Eur. Phys. J. A **15**, 13–16 (2002)
DOI 10.1140/epja/i2001-10215-y

THE EUROPEAN PHYSICAL JOURNAL A

A Hartree-Fock nuclear mass formula

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Received: 21 March 2002 /
Published online: 31 October 2002 –

Abstract. We recall the main features of the recently published mass formula, HFBCS-1, based on the Hartree-Fock-BCS method, and compare its extrapolations out to the neutron drip line with those given by the fine-range droplet model. A new Hartree-Fock-Bogolyubov mass formula, HFB-1, is described: the rms error of the fit to 1888 masses is 0.766 MeV, compared with 0 .738 MeV for HFBCS-1, but there are no substantial changes in the predictions relevant to the r-process. After a critical examination of various questions relating to the effective nucleon mass and to the requirements of the relativistic mean-field theory, we conclude that the greatest remaining ambiguity concerns the nature of the pairing force.

PACS. 21.10.Dr Binding energies and masses – 21.60.Jz Hartree-Fock and random-phase approximations – 21.65.+f Nuclear matter

1 Introduction

The r-process of nucleosynthesis depends crucially on the binding energies (among other properties) of heavy nuclei that are so neutron rich that there is no hope of being able to measure them in the laboratory. It thus becomes of the greatest importance to be able to make reliable extrapolations of nuclear masses (and other relevant properties, such as fission barriers) away from the known region, relatively close to the stability line, out towards the neutron drip line. This means that one should have a mass formula that not only gives a good fit to the data, but also has a sound theoretical basis; generally speaking, the more microscopically grounded is a mass formula, the better one would expect its theoretical basis to be.

Until recently the masses and barriers used in all studies of the r-process were calculated on the basis of one form or another of the liquid-drop model, the most sophisticated version of which is the "finite-range droplet model" (FRDM) [1]. Despite the great empirical success of this formula (it fits 1654 masses with an rms error of 0.669 MeV), there is still an obvious need to develop a mass formula that is more closely connected to the basic nuclear interactions. Two such approaches are feasible at the present time: one is the non-relativistic Hartree-Fock (HF) method and the other the relativistic mean-field (RMF) method, though so far only the first has been fully exploited in the sense of complete mass formulas being constructed, with essentially all the mass data being fitted.

The first such mass formula is the recently published HFBCS-1 [2,3], the main features of which we recall in sect. 2, with the rest of the paper being devoted to a critical evaluation of this mass formula. In sect. 3 we deal with pairing, and in particular describe a new HF-Bogolyubov (HFB) mass formula. Various questions relating to the effective nucleon mass are discussed in sect. 4, while in sect. 5 we consider the relation of these Skyrme-based mass formulas to RMF theory. Finally, in sect. 6 we attempt to anticipate future developments.

2 The HFBCS-1 mass formula

This mass formula is based on a Skyrme-type HF force with the usual form

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

where P_σ is the two-body spin-exchange operator, and a δ-function pairing force,

$$v_{\text{pair}}(\mathbf{r}_{ij}) = V_{\pi q}\ \delta(\mathbf{r}_{ij})\,, \tag{2}$$

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is treated in the BCS approximation. The Wigner effect is handled purely phenomenologically by adding to the HF-BCS energy a term of the form

$$E_{\mathrm{W}} = V_{\mathrm{W}} \exp(-\lambda |N - Z|/A)\,. \tag{3}$$

In the HF part of the calculation we impose the constraint of axial and left-right symmetry on deformations, with corrections made for the spurious centre-of-mass and rotational energies. As for the pairing part of the calculation, the pairing-strength parameter $V_{\pi q}$ is allowed to be different for neutrons and protons, and also to be slightly stronger for an odd number of nucleons ($V_{\pi q}^{-}$) than for an even number ($V_{\pi q}^{+}$), *i.e.* the pairing force between neutrons, for example, depends on whether the neutron number N is even or odd [4]. The BCS calculations are performed with blocking, and a sharp cutoff energy of $\hbar\omega = 41A^{-1/3}$ is adopted; the Lipkin-Nogami variant of the BCS method has not been used so far in these calculations.

