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Further explorations of Skyrme-Hartree-Fock-Bogoliubov mass formulas. VIII. Role of Coulomb exchange

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Following suggestions that the energy associated with Coulomb correlations and a possible charge-symmetry breaking of nuclear forces might largely cancel the Coulomb-exchange term, we refit the HFB-14 mass model without the Coulomb-exchange term to essentially all the mass data. The resulting mass model, HFB-15, gives a better fit to the 2149 mass data, $\sigma_{\rm rms}$ falling from 0.729 to 0.678 MeV. The improvement in the energy differences between mirror nuclei is particularly striking: the Nolen-Schiffer anomaly, which is strong for HFB-14, is essentially eliminated. As for the extrapolation to highly neutron-rich nuclei, the HFB-15 model differs significantly from HFB-14, with up to 15 MeV less binding being predicted. However, the differences in the predicted values of differential quantities such as the neutron-separation energies, β-decay energies and fission barriers are very much smaller.

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Over the past several years we have constructed a series of mass models based on the Hartree-Fock-Bogoliubov (HFB) method with Skyrme forces and a δ-function pairing force, the force parameters being fitted to the mass data [1]. Of all our mass models, it is model HFB-8 [2] (for which the corresponding set of force parameters is labeled BSk8) that gives the best fit to the mass data: for the 2149 measured nuclei with $Z, N \geqslant 8$, the rms error is 0.635 MeV. With our more recent models the direction of our work has shifted: rather than seek ever-better fits to the mass data our concern has been more with the construction of a universal effective force adapted to the highly neutron-rich astrophysical environments that are inaccessible to direct nuclear-physics experiments, and to this end we have been imposing on our mass models extra physical constraints.

Our latest published model [3], HFB-14 (force BSk14), was subjected to the following constraints: (i) the energy-density curve of neutron matter was fitted, a requirement that is relevant not only to neutron-star applications but also to the reliability of finite-nucleus extrapolations out toward the neutron drip line; (ii) the strength of the pairing force was held considerably below the value that would emerge from an optimal fit to the mass data, thereby improving considerably the predictions for level densities; and (iii) a vibrational term was added to the phenomenological collective correction, fitting it to measured fission-barrier heights. Because of these extra constraints the rms error of the mass fit was somewhat worse than for HFB-8: 0.729 rather than 0.635 MeV, but the physical constraints that it satisifies make it more reliable for extrapolation to the neutron-rich region.

In the present note we turn to the device of omitting the Coulomb-exchange (CE) term from our HFB calculations. This has been shown by Brown *et al.* [4,5] in HF calculations on a highly restricted set of nuclei to lead to a significant improvement in energy differences between pairs of mirror nuclei and in particular to a resolution of the Nolen-Schiffer anomaly. Some microscopic justification for this procedure is found in the energy associated with Coulomb correlations, a long-range surface effect that arises from an interplay between the Coulomb and nucleonic interactions and that is not included in the usual HF(B) framework. Microscopic calculations [6,7] showed that this correlation energy has the opposite sign to that of the CE energy but *roughly* the same magnitude. We shall return below to the question of how exact is the cancellation between the CE and Coulomb-correlation terms, but first we investigate the implications for HFB mass models of dropping the CE term, thereby effectively generalizing the work of Refs. [4,5] to essentially all nuclei.

Our starting point is force BSk14 [3], which we refit to the same 2149 mass data as before but with the CE term dropped and the following constraints imposed: (i) neutron matter is fitted as before (this is assured by fixing the nuclear-matter symmetry coefficient J at 30 MeV, (ii) the pairing strengths are fitted to the same spectral gaps as before [3,8], and (iii) the collective correction is as for model HFB-14 [3]. Furthermore, we impose the same value of the isoscalar effective mass at the equilibrium density ρ_0 of symmetric infinite nuclear matter as for BSk14, i.e., $0.8M$; we likewise retain the Bulgac-Yu [9] treatment of pairing. The new force parameters are shown in the first column of Table I, being labeled BSk15; the corresponding mass table will be referred to as HFB-15. For comparison we also show the BSk14 parameters (note that there were errors in the pairing parameters given in Table I of Ref. [3]).

