Hartree-Fock mass formulas and extrapolation to new mass data

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The two previously published Hartree-Fock (HF) mass formulas, HFBCS-1 and HFB-1 (HF-Bogoliubov), are shown to be in poor agreement with new Audi-Wapstra mass data. The problem lies first with the prescription adopted for the cutoff of the single-particle spectrum used with the δ-function pairing force, and second with the Wigner term. We find an optimal mass fit if the spectrum is cut off both above E_F+15 MeV and below E_F-15 MeV, E_F being the Fermi energy of the nucleus in question. In addition to the Wigner term of the form $V_W \exp(-\lambda|N-Z|/A)$ already included in the two earlier HF mass formulas, we find that a second Wigner term linear in $|N-Z|$ leads to a significant improvement in lighter nuclei. These two features are incorporated into our new Hartree-Fock-Bogoliubov model, which leads to much improved extrapolations. The 18 parameters of the model are fitted to the 2135 measured masses for $N,Z\geqslant 8$ with an rms error of 0.674 MeV. With this parameter set a complete mass table, labeled HFB-2, has been constructed, going from one drip line to the other, up to $Z=120$. The new pairing-cutoff prescription favored by the new mass data leads to weaker neutron-shell gaps in neutron-rich nuclei.

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I. INTRODUCTION

Since the turn of the millenium it has become possible to base complete mass tables on the Hartree-Fock (HF) method, with the parameters of the underlying forces being fitted to essentially all of the nearly 2000 nuclei whose masses had been measured and compiled in the 1995 Atomic Mass Evaluation of Audi and Wapstra [1]. Two such mass formulas have been published so far, both based on a conventional form of Skyrme force,

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

and a δ-function pairing force acting between like nucleons,

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

in which we allow the pairing-strength parameter $V_{\pi q}$ 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 N is even or odd. This "staggered pairing" device was introduced in Ref. [2], and further discussed in Ref. [3]. Both mass formulas add to the energy corresponding to the above forces the Coulomb energy and a phenomenological Wigner term of the form

$$E_W = V_W\exp(-\lambda|N-Z|/A), \quad (3)$$

in which V_W is always negative, so that this term is attractive.

The first of these mass formulas is the HFBCS-1 formula of Goriely *et al.* [4], in which the pairing force was treated in the BCS approximation, and the other the HFB-1 formula of Samyn *et al.* [5], which involves a full HF-Bogoliubov (HFB) calculation. These two mass formulas give comparable fits to the 1768 measured masses of nuclei with $N,Z\geqslant 8$ that appear in the 1995 compilation [1] (Table I); these fits are roughly of the same quality as the one given by the "finite-range droplet model" (FRDM), a sophisticated macroscopic-microscopic mass formula with at least five more adjustable parameters than either of the HF mass formulas [6]. (Actually, both of the HF mass formulas were fitted to the 1888 measured masses with $N,Z\geqslant 8$ given in the unpublished Audi-Wapstra file mass_exp.mas95, but 120 of these experimental masses, marked by a black diamond in the published tables [1], are not "recommended," being inconsistent with local systematics. On the other hand, the FRDM was fitted to only 1654 masses.)

Since the time that these two HF mass formulas were constructed an extensive preliminary version of a new Atomic Mass Evaluation was kindly made available to us by Audi and Wapstra [7]. This new compilation contains 2135 measured masses of nuclei with $N,Z\geqslant 8$, but since 15 of the nuclei that originally appeared in the 1995 compilation [1] have now been removed there are actually 382 "new" nuclei, out of which 337 are located in the proton-rich region of the nuclear chart and only 45 in the neutron rich. We show in Table I the errors of the various mass formulas for this set of

TABLE I. Errors of fits to the masses of the 1768 nuclei of the 1995 data compilation [1] and of extrapolations to the 382 new nuclei of the 2001 data compilation [7]. σ denotes rms error, ϵ denotes mean error; all errors in MeV. R is the ratio of the rms error for the 382 new nuclei to the rms error of the 1768 nuclei of the 1995 compilation.

	1995 data	(1768 nuclei)	New data (382 nuclei)		
	σ	ϵ	σ	ϵ	R
FRDM	0.678	0.023	0.655	0.247	0.966
HFBCS-1	0.718	0.102	1.115	0.494	1.552
HFB-1	0.740	0.040	1.123	0.510	1.518
HFB-1($W1$)	0.733	0.016	1.088	0.456	1.484
HFB-1($W2$)	0.702	−0.036	1.029	0.415	1.466
HFB-2′	0.651	−0.039	0.857	0.470	1.316

new data [see Sec. III for HFB-1($W1$) and HFB-1($W2$), and Sec. IV for HFB-2′]; R is the ratio of the rms error for the 382 new nuclei to the rms error of the 1768 nuclei of the 1995 compilation, and is a measure of the predictive power of the mass formula in question. It will be seen that both of the above HF formulas extrapolate rather badly to these new data, particularly in comparison to the FRDM, which actually fares better on the new data than in the original fit. The problem with the two previously published HF formulas lies in a tendency to overbind both highly neutron-rich and highly proton-rich nuclei, particularly the $Z \simeq 82$ isotopes and $N \simeq 110$ isotones. Actually, the beginnings of this problem can already be discerned in Figs. 2 of Refs. [4,5], but the new data far from the stability line that have become available in the meantime [7] have rendered the situation acute, and reveal serious deficiencies in the HFBCS-1 and HFB-1 models.