The 10 Skyrme parameters are constrained by the condition that the isoscalar and isovector effective nucleon masses be equal, $M_s^* = M_v^* = M^*$. (We recall that these two quantities are defined such that the effective mass of a nucleon of charge type q in nuclear matter at the equilibrium density ρ_0 is given by

$$\frac{\hbar^2}{2M_q^*} = \frac{2\rho_q}{\rho_0}\frac{\hbar^2}{2M_s^*} + \left(1 - \frac{2\rho_q}{\rho_0}\right)\frac{\hbar^2}{2M_v^*}\,, \tag{4}$$

where ρ_q is the density of nucleons of charge type q.) Thus with four pairing and two Wigner parameters there are 15 degrees of freedom in all. The final parameter set, labelled MSk7, is determined by fitting to the 1772 measured masses given in the 1995 compilation [5] for nuclei with $A \geq 36$. Nuclei with $A < 36$ were excluded from the fit because the HF-BCS method is not expected to work well for such light nuclei, and we wanted to avoid contaminating the force by including inappropriate data in its determination. The rms error of this fit is 0.683 MeV. If we now add to our data set the measured nuclei with $A < 36$ and $Z, N \geq 8$ without any further adjustment of the force, the rms error rises to 0.738 MeV (for 1888 nuclei).

Charge radii. For each nucleus we calculate the rms charge radius given by our model. Comparison with the measured charge radii of the 523 nuclei listed in the 1994 data compilation [6] shows an rms error of only 0.024 fm. We stress that this agreement has been achieved without any further parameter adjustment, all our parameters having been determined by the mass fit. This is a sensitive test of the overall quality of the underlying model. A similar check is provided by a comparison of the calculated deformations with experiment [3].

Nuclear-matter symmetry coefficient J. The value of this coefficient for our final parameter set MSk7 is 27.95 MeV, which is somewhat smaller than the values of 32.73 MeV for the macroscopic part of the FRDM and 35.00 MeV for its microscopic part. This low value of J is however quite robust within the framework of Skyrme-force fits to *all* the mass data, and is in any case in good agreement with nuclear-matter calculations based on modern realistic nucleonic interactions [7,8], which give values over the range 28–30 MeV. It is noteworthy that our value of J is close to the lower limit that is compatible with the stability of neutron matter: see fig. 1, in which FP denotes the realistic calculations of ref. [9], and also ref. [10].

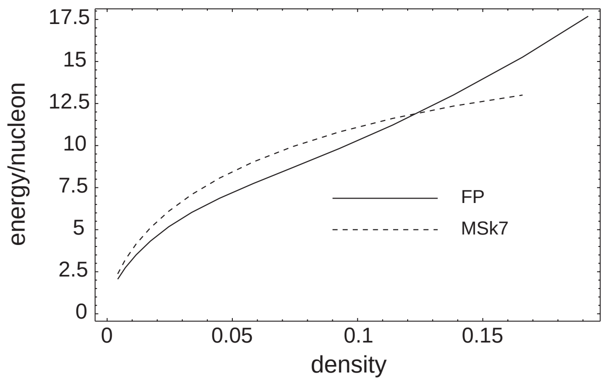

Fig. 1. Energy per nucleon (MeV) of neutron matter as a function of density (nucleons $\cdot$ fm^{-3}).

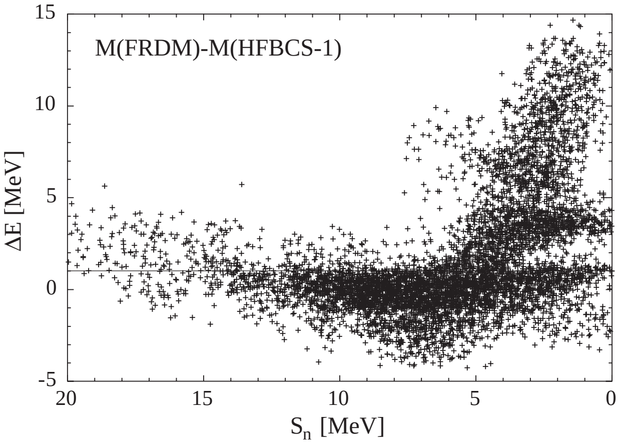

Fig. 2. Differences between HFBCS-1 and FRDM mass formulas, as a function of the neutron separation energy S_n.

Comparison with the FRDM. For our final set of 1888 masses the rms error given by the FRDM [1] is 0.689 MeV, and might have been still lower had the model been fitted to this set. With our own rms error of 0.738 MeV, the differences between the two mass formulas are very small over the known region of the nuclear chart, but become pronounced on extrapolating to the neutron drip line, as can be seen in fig. 2, where we plot the differences as a function of the neutron separation energy, S_n (this figure also shows that the divergence is much smaller on the proton-rich side). This strong divergence is associated with bigger shell gaps near the neutron drip line for FRDM at $N_0 = 50$ and 82, and for HFBCS-1 at $N_0 = 184$; we are here defining the neutron shell gap by

$$\Delta(N_0, Z) = S_{2n}(N_0, Z) - S_{2n}(N_0 + 2, Z)\,. \tag{5}$$

The stronger gap for HFBCS-1 at $N_0 = 184$ will imply higher fission barriers for very heavy, very neutron-rich nuclei, which could lead to the r-process evolving to much heavier nuclei than previously believed [11].