Table II shows the resulting parameters of infinite and semi-infinite nuclear matter for forces BSk15 and BSk14, as defined in Ref. [8]. Appreciable shifts arise for the volume-related coefficients a_v and L and for the surface-stiffness coefficient Q, with the first two favoring stronger binding for BSk15 and the last to weaker binding (we recall that J, like M_s^*, was constrained to take the same values in BSk15 as in BSk14).

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TABLE I. Parameter set BSk15 (for convenience we also show parameter set BSk14 [3]).

	BSk15	BSk14
t_0 (MeV fm^3)	−1832.91	−1822.67
t_1 (MeV fm^5)	372.552	377.470
t_2 (MeV fm^5)	17.9820	−2.41056
t_3 (MeV fm$^{3+3\gamma}$)	11483.0	11406.3
x_0	0.436279	0.302096
x_1	−0.785263	−0.823575
x_2	−9.53228	61.9411
x_3	0.675865	0.473460
W_0 (MeV fm^5)	135.012	135.565
γ	0.3	0.3
V_n^+ (MeV fm^3)	−240.0	−240.0
V_n^- (MeV fm^3)	−251.3	−252.4
V_p^+ (MeV fm^3)	−262.9	−265.5
V_p^- (MeV fm^3)	−271.2	−275.2
ε_Λ (MeV)	7.0	7.0
V_W (MeV)	−2.3	−1.70
λ	200.0	400.0
V'_W (MeV)	0.54	0.75
A_0	34.0	30.0

The rms and mean (data-theory) values of the deviations between the measured masses and the HFB-15 predictions are given in the first and second lines, respectively, of Table III, where we also compare with HFB-14 and with our "best-fit" model HFB-8 [2]. It will be seen that the new feature of dropping CE has lead to a considerable improvement over HFB-14, although we still do not do as well as does HFB-8 (which, however, does not satisfy any of the physical constraints that we subsequently imposed). However, in the next pair of lines we show the rms and mean deviations for the subset of the mass data consisting of the 185 neutron-rich nuclei having a neutron-separation energy $S_n \leqslant 5.0$ MeV, and we see that in this astrophysically crucial region the new mass model does better than any of the others. Actually, the S_n and the β-decay energies Q_β, being differential quantities, are astrophysically more relevant than the absolute masses M, so in the next four lines of Table III we give the rms and mean deviations for these quantities, using the full data set of 2149 measured masses. Again we see how the new mass model performs better than HFB-14; in fact it does almost as well as HFB-8, despite the extra physical constraints. The improvement brought about by dropping the CE term becomes particularly apparent on considering the energy differences between pairs of mirror nuclei. There are 62 such pairs for which mass data exist, and in lines 9 and 10 we give the rms and mean deviations for this quantity. Lines 11 and 12 show the rms and mean deviations between measured charge radii [10] and model predictions; dropping CE is seen to have a negligible effect once the masses are refitted. The last line of Table III gives the neutron-skin thickness $\theta \equiv R_n^{\mathrm{rms}} - R_p^{\mathrm{rms}}$, where R_n^{rms} is the rms radius of the neutron distribution and R_p^{rms} that of the point-proton distribution.

TABLE II. Macroscopic parameters for force BSk15 (for convenience we also show force BSk14 [3]). The first 12 lines refer to infinite nuclear matter and the last 2 to semi-infinite nuclear matter.