The first objective of the present paper is to respond to the unfavorable situation shown in Table I by introducing two different modifications to our HFB model, which is otherwise exactly as described in Ref. [5]: (a) a new prescription for the cutoff of the spectrum of single-particle (SP) states over which the pairing force acts (Sec. II), and (b) a new Wigner term (Sec. III). Making use of these two new features, and making a finer parameter search than in our two previous HF mass formulas, we then (Sec. IV) generate a new mass formula, HFB-2, which is fitted to all of the 2135 masses of nuclei with $N,Z \geqslant 8$ in the new compilation [7]. Various aspects of the newly developed Skyrme force and mass table are discussed in this same section, particularly with respect to their suitability for calculations of the r process of nucleosynthesis, for which it is only the neutron-rich part of the nuclear chart that is relevant.

II. THE PAIRING CUTOFF

Both BCS and Bogoliubov calculations will diverge if the space of SP states over which a δ-function pairing force is allowed to act is not truncated. Making such a cutoff is, however, not simply a computational device but is an essential part of the physics, since the pairing interaction between two nucleons is really a long-range phenomenon mediated at least in part by the exchange of surface phonons [8]. To represent such an interaction by a δ-function force is thus legitimate only to the extent that all high-lying excitations are suppressed, although how exactly the truncation of the pairing space should be made will depend on the precise nature of the real, long-range pairing force. Since this is badly known one has considerable latitude in making the cutoff, and one might hope to use the data to limit the range of possibilities. The question of a cutoff need not arise if one uses a finite-range pairing force, such as the Gogny force [9], in the BCS or Bogoliubov calculations. However, to obtain convergence of the pairing energy with the Gogny force it is necessary to include contributions up to more than 100 MeV above the Fermi level, essentially because of the short-range part of the interaction [10]. And even if convergence is achieved in this way, it is doubtful that the choice of a simple static energy-independent force such as the Gogny force is much closer to the complicated underlying reality than is the "truncated δ-function" representation.

In both the HFBCS-1 formula and the HFB-1 formula the spectrum of SP states included in the pairing calculation was cut off at a SP energy of $\hbar\omega = 41A^{-1/3}$ MeV. This means that as one moves towards the neutron-drip line the available spectrum for neutrons above the Fermi surface is narrowed, while that for protons is widened; the opposite situation will prevail as one moves towards the proton-drip line. An alternative, and physically more plausible, scenario is that the height of the spectrum above the Fermi surface is constant, at

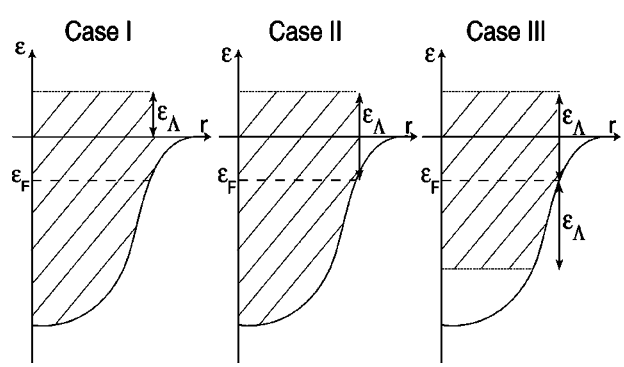

FIG. 1. Schematic representation in the single-particle space of the three cutoff prescriptions considered in the present work. ε_F corresponds to the Fermi energy and ε_Λ to the height of the cutoff energy.

TABLE II. Errors (rms, in MeV) of fits to 780 nuclei for different pairing cutoffs ε_Λ for the three different prescriptions considered and illustrated in Fig. 1.

Cutoff energy (ε_Λ)	Case I	Case II	Case III
$1\hbar\omega$	0.704	0.799	0.992
$2\hbar\omega$	0.716	0.737	0.774
$3\hbar\omega$	0.768	0.775	0.812
5 MeV	0.784	1.005	0.973
10 MeV	0.699	0.818	0.817
15 MeV	0.732	0.678	0.662
20 MeV	0.767	0.799	0.785

least for a given mass number A.

To study the sensitivity of the results to the choice of cutoff condition, three different prescriptions are considered, as illustrated in Fig. 1. In case I the cutoff energy height is taken relative to zero energy while the spectrum is extended down to the bottom of the potential well. In case II the cutoff energy height is taken relative to the Fermi energy of the nucleus in question, but again the spectrum is extended down to the bottom of the potential well. Now the same physical insight that suggests a constant cutoff height above the Fermi energy also suggests that the pairing spectrum of SP states should be cut off at a certain depth below the Fermi energy as well. Thus in case III the SP spectrum is cut off equidistantly above and below the Fermi energy. For each of these three prescriptions seven different cutoff energies ε_Λ are tested by fitting in each case all the force parameters to a data set of 780 nuclei drawn from the new compilation [7] as follows. To save the computer time, we calculate all nuclei in the spherical configuration, and thus limit these fits to quasispherical nuclei, imposing as always the constraint $N,Z \geqslant 8$. We consider that a nucleus is quasispherical if its deformation energy E_{def}, as defined in Eq. (13) of Ref. [3], is less than 0.2 MeV, as calculated according to the HFB-1 mass formula. We always subtract E_{def} from the energy calculated in the spherical configuration, assuming that the changes in this small correction from its HFB-1 value as the force parameters change are negligible. Also, with a view to avoiding problems with the Wigner effect (see Sec. III) we exclude nuclei with $|N-Z| \leqslant 2$, leaving us finally with 780 nuclei.

