Predictive power of nuclear-mass models

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The predictive power of modern nuclear-mass models is studied. To quantify this property, we compare the description of masses which were not experimentally known at the time of the model adjustment to that of older masses. For the latter, the masses evaluated in 2003 are taken. The masses evaluated in 2012 and not present in the earlier evaluation of 2003 are considered as the new ones. The predictive power is analyzed for ten often-used models of various natures and also for five different regions in the nuclear chart. A strong dependence of predictive power on the model as well as on the considered region of nuclei is observed. No clear correlation between the accuracy of the description of masses by a model and its predictive power is found.

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Understanding of many nuclear structure effects and nucleosynthesis processes in astrophysics requires accurate knowledge of nuclear masses. The importance of the masses is also indirectly emphasized by huge efforts in building novel instrumentation and methods aiming at measuring masses of nuclei more distant from the region of stability as well as at essentially increasing the accuracy of these measurements (see, e.g., Refs. [1–12]). Also the progress in the development of nuclear-mass models as well as theoretical methods using data on masses for the extension of our knowledge of nuclear structure and astrophysical processes is impressive (e.g., Refs. [13–28]).

The importance of nuclear masses stresses particularly the need for models describing the mass surface as accurately as possible. Also essential is the ability of a model to accurately predict as-yet-unknown masses. One usually expects that a model which accurately describes masses of many nuclei should thus have also good predictive power. Indeed, for making predictions, one usually uses models which provide the best description of the known masses.

However, is there a clear correlation between these two properties of a model? The objective of this paper is to address this question.

Ten models of various kinds are taken for the study. These are the same models as were used in our recent analysis of the accuracy of the description of nuclear masses in different regions in the nuclidic chart [29]. As a measure of the accuracy of a model, we employ the rms (root mean square) of discrepancies between the measured masses and the corresponding ones calculated with this model. We define the predictive power of a model as a difference between the rms value obtained for new masses, rms(new), to which the model was not adjusted, and the rms for older masses, rms(2003): $\delta\text{rms} = \text{rms(new)} - \text{rms(2003)}$.

The masses evaluated within the framework of the atomic mass evaluation (AME) in 2003, AME'03 [30] are treated here as the old ones, while the new masses are those from the recent evaluation of 2012, AME'12 [31], which were not included in the evaluation of 2003. Here, we should add that we removed from the AME'03 15 nuclei, which do not appear in the later AME'12.

An earlier preliminary analysis of the predictive power of nuclear-mass models can be found in Ref. [32]. The present study is a considerable extension of that analysis and is based on the more recent data.

As stated above, we consider ten models in this analysis. These are the same ones studied for accuracy in description of nuclear masses [29]. These are six macroscopic-microscopic models, two purely microscopic (self-consistent) ones, and two other kinds. The six macroscopic-microscopic models are the finite-range droplet model (FRDM) [33], the finite-range liquid drop model (FRLDM) [33], the nuclear Thomas-Fermi (TF) model [34], the Lublin-Strasbourg drop (LSD) model [35], and the recent models of Liu et al. (WS3.6) [19] and Wang et al. (WS3.3) [20]. Important for the WS3.3 model is the inclusion of the radial basis function (RBF) (see Ref. [20], where the two latter models are discussed in detail). The purely microscopic models are the Hartree-Fock-Bogoliubov mean field models: one with the BSk21 Skyrme interaction (HFB21) [15] and the other with the D1M Gogny forces (GHFB) [14]. The last two models are those of Duflo and Zuker (DZ) [36] (see also Ref. [16]) and Koura *et al.* (KTUY) [37], which use a large number of parameters directly adjusted to experimental masses. The DZ model uses 28 and the KTUY uses 34 parameters.

Table I gives two rms values of the discrepancies between the calculated masses and two sets of the experimental ones. One corresponds to the old measured masses, evaluated in 2003 [30], rms(2003), and the other one corresponds to the new masses evaluated in 2012 [31], which were not known in 2003, rms(new). The difference between the two, $\delta\text{rms} \equiv \text{rms(new)} - \text{rms(2003)}$, is also specified. We consider the latter quantity as a measure of the predictive power of a model. Its positive value means that new masses are described worse than the old ones, while the negative value tells us that the new masses are reproduced even better than the old masses. If the δrms is lower, it means the predictive power of the

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TABLE I. The rms values of the discrepancies between the masses calculated by considered models and the masses from AME'03, rms(2003), and the new masses, rms(new). The differences, δrms, are specified as well. The values are given separately for the global ($Z, N \geqslant 8$), light ($8 \leqslant Z < 28, N \geqslant 8$), medium I ($28 \leqslant Z < 50$), medium II ($50 \leqslant Z < 82$), and heavy ($Z \geqslant 82$) regions of nuclei. Also shown are the corresponding numbers of used nuclei: N_{nucl}(2003) and N_{nucl}(new).