	BSk15	BSk14
a_v (MeV)	−16.037	−15.853
ρ_0 (fm^{-3})	0.1589	0.1586
J (MeV)	30.0	30.0
M_s^*/M	0.80	0.80
M_v^*/M	0.77	0.78
K_v (MeV)	241.5	239.3
L (MeV)	33.60	43.91
G_0	−0.67	−0.63
G'_0	0.54	0.51
G_1	1.47	1.49
G'_1	0.41	0.44
$\rho_{\mathrm{frmg}}/\rho_0$	1.24	1.24
a_{sf} (MeV)	17.7	17.6
Q (MeV)	39.7	35.0

TABLE III. Rms (σ) and mean ($\bar{\epsilon}$) deviations (in MeV) between data and predictions for model HFB-15; for convenience we also show models HFB-14 [3] and HFB-8 [2]. The first pair of lines refers to all the 2149 measured masses M, the second pair to the masses M_{nr} of the subset of 185 neutron-rich nuclei with $S_n \leqslant 5.0$ MeV, the third pair to the neutron separation energies S_n (1988 measured values), the fourth pair to β-decay energies Q_β (1868 measured values), the fifth pair to mirror-nuclei difference (62 values), and the sixth pair to charge radii (782 measured values). The last line shows the calculated neutron-skin thickness of ^{208}Pb for these models.

	HFB-15	HFB-14	HFB-8
$\sigma(M)$ (MeV)	0.678	0.729	0.635
$\bar{\epsilon}(M)$ (MeV)	0.026	−0.057	0.009
$\sigma(M_{nr})$ (MeV)	0.809	0.833	0.838
$\bar{\epsilon}(M_{nr})$ (MeV)	0.173	0.261	−0.025
$\sigma(S_n)$ (MeV)	0.588	0.640	0.564
$\bar{\epsilon}(S_n)$ (MeV)	−0.004	−0.002	0.013
$\sigma(Q_\beta)$ (MeV)	0.693	0.754	0.704
$\bar{\epsilon}(Q_\beta)$ (MeV)	0.024	0.008	−0.027
σ(mirror) (MeV)	0.515	1.186	0.879
$\bar{\epsilon}$(mirror) (MeV)	0.181	0.945	0.757
$\sigma(R_c)$ (fm)	0.0302	0.0309	0.0275
$\bar{\epsilon}(R_c)$ (fm)	−0.0108	−0.0117	0.0025
$\theta(^{208}\mathrm{Pb})$ (fm)	0.15	0.16	0.12

Even if it is not clear that the device of dropping CE can be entirely justified in microscopic terms there can be no doubt as to its efficacy. We therefore examine the predictions of the new mass model beyond the known region, summarizing the differences compared to HFB-14 in Fig. 1. We see that although the impact of the neglect of CE on the data fit has been well compensated in the mass model HFB-15, considerable differences emerge on extrapolating beyond the known region, with HFB-15 systematically predicting less binding than HFB-14; in fact, no two of all our earlier models differ so much in their mass extrapolations (the sign of the difference is related to the larger surface-stiffness coefficient Q for force BSk15). To see quantitatively what happens on the neutron-rich side we compare the predictions made by the

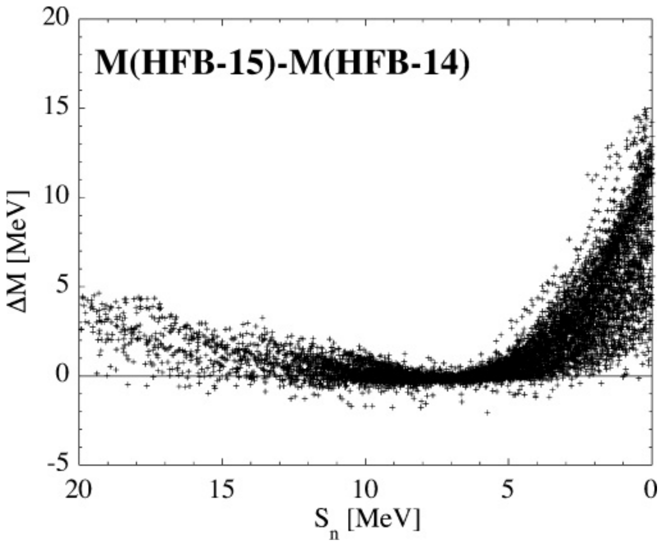

FIG. 1. Differences of mass predictions between models HFB-15 and HFB-14, plotted as a function of the neutron-separation energy S_n.