The rms errors of these fits for the 21 different cutoffs are shown in Table II. It will be seen that the best fit is obtained for $\varepsilon_\Lambda = 15$ MeV with prescription III, i.e., a double cutoff at $E_F \pm 15$ MeV, which we henceforth adopt. Actually, a fit that is almost as good is obtained for the same value of ε_Λ used with prescription II, i.e., a simple cutoff at $E_F + 15$ MeV, but our preference for the former prescription is strengthened by the fact that the force for the latter fit has an isovector effective mass of $M_v^* = 1.06M$, while the former fit leads to the more realistic value of $M_v^* = 0.86M$ (see Sec. IV). We should point out also that the best force obtained in case II is characterized by a symmetry coefficient $J = 27.8$ MeV, while in case III we obtain $J = 28.3$ MeV which favors the stability of neutron matter at nuclear densities (see Sec. IV).

In the case where the baseline for the cutoff is taken at zero energy (case I), we find that the optimal cutoff energy is reduced to 10 MeV, with $1\hbar\omega$ being almost as good (it is quite fortuitous that this is the value adopted already in the HFBCS-1 and HFB-1 mass formulas). Taking any multiple of $\hbar\omega$ for the cutoff energy implies, of course, a $A^{-1/3}$ dependence. Other powers of A were also considered, but none led to any improvement over the best cases shown in Table II.

It is rather fortunate from the computational point of view that our optimal cutoff energy is as low as 15 MeV; adopting a much higher cutoff would not only be unnecessary but would actually degrade the fit, as would too low values of the cutoff energy.

III. THE WIGNER TERMS

Even when pairing between like nucleons is correctly taken into account, HF and other mean-field calculations systematically underbind nuclei with $N \simeq Z$ by about 2 MeV, especially for N and Z even. This effect is strikingly evident in the mass tables of Ref. [11], which were based on the ETFSI approximation (extended Thomas-Fermi plus Strutinsky integral) to the HF method, with nn and pp pairing included. It is also conspicuous in macroscopic-microscopic approaches to the mass formula, and it was in this framework that Myers and Swiatecki [12], stressing that the effect dies out rapidly as $|N-Z|$ increases from 0, proposed the phenomenological representation (3). However, there is nothing compelling about this exponential representation, and *a priori* a Gaussian representation,

$$E_W = V_W \exp\left\{ -\lambda \left(\frac{N-Z}{A} \right)^2 \right\}, \quad (4)$$

is just as acceptable. We find, in fact that adopting this form permits a slight improvement to the HFB-1 fit, as evidenced by the line labeled HFB-1($W1$) in Table I (the corresponding parameters are $\lambda = -400.0$, $V_W = -2.327$ MeV).

Whichever of these two representations is adopted [and henceforth we retain the Gaussian form (4)] implies nothing about the underlying microscopic origins of the effect, but it is likely that it arises from $T=0$ np pairing, the contribution of which rapidly vanishes as N moves away from Z [13–15]. However, associating this effect with the name of Wigner suggests that historically a quite different origin was imputed to this term, namely, Wigner's supermultiplet theory, based on SU(4) spin-isospin symmetry, which gives rise to a similar sharp cusp for nuclei with $N=Z$ [16,17]. But the cusp of supermultiplet theory arises from repulsive terms that are linear in $|N-Z|$, which become increasingly important as one moves away from the $N=Z$ line, in contrast to the highly localized phenomenon that is strikingly apparent in the absence of any Wigner term at all. For this reason, and the inconvenient entanglement of an $|N-Z|$ term with the mean-field contributions, we prefer to adopt a term of the form (3) or (4), which simulates the $|N-Z|$ dependence of a $T=0$ pairing term. Nevertheless, this does not preclude a residual SU(4) effect [it will be recalled that the Wigner term in the FRDM [6] is *exclusively* of SU(4) form], and we find that adding a term of the form

$$E'_W = V'_W |N-Z| \exp\left\{-\left(\frac{A}{A_0}\right)^2\right\} \quad (5)$$

leads in fact to a significant improvement in the HFB-1 fit, as evidenced by the line labeled HFB-1($W2$) in Table I, the optimal value of A_0 being 26 and of V'_W 0.670 MeV; the improvement is even more marked for the extrapolation to the 382 new masses than for the original 1768 masses to which the fit was actually made. The Gaussian cutoff factor is compatible with SU(4) symmetry being expected to be most relevant to light nuclei, but while the presence of a term of the form (5) seems to be well established, we cannot exclude the possibility that it has an origin other than SU(4) symmetry.

One possibility is that this *repulsive* term is compensating for the absence of $T=1$ np pairing in our model, which acts only when valence neutrons and protons are filling the same shell, and is thus restricted to relatively light nuclei. In our model the role of the missing $T=1$ np pairing will be compensated in these nuclei by an excessively strong nn and pp pairing, leading thereby to too much attraction in nuclei with $|N-Z| \gg 1$, where the $T=1$ np pairing is weaker.