Model	LSD (2003) 1	FRDM (1995) 2	TF (1996) 3	FRLDM (1995) 4	HFB21 (2010) 5	GHFB (2009) 6	DZ (1995) 7	KTUY (2005) 8	WS3.6 (2011) 9	WS3.3 (2011) 10
				Global						
N_{nucl}(2003)	2127	2134	2134	2134	2134	2134	2134	2134	2134	2134
N_{nucl}(new)	189	219	217	219	219	219	219	219	219	219
rms(2003)	0.620	0.655	0.638	0.768	0.578	0.799	0.358	0.651	0.338	0.217
rms(new)	0.627	0.765	0.805	0.910	0.646	0.764	0.673	1.092	0.424	0.374
δrms	0.007	0.110	0.167	0.142	0.068	–0.035	0.315	0.441	0.088	0.157
				Light						
N_{nucl}(2003)	319	319	319	319	319	319	319	319	319	319
N_{nucl}(new)	13	16	16	16	16	16	16	16	16	16
rms(2003)	1.068	1.154	0.990	1.194	0.933	1.053	0.543	0.731	0.495	0.326
rms(new)	1.236	1.558	1.923	1.660	1.021	1.782	0.889	1.092	0.852	0.579
δrms	0.168	0.404	0.933	0.466	0.088	0.729	0.346	0.361	0.357	0.253
				Medium I						
N_{nucl}(2003)	508	508	508	508	508	508	508	508	508	508
N_{nucl}(new)	66	67	67	67	67	67	67	67	67	67
rms(2003)	0.669	0.679	0.725	0.652	0.613	0.800	0.363	0.643	0.369	0.213
rms(new)	0.654	0.721	0.715	0.648	0.529	0.466	0.649	1.368	0.399	0.457
δrms	–0.015	0.042	–0.010	–0.004	–0.084	–0.334	0.286	0.725	0.030	0.244
				Medium II						
N_{nucl}(2003)	894	895	895	895	895	895	895	895	895	895
N_{nucl}(new)	67	75	75	75	75	75	75	75	75	75
rms(2003)	0.445	0.461	0.481	0.655	0.439	0.549	0.300	0.543	0.278	0.193
rms(new)	0.533	0.598	0.676	0.828	0.611	0.617	0.567	0.532	0.374	0.309
δrms	0.088	0.137	0.195	0.173	0.172	0.068	0.267	–0.011	0.096	0.116
				Heavy						
N_{nucl}(2003)	406	412	412	412	412	412	412	412	412	412
N_{nucl}(new)	43	61	59	61	61	61	61	61	61	61
rms(2003)	0.343	0.401	0.442	0.705	0.416	1.000	0.279	0.797	0.240	0.159
rms(new)	0.407	0.673	0.467	0.972	0.676	0.744	0.749	1.250	0.327	0.263
δrms	0.064	0.272	0.025	0.267	0.260	–0.256	0.470	0.453	0.087	0.104

model is better. All the data are given for five regions of nuclei specified in the table caption. For each region and each model, the number of nuclei with both calculated and evaluated masses in 2003, N_{nucl} (2003), and new ones, N_{nucl}(new), are also shown. They give us the information about how many new masses are involved in the description, in comparison to masses known in 2003. For each model, the year of its publication is also shown.

One can see in Table I that the number of new nuclei in the global region is 219. It is large enough to get a good idea of the ability of the considered models to describe the masses to which they were not adjusted. It is about 10% of the number of nuclei with masses evaluated in 2003. The distribution of this number in the five subregions differs from one subregion to another: from 16 (about 5% of the nuclei with masses evaluated in 2003) in the region of light nuclei to 75 (about 8%) in the medium II region.

It is seen in the table that both rms(2003) and δrms depend strongly on the model and on the region of nuclei. These dependencies, however, are better seen when presented in the graphical form.

Figure 1 shows the dependencies of rms [each rms means rms(2003)] and δrms on the model for the global region of nuclei. Each model is identified by the number (from 1 to 10) ascribed to it in Table I. One can see that both rms and δrms depend quite strongly on the model. No clear correlation between the two properties can be seen. A priori, one could expect that a good model (low rms) should also have a low δrms (good predictive power), and a poor model (large rms) should also show a large δrms (poor predictive power), but this is seldom the case. Only for the KTUY (8) model is a large rms accompanied by a large δrms, in the illustrated global region. For GHFB (6), however, it is just the opposite: a very large rms is connected with a very small δrms. For the DZ (7) and the WS3.3 (10) models, low rms are accompanied by large δrms.