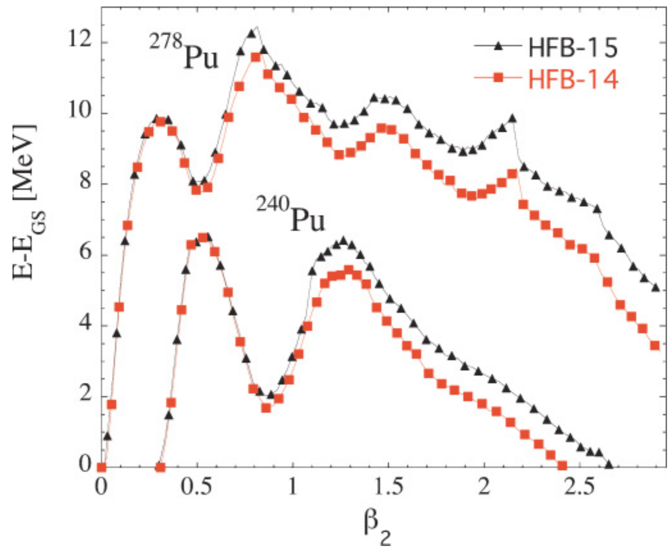

FIG. 2. (Color online) Fission barriers of ^{240}Pu and ^{278}Pu for models HFB-14 and HFB-15. The difference between the energy E at a given deformation β_2 and the ground-state energy E_{gs} is plotted as a function of β_2.

two models for all those nuclei with $26 \leqslant Z \leqslant 110$ for which $S_n < 4.0$ MeV, summarizing the results in Table IV. This table shows that for the more astrophysically relevant quantities S_n and Q_β the rms difference between the two models is much smaller than for the absolute masses. Indeed, referring to lines 5–8 of Table III it is seen that the rms difference between the predictions of the two models for S_n and Q_β are smaller than the deviations between each model and the data. As for possible local differences between the two models, we have checked that they give very similar neutron-shell gaps right out to the neutron drip line.

The fission barriers of experimentally inaccessible highly neutron-rich nuclei are another differential quantity of crucial importance for the *r* process of stellar nucleosynthesis. Now in model HFB-14, by adjusting the phenomenological collective correction at large deformations, we succeeded in fitting the experimental fission barriers without destroying the quality of the mass fits found in our earlier models. Accordingly we recalculated with model HFB-15 some 20 fission barriers for U and Pu isotopes in the same way as described in Ref. [3] for model HFB-14. The two cases shown in Fig. 2, the measured nucleus ^{240}Pu and the closed-shell neutron-rich nucleus ^{278}Pu, are representative of all these calculations: we see that although the HFB-15 inner barriers are systematically close to those of the HFB-14 model, the outer barriers are higher by about 1 MeV. Because we have taken for model HFB-15 the phenomenological collective correction of model HFB-14, this comparison shows that a new fit of the HFB-15 collective correction might be needed to optimize the prediction of experimental fission barriers. Only after such a readjustment is performed will it be possible to confirm that the fission barriers are unaffected by the neglect of the CE term. However, it is already clear that the deviation between the predictions of the two models for the outer barriers is roughly the same for all the nuclei we have considered, regardless of whether they are close to the stability line or the neutron drip line: this stands in sharp contrast to the mass predictions, for which the two models agree closely in the case of measured nuclei but can differ by up to 15 MeV for highly neutron-rich nuclei.