A possible objection to include a term of the form (5) is that it is simply correcting for an error in the fitted value of the symmetry coefficient J, i.e., it is simulating a term of the form $\delta J(N-Z)^2/A$. We checked this point by fitting such a term to the errors of the $W1$ version of the HFB-1 mass formula, and found that it reduced the rms error by no more than 0.001 MeV (the corresponding error in our original value of 27.81 MeV for J is 0.008 MeV).

While dealing with the topic of residual terms that are linear in $|N-Z|$, it is appropriate to recall that the FRDM [6] introduces a "charge-asymmetry" term $-c_a(N-Z)$, in which the optimal value of c_a is 0.436 MeV. The errors in our mass formulas show a much weaker correlation with such a term; in the case of HFB-1($W1$) the optimal value of c_a is 0.001 MeV, for which the rms error is reduced by only 0.001 MeV.

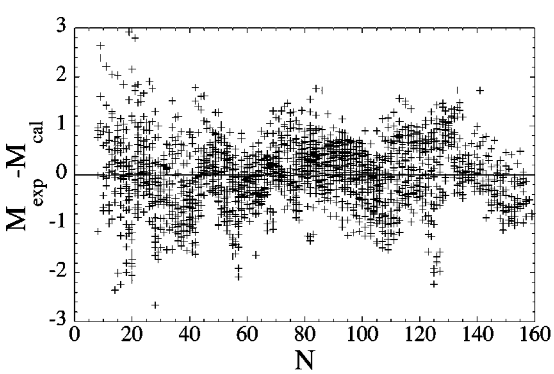

FIG. 2. Difference between experimental and calculated mass excesses, $M_{exp}-M_{cal}$ (MeV) as a function of the neutron number N.

TABLE III. Errors in the fit of the HFB-2 mass formula (force BSk2) to the 2135 nuclei with $Z,N \geqslant 8$ for which measured masses are given in the 2001 compilation [7]. $\sigma(M),\sigma(S_n)$, and $\sigma(Q_\beta)$ denote, in MeV, the rms errors in the fit to the absolute masses, the neutron-separation energies, and the β-decay energies, respectively, while the ϵ quantities refer to the corresponding mean errors.

$\sigma(M)$	0.674
$\epsilon(M)$	0.000
$\sigma(S_n)$	0.487
$\epsilon(S_n)$	0.018
$\sigma(Q_\beta)$	0.606
$\epsilon(Q_\beta)$	−0.042

IV. THE HFB-2 MASS FORMULA

We now incorporate the two new features discussed above into our HFB model, i.e., while retaining the form (1) of the Skyrme force, and the form (2) of the pairing force, we impose a double cutoff at $E_F \pm 15$ MeV on the latter, while for the Wigner term we take

$$E_W = V_W \exp\left\{-\lambda\left(\frac{N-Z}{A}\right)^2\right\} + V'_W |N-Z| \exp\left\{-\left(\frac{A}{A_0}\right)^2\right\}, \quad (6)$$

in place of the form (3). Then varying all the 10 Skyrme parameters, 4 pairing parameters, and 4 Wigner parameters, we fit the 2135 measured masses of the new compilation [7] with an rms error of 0.674 MeV: see Fig. 2 and Table III, which also give the errors for the neutron-separation energies S_n, and the β-decay energies Q_β. In Table IV we show the 18 parameters of the corresponding force, identified as BSk2, while the nuclear-matter parameters for this force are given

TABLE IV. Parameters of the forces BSk2 and BSk2′ (HFB-2 and HFB-2′ mass formulas, respectively).

	BSk2	BSk2′
t_0 (MeV fm^3)	−1790.62	−1792.71
t_1 (MeV fm^5)	260.996	259.053
t_2 (MeV fm^5)	−147.167	−146.768
t_3 (MeV fm$^{3(1+\gamma)}$)	13 215.1	13 267.9
x_0	0.498 986	0.498 612
x_1	−0.089 752 1	−0.089 757 2
x_2	0.224 411	0.242 854
x_3	0.515 675	0.509 818
W_0 (MeV fm^5)	119.047	119.985
γ	0.343 295	0.343 295
$V^+_{\pi n}$ (MeV fm^3)	−237.6	−237.6
$V^+_{\pi p}$ (MeV fm^3)	−265.3	−265.3
$V^-_{\pi n}$ (MeV fm^3)	−246.9	−246.9
$V^-_{\pi p}$ (MeV fm^3)	−277.8	−277.8
V_W (MeV)	−2.05	−2.01
λ	485.0	500
A_0	28	23
V'_W (MeV)	0.697	0.651

TABLE V. Nuclear-matter parameters of force BSk2 (see text).

a_v (MeV)	-15.79
ρ_0 (fm^{-3})	0.1575
J (MeV)	28.00
K_v (MeV)	233.6
M_s^*/M	1.042
M_v^*/M	0.8602
G_0	-0.705
G_0'	0.446
ρ_{frmg}/ρ_0	1.1

in Table V, as follows: a_v is the energy per nucleon at equilibrium in symmetric nuclear matter, ρ_0 the corresponding density, J the symmetry coefficient, K_v the incompressibility, M_s^*/M the ratio of the isoscalar effective nucleon mass at density ρ_0 to the real nucleon mass M, M_v^*/M the corresponding quantity for the isovector effective mass, G_0 and G_0' are the Landau parameters defined in Ref. [18], and, finally, ρ_{frmg} is the density at which neutron matter flips over into a ferromagnetic state that has no energy minimum and would collapse indefinitely [19]. We now comment on the values of some of these parameters.