3 Pairing considerations

The most questionable aspect of the HFBCS-1 mass formula is the use of the BCS method to calculate pairing, the superiority of the Bogolyubov method at the neutron drip line having been stressed many times: see, for example, ref. [12]. Samyn *et al.* [13] have therefore constructed a new mass formula, HFB-1, very much on the lines of HFBCS-1, except that pairing is handled with the Bogolyubov method. (Working as always in a harmonic-oscillator basis, we do not make the transformation of Stoitsov *et al.* [14], since binding energies are expected to be insensitive to such asymptotic considerations.) The Skyrme and pairing forces, as well as the Wigner term, have the same forms as before, and the same cutoff is adopted in the pairing channel. With the HFB method replacing the HF-BCS method it was found that there was a deterioration in the data fit with the original force MSk7. A new fit was accordingly made in the HFB model, with the final parameter set, labelled BSk1, giving an rms error of 0.766 MeV to the same data set of 1888 nuclei as before, only slightly worse than the original error of 0.738 MeV. The values of the BSk1 parameters are

$$
\begin{aligned}
&t_0 = -1831.65\ \mathrm{MeV}\cdot\mathrm{fm}^3\,, \quad t_1 = 263.318\ \mathrm{MeV}\cdot\mathrm{fm}^5\,,\\
&t_2 = -296.824\ \mathrm{MeV}\cdot\mathrm{fm}^5\,, \quad t_3 = 13458.2\ \mathrm{MeV}\cdot\mathrm{fm}^4\,,\\
&x_0 = 0.596663\,, \quad x_1 = x_2 = -0.5\,, \quad x_3 = 0.817748\,,\\
&W_0 = 117.984\ \mathrm{MeV}\cdot\mathrm{fm}^5, \quad \gamma = 0.333333\,,\\
&V_{\pi n}^{+} = -227\ \mathrm{MeV}\cdot\mathrm{fm}^3\,,\\
&V_{\pi n}^{-} = -236\ \mathrm{MeV}\cdot\mathrm{fm}^3\,,\\
&V_{\pi p}^{+} = -251\ \mathrm{MeV}\cdot\mathrm{fm}^3\,, \quad V_{\pi p}^{-} = -260\ \mathrm{MeV}\cdot\mathrm{fm}^3\,,\\
&V_{\mathrm{W}} = -2.90\ \mathrm{MeV}\,, \quad \lambda = 30.0\,.
\end{aligned}
$$

Extrapolating out to the neutron drip line, it was found that the shift in the HFB-1 masses with respect to the HFBCS-1 masses was almost invariably less than 2 MeV, while the shifts in the S_n and the beta-decay energies Q_β, the quantities of ultimate interest for the r-process, are much smaller. Of particular interest in this respect is the almost negligible difference between the shell gaps for the two methods, as shown in fig. 3.

We conclude that replacing the BCS method by the Bogolyubov method will have very little impact on masses, insofar as they are relevant to the r-process. However, this is not to say that there are no important ambiguities associated with the pairing. Indeed, it has been known for some time that making the pairing force density dependent in such a way that it is concentrated in the nuclear surface can lead to a stronger quenching of the shell gap as the neutron drip line is approached [15]. However, such a modification of the pairing force may not lead to any significant improvement in the data fit: in this case one would have to be guided by more microscopic studies of the origin of the pairing force. It will also be necessary to study the sensitivity of the extrapolated masses to the cutoff in the pairing channel. However, to the extent that the pairing force originates through the exchange of surface phonons it will be long ranged, which means that in a δ-function representation a low-energy cutoff is indicated. Finally, we intend to see what happens when the Lipkin-Nogami procedure is implemented.