Figure 2 presents the same dependencies obtained for the region of light nuclei. Again, no clear correlation between rms and δrms is obtained. A particularly large δrms value is

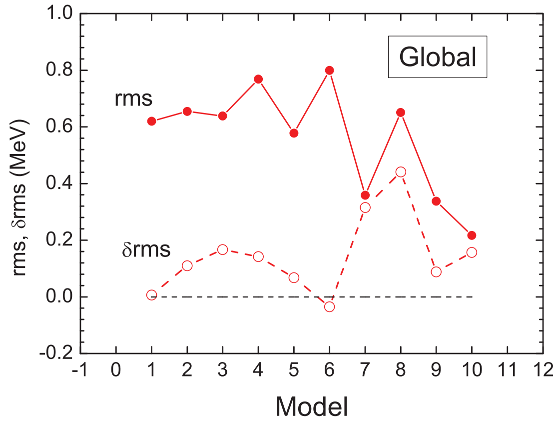

FIG. 1. (Color online) The dependencies of rms and δrms on the model for the global region of nuclei. Each model is identified by the number (from 1 to 10) ascribed to it in Table I.

obtained for the TF (3) model. This means that the description of new masses by this model in the light region of nuclei is especially poor, about two times worse than that of the old nuclei. Also large δrms is obtained for the GHFB (6) model, in a strong distinction to HFB21 (5), for which δrms is very small. It is interesting because the models use the same (Hartree-Fock-Bogoliubov) approach. However, besides the different forces, they also differ by other factors, e.g., by different ways of introducing the correlations, which may result in significant differences in their properties.

Generally, the description of masses in the light-nuclei region by the studied models is relatively poor, as observed already in our previous analysis [29]. The rms obtained for six models (1–6) are close or even larger than 1 MeV. This poor description may be interpreted such that the condition of a good average field, on which all the models are based, is not satisfactorily fulfilled for these relatively light nuclei.

The discussed dependencies, calculated for the medium I region, are shown in Fig. 3. Here, interesting results are the negative values of δrms for the HFB21′ (5) and GHFB (6) models, especially low for the latter one. It is also worth noticing a good predictive power ($\delta\text{rms} \approx 0$, i.e., the new masses are described approximately as well as the old ones) of five macroscopic-microscopic models: LSD (1), FRDM (2), TF (3), FRLDM (4), and WS3.6 (9). On the other hand, δrms for the KTUY model is very large in this region, even larger than rms itself. A rather unexpected result is the relatively large δrms (close to rms) for the models DZ (7) and WS3.3 (10), known for their good description quality of known nuclear masses.

Figure 4 illustrates the dependencies for the medium II region. In this region, δrms values are not very different for all models. An especially low value (close to zero) is obtained for the KTUY (8) model and a relatively large one is found for the DZ (7) one.

Finally, Fig. 5 shows the dependencies for the region of heavy nuclei. Here, a strong negative correlation appears for the GHFB (6) model, similar to that observed for this model in the medium I region. Just the opposite situation is observed for the DZ (7) model. Its predictive power is poor; the description of new masses is more than twice worse than that of the old ones.

Figures 1 to 5 tell us that both the accuracy of the description of known masses, rms, and the predictive power, δrms, strongly

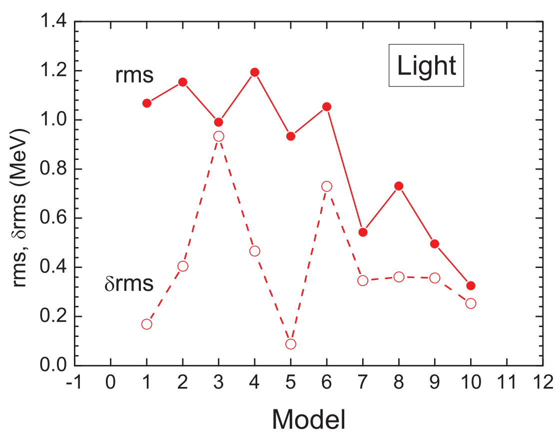

FIG. 2. (Color online) Same as in Fig. 1, but for the light region of nuclei.

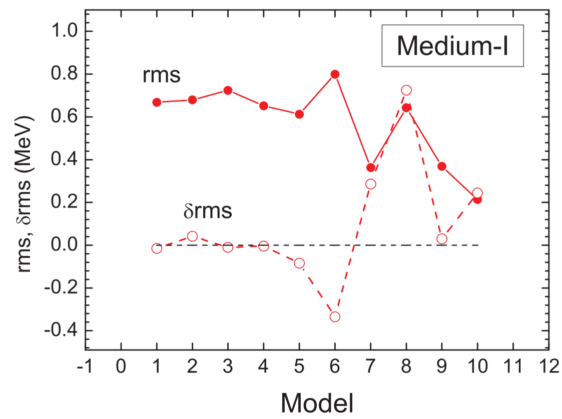

FIG. 3. (Color online) Same as in Fig. 1, but for the medium I region of nuclei.