Comments on nuclear-matter parameters. The value $J = 28.00$ MeV appearing in Table V was actually set as a lower limit in the search on the Skyrme parameters. It is possible that a slightly better mass fit could have been obtained with a value somewhat closer to 27.5 MeV, but this might have engendered an unphysical collapse of neutron matter at nuclear densities. The actual situation in neutron matter for our force is as shown in Fig. 3; the solid curve labeled FP shows the results of Friedman and Pandharipande [20] for the realistic force v_{14} and TNI, containing two- and three-nucleon terms. More recent realistic calculations of neutron matter [21–23] give similar results up to nuclear densities; higher densities do not concern us here. Both previous HF mass formulas [4,5] lead to similar values of J, and are very close to a collapse of neutron matter at unphysically low densities. It is worth noting that nuclear-matter calculations based on modern realistic nucleonic interactions give values of J in the range 28–30 MeV in the case of Ref. [24], while Ref. [25] finds 28.7 MeV. However, very recent calculations based on chiral perturbation theory [26] yield 33.8 MeV.

Our value of K_v is in excellent agreement with the experimental value of 231 ± 5 MeV extracted from breathing-mode measurements [27], even though it emerges entirely from the mass fits.

The value that we find for the isoscalar effective mass M_s^* is consistent with the observation that unless $M_s^*/M \simeq 1.0$ the density of SP states in the vicinity of the Fermi surface will be wrong [28], which would make it impossible to fit the masses of open-shell nuclei. As for the isovector effective mass, our value of $M_v^*/M = 0.86$ is to be compared with the range 0.83 ± 0.08 found from the enhancement of the integrated cross section for electric-dipole photoabsorption over the value given by the Thomas-Reiche-Kuhn sum rule [29]. Our result also agrees remarkably well with the value of 0.83 that we infer from the nuclear-matter calculations of Zuo *et al.* [25] with modern realistic nucleonic interactions (see especially their Fig. 9). Nevertheless, a word of caution is necessary here. In the first place, it is known from Ref. [30] that the rms error of the mass fit varies only very slowly with M_v^*. Second, it is the value of M_v^* for SP states in the vicinity of the Fermi surface that is relevant to the mass fit, and it is not clear that either the $E1$ photoabsorption measurements or nuclear-matter calculations give this quantity. Indeed, it is known from Refs. [31] and [32] that the Fermi-surface effective mass is renormalized by coupling with surface-vibration random-phase approximation modes, but unfortunately these calculations have been confined to nuclei close to the stability line, where the isoscalar effective mass dominates: extending the calculations [31] and [32] to nuclei far from stability would be an interesting contribution.

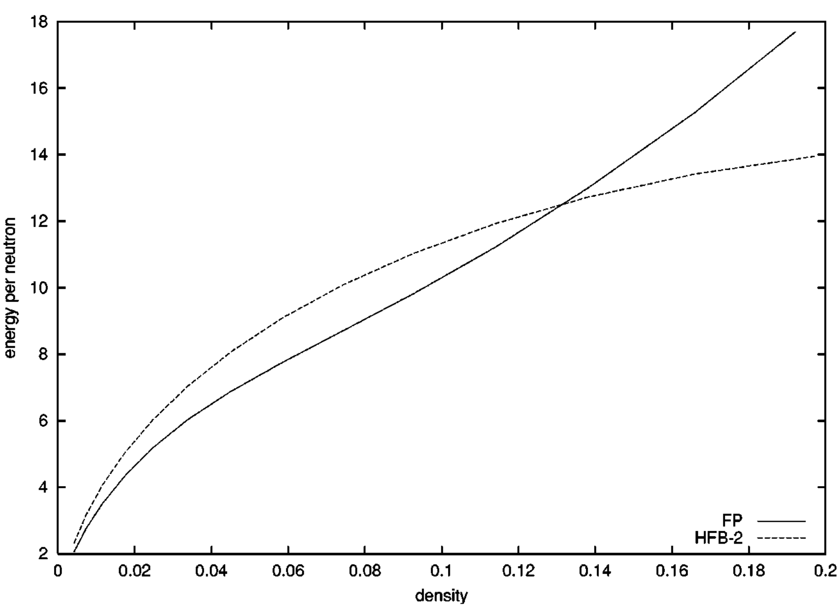

FIG. 3. Energy per nucleon (MeV) of neutron matter as a function of density (nucleons fm^{-3}) for force BSk2, and for the calculations of Ref. [20].

As for the values of our Landau parameters, these do not agree very well with the experimental values of approximately zero in the case of G_0 and 1.80 for G_0' [33]. Attempting to better reproduce these parameters always leads to a worse mass fit. However, we do at least satisfy the condition $G_0, G_0' > -1$, necessary for the stability of symmetric nuclear matter against spin and spin-isospin flips, respectively [34].

Finally, the last line of Table V shows that with our force neutron matter flips over into a collapsing ferromagnetic state only at supernuclear densities, for which the nonrelativistic Skyrme-form force is expected to be invalid anyway.