Cancellation of the Coulomb-exchange term. In view of the improved fit to the data given by the new model, we have to understand how an apparent cancellation of the CE term could arise. We have already mentioned the Coulomb-correlation energy as a possible mechanism, and now we examine it more closely. In Eq. (21) of Ref. [6] the contribution of Coulomb correlations is parametrized as

$$E_{corr} = b_v Z + b_s Z^{2/3}, \tag{1}$$

with the values $b_v = -0.1 \pm 0.1$ MeV and $b_s = 1.1 \pm 0.1$ MeV being determined by microscopic calculations on semi-infinite nuclear matter. However, the finite-nucleus results of Table II of Ref. [6] suggest rather 0.055 and 0.14 MeV for the respective parameters, which implies enough

TABLE IV. Rms and mean differences between predictions for highly neutron-rich nuclei ($4.0\,\text{MeV} \geqslant S_n \geqslant 0$) given by different pairs of mass models. Mean differences are given in parentheses.

	M	S_n	Q_β
HFB-14–HFB-15	4.060 (−3.433)	0.270 (0.178)	0.517 (−0.454)
HFB-14–HFB-8	3.323 (−2.639)	0.557 (0.231)	0.974 (−0.547)

ambiguity for us to treat them as free parameters. Fitting then these two free parameters to the CE term in all 8382 nuclei having $8 \leqslant Z \leqslant 110$, $N \geqslant 8$, and lying between the drip lines, we found $b_v = 0.394$ MeV and $b_s = 0.159$ MeV, values that are somewhat different from those implied by Ref. [6]; in fact this fit implies that the Coulomb-correlation energy is dominated by the volume term. However, we should take into account also the vacuum-polarization energy [11],

$$E_{vp} = 0.0035 Z^2 A^{-1/3} \text{ MeV} \tag{2}$$

(we included this in mass model HFB-9 [12] but not in any other). Refitting then the two free parameters in E_{corr} leads to the values $b_v = 0.275$ MeV and $b_s = 0.466$ MeV, much closer to those of Ref. [6]. The rms value of the fractional error with which this correction reproduced the CE term in each of the 8382 nuclei is 5.8%. That is to say, the correction $E_{\mathrm{corr}} + E_{vp}$ could reproduce more than 94% of the CE term. It would be interesting to have more detailed microscopic calculations of the Coulomb-correlation energy to see whether our fitted values of b_v and b_s might be possible. At the same time one should look around for other effects not previously mentioned here that oppose the CE term.

Charge-symmetry breaking. One such possible effect is that of a breaking of the charge-symmetry (CSB) of nuclear forces [13]. Actually, in the articles in which they studied the impact of dropping CE, Refs. [4,5] made a parallel study of CSB. They showed that it is not necessary to drop CE to account for the Nolen-Schiffer anomaly, a comparable improvement being found when the t_0 component of the Skyrme force was given a CSB degree of freedom. It would be of considerable interest to construct a complete mass model in this way, retaining CE (corrected for vacuum polarization) and seeing whether it is possible by invoking CSB to obtain the same improvement on mass model HFB-14 as we have achieved here in constructing mass model HFB-15. Of course, there is no guarantee that the particular form of CSB adopted in Refs. [4,5] would lead to an effective cancellation of the CE term and hence to a global mass model that works as well as model HFB-15, but there are many other forms of CSB to consider. Even if eventually it proved impossible to obtain such an improvement with CSB, it is likely that CSB could supplement Coulomb correlations and vacuum polarization in effectively cancelling the CE term. In any case, we do not regard CSB as an alternative to dropping the CE term; rather we regard it as one possible physical mechanism contributing to the apparent cancellation of the CE term.

Summary. We have shown that the device of dropping the CE term in Skyrme-HFB models leads to an improvement in the global fit to the mass data, particularly on the neutron-rich side of the stability line. In particular, the errors with which the energy differences between mirror pairs are reproduced is drastically reduced (as shown earlier in Refs. [4,5,14] within the framework of restricted mass fits). We have also found that on extrapolating from the data out toward the neutron drip line, the neglect of the Coulomb-exchange term can lead to a shift of up to 15 MeV in the predicted masses. However, as far as the differential quantities S_n, Q_β and fission barriers are concerned, the differences between the two models are much smaller. Real physical processes that could account for the apparent cancellation of the CE term include Coulomb correlations, CSB effects, and vacuum polarization; considerable work remains to be done on the first two of these.

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