., In: S. Wender (ed.), *Proceedings of the 10th International Symposium on Capture Gamma-Ray Spectroscopy and Related Topics*, Santa Fe, New Mexico, USA, September 1999; *A.I.P. Proceedings* **529** (2000), 287.
33. Mamdouh, A., Pearson, J. M., Rayet, M. and Tondeur, F., *Nucl. Phys. A* **644** (1998), 389.
34. Mamdouh, A., Pearson, J. M., Rayet, M. and Tondeur, F., *Nucl. Phys. A* **679** (2001), 337.
35. Myers, W. D. and Swiatecki, W. J., *Nucl. Phys. A* **601** (1996), 141.
36. Onsi, M., Nayak, R. C., Pearson, J. M., Freyer, H. and Stocker, W., *Phys. Rev. C* **55** (1997), 3166.
37. Nayak, R. C. and Pearson, J. M., *Phys. Rev. C* **58** (1998), 878.
38. Dobaczewski, J., Hamamoto, I., Nazarewicz, W. and Sheikh, J. A., *Phys. Rev. Lett.* **72** (1994), 981.
39. Dobaczewski, J., Nazarewicz, W. and Werner, T. R., *Phys. Scr. T* **56** (1995), 15.
40. Pearson, J. M., Nayak, R. C. and Goriely, S., *Phys. Lett. B* **387** (1996), 455.
41. Barranco, F., Broglia, R. A., Gori, G., Vigezzi, E., Bortignon, P. F. and Terasaki, J., *Phys. Rev. Lett.* **83** (1999), 2147.
42. Garrido, E., Sarriguren, P., Moya de Guerra, E. and Schuck, P., *Phys. Rev. C* **60** (1999), 064312.
43. Bertsch, G. F. and Esbensen, H., *Ann. Phys.* **209** (1991), 327.