Charge radii. HF calculations (either HFBCS or HFB) with a given force automatically yield a unique value of the charge radius of the nucleus in question. For the 523 nuclei listed in the 1994 compilation of measured charge radii [35] the HFB-2 values show an rms deviation of only 0.028 fm (for further details see Ref. [36]). This excellent agreement of the HFB-2 calculations with the measured charge radii, without any further parameter adjustment, provides a sound test of the HFB-2 model and its parameters.

Predictive power. Since the parameters of the new mass formula HFB-2 have been fitted to all of the available data it is impossible to make a direct assessment of its "extrapolatability," i.e., the reliability of its extrapolations. However, we have tested the reliability of the underlying model by refitting the parameter set BSk2 to the original 1768 measured masses referred to in Table I, and then inspecting the predictions of this modified version of the mass formula HFB-2, labeled HFB-2′, for the 382 new data (the modified parameter set, BSk2′, is shown in Table IV). We see from the last line of Table I that the new model leads to a drastic improvement on the mass formula HFB-1.

The HFB-2 mass table. In view of these successful results of the HFB-2 model we have constructed a complete mass table of all nuclei with $Z,N \geq 8$ lying between the drip lines, up to $Z=120$. This table is available on the Web at *http://www-astro.ulb.ac.be*. We see from Fig. 4 that the differences between the new mass table and the HFB-1 table become particularly pronounced close to the neutron-shell closures, principally for the exotic neutron-rich nuclei with $S_n < 3$ MeV, the region of relevance to the *r* process. Similar differences with respect to the HFBCS-1 mass formula are found.

Shell-model gaps. These differences between the predictions of the HFB-2 mass formula, on the one hand, and the HFBCS-1 and HFB-1 mass formulas, on the other, become particularly striking when expressed in terms of the shell-model gaps $\Delta(N_0)$ for the various magic neutron numbers N_0, defined as

$$\Delta(N_0) \equiv S_{2n}(Z,N_0) - S_{2n}(Z,N_0+2) = M(Z,N_0-2) + M(Z,N_0+2) - 2M(Z,N_0), \quad (7)$$

where $M(Z,N)$ is the mass and $S_{2n}(Z,N)$ the two-neutron separation energy of the nucleus (Z,N). In Figs. 5 and 6 we show for all three HF mass formulas how the canonical gaps

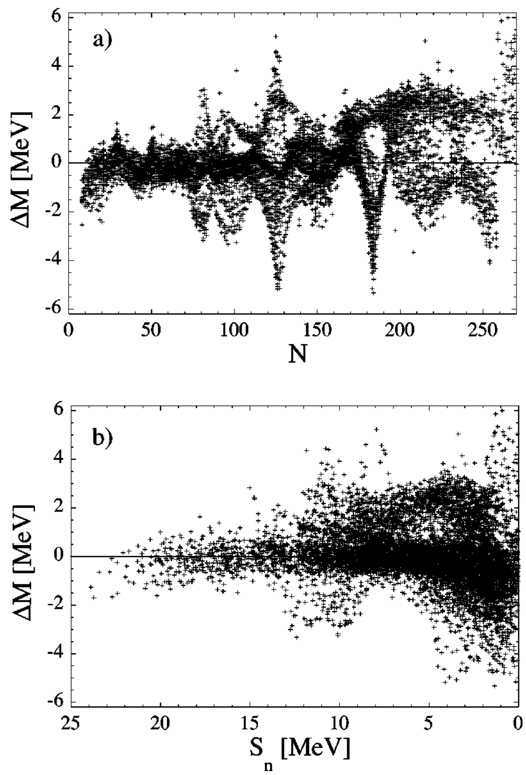

FIG. 4. Differences between HFB-1 and HFB-2 masses, shown as a function of the neutron number *N* (a) and the neutron separation energy (b).

at $N_0 = 50$, 82, and 126, and the putative gap at 184 vary with Z. It will be seen that while the HFB-1 neutron-shell gaps follow closely those of the HFBCS-1 mass formula, the neutron-shell gaps corresponding to the HFB-2 mass formula tend to follow a more distinctive trend as N_0 increases: while all the mass formulas shown in these figures more or less agree at the stability line (as they should, since they have been fitted to the data), the HFB-2 neutron-shell gaps become smaller and smaller relative to those of the HFBCS-1 and HFB-1 mass formulas as Z decreases, i.e., as the neutron-drip line is approached.

These striking differences between the HFBCS-1 and HFB-1 mass formulas, on the one hand, and the HFB-2 formula, on the other, can only be attributed to the pairing-cutoff prescriptions that have been adopted: the two former formulas use the same prescription while the HFB-2 formula uses a different one, and this fact seems to be more important than the replacement of the HFBCS method by the HFB method (assuming always that the force is refitted appropriately). To understand what happens, we first note that with the new prescription the available SP spectrum is narrower than before for nuclei close to the stability line, which accounts for the fact that the pairing parameters resulting from the data fit are larger. But for highly neutron-rich nuclei the SP spectrum entering the neutron-pairing calculation is *wider* than with the old prescription, so that for these nuclei the neutron pairing will be strongly enhanced, with the result that the neutron-shell gaps are weakened.