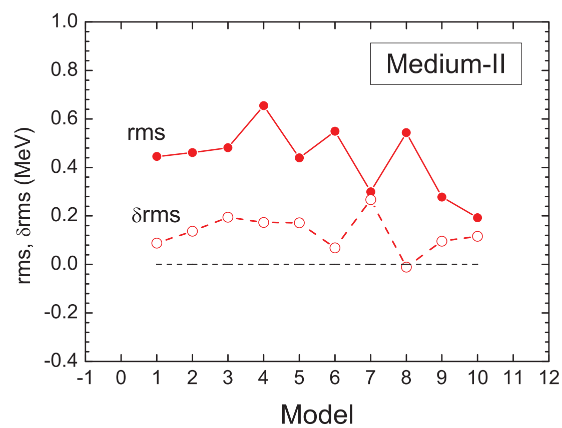

FIG. 4. (Color online) Same as in Fig. 1, but for the medium II region of nuclei.

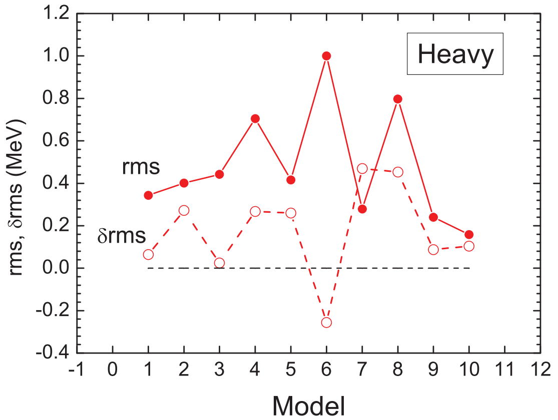

FIG. 5. (Color online) Same as in Fig. 1, but for the region of heavy nuclei.

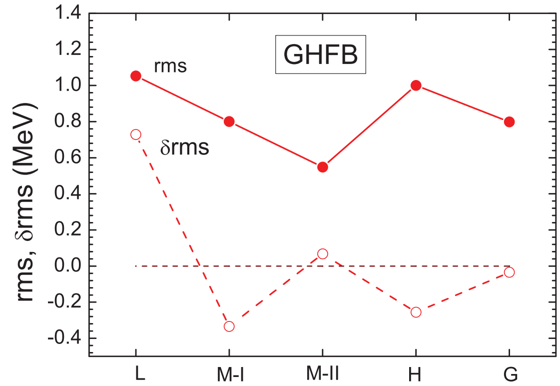

FIG. 6. (Color online) The dependencies of rms and δrms on the region of nuclei for the GHFB model.

depend on the model. Additionally, they show that there is no clear correlation between these two important quantities. It appears that the model which describes known masses quite well may have rather poor predictive power, and the opposite, that poor accuracy of description of known masses may be accompanied by rather good predictive power.

The dependence of rms and δrms on the region of nuclei is illustrated in Fig. 6 for the GHFB model, which shows especially good predictive power. Here, L, M-I, M-II, H, and G denote the light, medium I, medium II, heavy, and global regions of nuclei, respectively. One can see that the predictive power of GHFB is very good for all regions except the region of light nuclei. Similarly to other models, no clear correlation between the rms and δrms is obtained. In particular, poor accuracy (large rms) is accompanied by a good predictive power (negative δrms) for the regions of the medium I and heavy nuclei.

Summarizing our study, one can say the following:

Ten recently used nuclear-mass models of different kinds are studied for their ability to predict masses of new nuclei, to which they were not adjusted. This property of the models is analyzed in five different regions of the nuclear chart. Much attention is given to the relation between the accuracy of a given model in description of masses and its predictive power and also to the dependence of this relation on the region of the nuclei considered.

The following conclusions may be drawn from the study:

(i) Both the accuracy of description of masses and also the predictive power of a model vary quite strongly from one model to the other.
(ii) For a given model, both these quantities strongly depend on the region of the nuclei considered.
(iii) No clear correlation between these two quantities is found.
(iv) A striking property is obtained for the GHFB model. With a rather poor description of known masses (to which the model was adjusted), it shows a good (the best among the studied models) predictive power for new masses. This is especially clearly seen for the regions of the medium I and heavy nuclei (see Fig. 6).

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