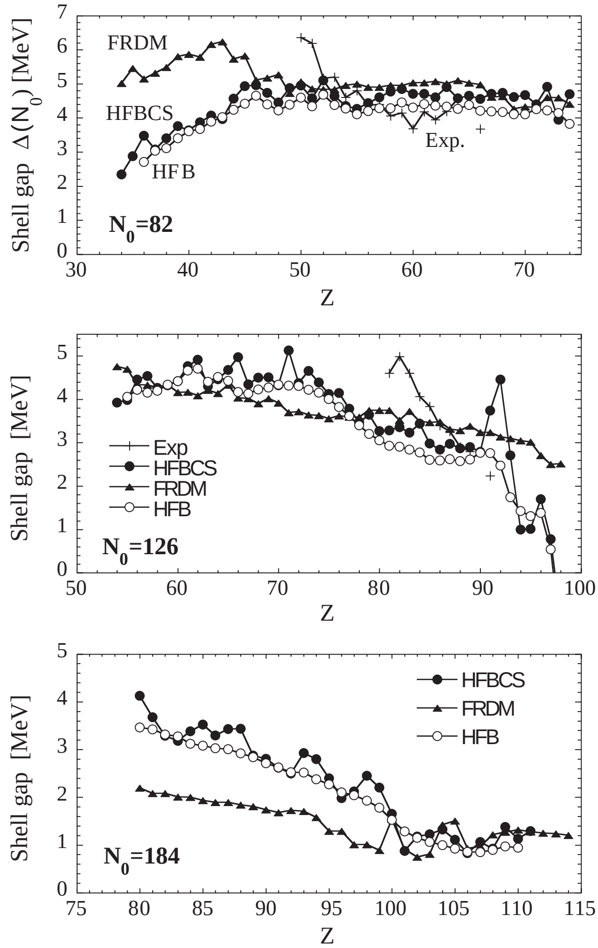

Fig. 3. Neutron shell gaps for N_0 = 82, 126, and 184, as a function of Z.

4 On the effective nucleon mass

In all the above data fits we have imposed the constraint $M_s^* = M_v^*$, and for the final forces the common value of these two effective masses is $M^* = 1.05M$. Releasing this constraint, we find that the optimal value, as determined by the data fit, of M_s^*, the isoscalar effective mass, remains very close to $1.05M$, while that of M_v^*, the isovector effective mass, is badly determined by the mass data, falling in the rather wide range of $0.90 \pm 0.20M$. However, the extrapolated masses at the neutron drip line are much more sensitive to M_v^* (see eq. (4)), but the associated ambiguities in the S_n and Q_β are inconsequential for the r-process [16].

5 Relation to RMF theory

For a Skyrme force of the form (1) the spin-orbit (s.o.) field for nucleons of charge type q is given approximately by

$$\mathbf{W}_q = \frac{1}{2} W_0 \boldsymbol{\nabla}(\rho+\rho_q) = \frac{3}{4} W_0 \boldsymbol{\nabla} \left\{ \rho \pm \frac{1}{3}(\rho_n - \rho_p) \right\} , \quad (6)$$

where $\rho = \rho_p + \rho_n$, and the upper sign corresponds to $q = n$, the lower to $q = p$. But in RMF theories the s.o. field can depend on $(\rho_n - \rho_p)$ only through the ρ-boson, and in view of the relatively weak coupling of this boson to the nucleon field it was suggested [17] that the s.o. field would have a much weaker isospin dependence in RMF models than in Skyrme-force models. Thus, it was argued, an RMF model and a Skyrme-force model that give comparable high-quality fits to the data might diverge when extrapolated far from the stability line. In fact, in view of the importance of the s.o. field for the determination of single-particle states, this was expected to be the principal difference between Skyrme-force and RMF methods, and it seemed that the former should fall into disfavour, since a theory that has manifest Lorentz invariance is inevitably to be preferred to one that does not.

However, in the case of the Skyrme force it is fairly easy to see that the isospin dependence arising from the second term of eq. (6) cannot be very large. In the first place we note that even at the neutron drip line the magnitude of $\frac{1}{3}(\rho_n - \rho_p)$ cannot exceed 10% of the first term ρ. Secondly, both of these terms are acted on by the gradient operator, and since the neutron and proton profiles are nearly everywhere parallel it follows that the isospin-dependent term in eq. (6) can make a non-zero contribution only over very restricted regions of the nucleus. Thus, there is reason to believe that the isospin dependence of the s.o. field will be similar in Skyrme-force and RMF models, provided both models are well fitted to the data. This has been confirmed in ref. [18], where it was shown that s.o. splittings in the HFBCS-1 model agree well with those given in the RMF approach, where available. The one counterexample that has been proposed [19] is that of ^{40}Ne, which actually lies beyond the neutron drip line.

6 Conclusions

It is shown that although the recently published mass formula HFBCS-1, the first to be based on the HF method, gives almost as good a fit to the mass data as does the FRDM mass formula, there are significant differences in their extrapolations to the neutron drip line. We have discussed ways in which the mass predictions for highly neutron-rich nuclei given by HFBCS-1 could be modified by future theoretical developments. It is shown that conclusions relevant to the r-process of nucleosynthesis are not changed in any substantial way either by replacing the BCS calculation of pairing effects with the Bogolyubov method, or by incorporating an improved understanding of the isovector dependence of the nucleon effective mass. Moreover, the isospin dependence of the spin-orbit field generated by the Skyrme forces underlying the two mass formulas is compatible with RMF theory. The most likely changes will be those associated with making the pairing force density dependent. Adding to the Skyrme force a t_4 term, *i.e.* a term with simultaneous density and momentum dependence, is expected to result in an improvement in the data fit [20].

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