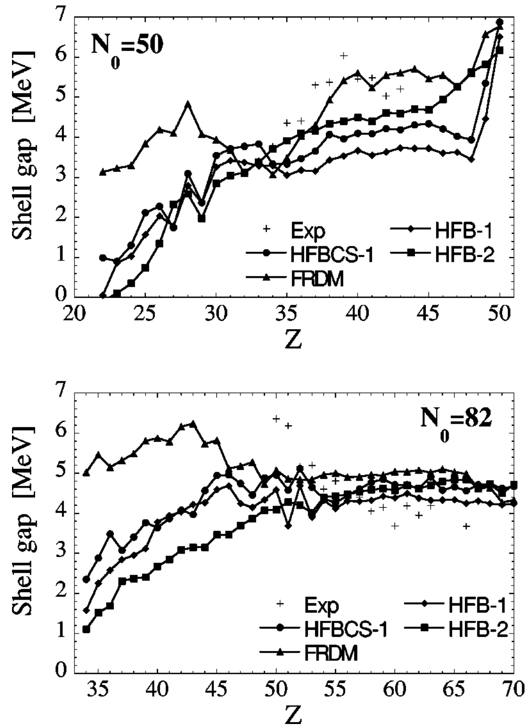

FIG. 5. Neutron-shell gaps at $N_0=50$ (upper panel) and 82 (lower panel) as a function of Z for the four mass tables HFBCS-1 (circles), HFB-1 (diamonds), HFB-2 (squares), and FRDM (triangles). Also included are the shell gaps based on experimental masses (crosses).

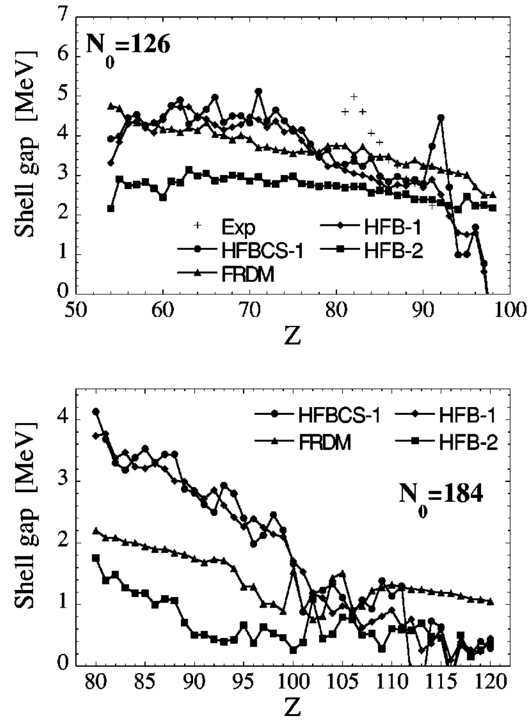

FIG. 6. Same as Fig. 5 for the neutron-shell gaps at $N_0=126$ (upper panel) and 184 (lower panel).

We now discuss in more detail Figs. 5 and 6, in which we have also shown for convenience the FRDM results. For $N_0=50$ all three HF mass formulas display a strong quenching of the gap as the neutron-drip line is approached, while for $N_0=82$ the quenching of all three HF gaps is weaker than for $N_0=50$, but is still stronger for HFB-2 than for the other mass formulas. This trend continues at $N_0=126$, for which the HFB-2 gap is quite unquenched, while for the other two HF mass formulas the gaps are actually enhanced at the neutron-drip line. Finally, at $N_0=184$ even the HFB-2 gap gets larger at the neutron-drip line, but significantly the gap for this mass formula is much weaker than for the other two HF formulas, and it is not clear that one can speak of a gap at all for this mass formula at $N_0=184$. This last observation has serious implications for the very high fission barriers found by Mamdouh *et al.* [37] for highly proton-deficient nuclei in the vicinity of $N_0=184$. These calculations used the ETFSI method with the SkSC4 force, which has the same pairing-cutoff prescription as adopted in the HFBCS-1 and HFB-1 calculations, and predict a $N_0=184$ gap that is even a little higher than we have found here for HFBCS-1 or HFB-1. Since there is an obvious correlation between a large gap and high fission barriers, it is clear that with the HFB-2 method the barriers of the highly proton-deficient nuclei with $N\simeq 184$ should be lower than reported in Ref. [37].

The possibility of one or other of the canonical neutron magic numbers being quenched for large neutron excesses can have some impact on the *r* process [38,39]. But the extent to which such quenching actually occurs depends, we have seen, on the pairing-cutoff prescription. Significantly, the prescription leading to the stronger quenching is the one favored by the new data [7]. At the same time, it has been shown [40] that if the pairing force is made to be density dependent in such a way that it is confined to the nuclear surface then the quenching of neutron-shell gaps will be still stronger than the one obtained by HFB-2. It remains to be shown that a density-dependent pairing force, while physically very appealing, can be fitted to the mass data with the same precision as the purely bulk pairing forces that have been adopted in all the HF mass formulas constructed so far.

Doubly magic nuclei. A striking feature of the HFB-2 mass formula is the strong underbinding of the doubly magic nuclei ^{48}Ca, ^{132}Sn, and ^{208}Pb, and their immediate neighbors formed by adding or removing not more than one nucleon of each kind. (Aside from ^{48}Ni, which does not show this effect, the only other known doubly magic nuclei have $N=Z$, and these have been compensated by the phenomenological Wigner terms.) There are 27 such nuclei, and their mean error (experiment−calculated) is -1.31 MeV, as compared to 0.000 MeV (to three decimal places) for the complete set of 2135 data. (A similar effect is found for the HFB-1 and HFBCS-1 mass formulas, although it is weaker in the latter case.) It is particularly to be noted that there is no tendency for singly magic nuclei to be underbound, so the problem of the doubly magic nuclei cannot simply be attributed to problems arising in the neutron and proton shells separately. Rather, one is apparently dealing here with the phenomenon of "mutually supporting magicities," for which the framework of the existing HF mass formulas is probably inadequate (see Zeldes *et al.* [41] for an extensive discussion and references to earlier papers). Fortunately, the anomalous re-

TABLE VI. Comparison between the standard deviation model error σ_{mod} and the mean model error ϵ_{mod}, as defined in Ref. [6], with the usual rms deviation σ and the mean error ϵ, for the 382 new nuclei of the 2001 data compilation [7], and for the 45 of these nuclei that are neutron rich. All errors in MeV.

	New nuclei	(382 nuclei)	New nuclei	(382 nuclei)	*n* rich	(45 nuclei)	*n* rich	(45 nuclei)
	σ_{mod}	ϵ_{mod}	σ	ϵ	σ_{mod}	ϵ_{mod}	σ	ϵ
FRDM	0.441	0.202	0.655	0.247	0.770	0.070	1.333	0.371
HFB-2	0.631	0.356	0.769	0.377	0.791	0.173	0.979	0.356
HFB-2′	0.657	0.437	0.857	0.470	0.873	0.335	1.201	0.575

gions are higly localized, and can be easily identified, even in extrapolation (once one has identified the local magic numbers).

Model errors. Our entire discussion of the relative accuracy of the different mass formulas was based on the rms deviations σ. However, these latter quantities do not take account of the experimental errors of the individual mass measurements, which are always cited in the Audi-Wapstra compilations [1,7]. This is a legitimate procedure when the experimental errors are small compared to the rms errors, but 4 of the 382 new nuclei have errors well in excess of 1 MeV. In such a case, a better assessment of the validity of a given mass formula can be had from Möller's ''theoretical'' or ''model'' errors, σ_{mod} and ϵ_{mod}, in which each data point is weighted in terms of its experimental error following a procedure based on the method of maximum likelihood [6]. In the first two columns of Table VI we accordingly show the σ_{mod} and ϵ_{mod} of the 382 new nuclei for mass formulas FRDM, HFB-2, and HFB-2′. Comparison with columns 3 and 4, where we show the corresponding rms errors σ and mean error ϵ, shows significant changes, but nothing that would lead to a change in the assessment of the relative performance of the different mass formulas.

However, to assess the suitability of different mass formulas for use in astrophysics applications related to the *r* process nucleosynthesis, it is of obvious interest to see how they perform in extrapolating to the neutron-rich members of the 382 new nuclei. There are only 45 such nuclei, and among them are all four nuclei with errors of over 1 MeV in their mass measurements. Comparing now columns 5 and 7 of Table VI, we see how σ and σ_{mod} can differ. This is a striking example of a case where it is absolutely essential to use the model error.

V. CONCLUSIONS

Our two HF mass formulas that had already been published, HFBCS-1 and HFB-1, have been found here to give a rather poor fit to new mass data that became available in late 2001 [7]. This problem has been shown to be partially a result of an inappropriate truncation of the SP spectrum used with the δ-function pairing force. We have made an extensive study of this question of the cutoff, and find an optimal mass fit if the spectrum is cut off both above E_F+15 MeV and below E_F-15 MeV, E_F being the Fermi energy of the nucleus in question. It is fortunate from the computational point of view that the cutoff energy is so low; adopting a much higher cutoff would not only be unnecessary but would actually degrade the fit, as would too low values. For light nuclei a second source of difficulty lies with the Wigner term. In addition to the term of the form $V_W\exp(-\lambda|N-Z|/A)$ already included in the two earlier HF mass formulas, we have found that a second Wigner term linear in $|N-Z|$ leads to a significant improvement.

We have incorporated these two features into a new HFB model, labeled HFB-2, which leads to much improved extrapolations. The 18 parameters of this model were fitted to the 2135 measured masses for $N,Z\geqslant 8$ with an rms error of 0.674 MeV. With this parameter set, labeled BSk2, a complete mass table has been constructed, going from one drip line to the other, up to $Z=120$. One feature of the new mass formula that shows up for highly neutron-rich nuclei whose masses have not yet been measured is that the neutron-shell gaps in these nuclei are weaker than with the earlier HF mass formulas. It should be realized that these weakened neutron-shell gaps are a consequence of the new pairing-cutoff prescription, which is itself strongly favored by the data.

Nevertheless, a word of warning is in order here. It was only with the *new* data that the evidence for the new pairing-cutoff prescription became compelling, even if some indications of a problem could have been (but were not) discerned in the older data. Thus we must bear in mind the possibility that future data could bring further surprising implications for the pairing. It follows that in addition to the obvious need for more and more mass data further and further from the stability line, there is, on the theoretical side, an equally compelling need for a better, i.e., a more microscopic, understanding of pairing. An important step in this direction has been achieved with the recent analysis by Duguet *et al.* [42] of the energy filters used to extract experimental information on pairing which is not obscured by other effects. A better microscopic understanding of the two phenomenological Wigner terms would likewise be welcome.

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