Accuracy of theoretical descriptions of nuclear masses

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The accuracy of current theoretical descriptions of nuclear masses is studied. Ten theoretical models of various kinds are taken for the study: the macroscopic-microscopic, purely microscopic (self-consistent), and models of other natures. Some of them are traditional, but still widely used, while the others are very recent. The most recently evaluated experimental masses of 2012 are taken for the test of the models. Much attention is given to the dependence of the accuracy on the region of nuclei described by the models. The macroscopic-microscopic approaches are still found to be the most accurate in the description of atomic masses. However, the recently developed purely microscopic models (the Hartree-Fock-Bogoliubov approach) reach comparable accuracy. A strong dependence of the accuracy on the region of nuclei described is found, knowledge of which is crucial for a realistic description of specific nuclei.

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I. INTRODUCTION

The masses of atomic nuclei are their basic properties. They are indispensable quantities for a number of branches of science, especially for nuclear physics and astrophysics [1–5]. Measurements of masses of more and more exotic nuclei (e.g., Refs. [6–11]) and also the increase of their accuracy (e.g., Refs. [12–16]) are a continuing process.

Parallel to the experimental progress, new or considerably improved conventional theoretical models are being developed (e.g., [17–24]). From time to time, the progress in the measurements is summarized by an evaluation of the measured values. The last evaluation was completed very recently [25], about a decade after the previous one [26]. In comparison to the number of nuclei with experimentally known masses in 2003 (2226), this number (2436) has now increased by 210 nuclei. This large number of new masses gives us an exceptional opportunity to perform an important test of the predictive power of various mass models.

The objective of the present paper is to provide (on the basis of these new data) a quantitative test of the ability of modern theoretical models to predict nuclear masses. This is a crucial test since the nuclei with newly measured masses lie at the outskirts of the nuclidic chart. They are either characterized by a strong asymmetry in their proton to neutron ratios (e.g., neutron-rich nuclei like ^{54}Ca [8] or ^{82}Zn [9]), lie at the proton drip-line or even beyond (e.g., ^{45}Cr [11] or ^{65}As [27]), or belong to very heavy elements (e.g., $^{252-255}$No [14,16] or $^{255-256}$Lr [16]), and, therefore, their theoretical descriptions are a challenge. To the best of our knowledge such a test is performed here for the first time, at least with the use of the latest data.

The quality of ten different models of global character (i.e., aiming at describing masses of all or almost all nuclei) is studied. These are six models of macroscopic-microscopic nature, two of a purely microscopic (self-consistent) character, and two of another kind. Several of the considered models have been widely used for a relatively long time, but the others are new, developed only recently. It is essential that all the models were proposed before the new data appeared. Thus, the present work is a real test of the predictive power of these models.

The accuracy of the description of nuclear masses by a given model is usually described by the rms (root-mean-square) value of the differences between the calculated and the experimental values of the mass for the global region of nuclei. However, such information, although important, is far from sufficient, because the accuracy of a model strongly depends on the region of nuclides considered. Due to this, we divided the whole region of nuclei under consideration into four subregions. This allowed us to illustrate the strong dependence of the accuracy of each of the models on the subregions considered.

Besides supplying general knowledge on the accuracy of the present theoretical description of masses, the results of the analysis may provide useful information for users of the models to help choose the most appropriate one when studying specific nuclei. For example, the choice of the proper model was crucial for the successful prediction of the properties of the decay chains of the nuclei of the as-yet-unobserved element $Z = 117$ [28]. A comparison of the predicted and experimentally obtained values was given in Ref. [29] describing the discovery of this element. Furthermore, as yet unknown masses are an indispensable nuclear physics input for modeling the nucleosynthesis processes in stars [22,30],

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understanding the composition of neutron stars [9,31], and investigating the evolution of shell closures [32], nucleon-nucleon correlations [33,34], fundamental symmetries [10] as well as the limits of nuclear existence [35,36]. Last but not least, the results of the present study may also be helpful for the authors of the models in improving them.

In our earlier, preliminary studies [37–39], older experimental mass evaluations were used.

In Sec. II, we specify the models used for the calculations of masses, while the results are presented in Sec. III. Section IV contains the summary of our study.

II. CONSIDERED MODELS

As already stated above, ten models are considered in the present study. The six macroscopic-microscopic models are the finite-range droplet model (FRDM) [40], the finite-range liquid drop model (FRLDM) [40], the nuclear Thomas-Fermi model (TF) [41], the Lublin-Strasbourg drop (LSD) model [42], and the recent models of Liu *et al*. (WS3.6) [19] and of Wang and Liu (WS3.3) [20]. Concerning the notation for the latter two models, the WS3.6 approach is also denoted sometimes by WS3, and the WS3.3 one is also labeled by WS3+RBF to stress the presence of the radial basis function (RBF) correction in it (see Ref. [20], where the two models are discussed in detail). The purely microscopic models are the Hartree-Fock-Bogoliubov mean field model with the BSk21 Skyrme interaction (HFB21) [18] and with the D1M Gogny interaction (GHFB) [17]. The last two models are that of Duflo and Zuker (DZ) [43] and that of Koura *et al*. (KTUY) [44].

III. RESULTS AND DISCUSSION

Table I gives the accuracy of the description of the experimental masses by each of the models for five regions of nuclei: global (all nuclei with $Z,N \geqslant 8$), light ($8 \leqslant Z < 28, N \geqslant 8$), medium-I ($28 \leqslant Z < 50$), medium-II ($50 \leqslant Z < 82$), and heavy ($Z \geqslant 82$) nuclei. As mentioned above, experimental masses are taken from the recent evaluation [25]. For each region and each model, the numbers of nuclei with both

TABLE I. The rms, average discrepancy, $\bar{\delta}$, and maximum of the absolute values of the discrepancies, max $|\delta|$, calculated 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 ($Z \geqslant 82$) nuclei, with the use of the specified models. The numbers of nuclei with both calculated and evaluated values in 2003, $N_{\text{nucl}}(2003)$, and in 2012, $N_{\text{nucl}}(2012)$, are also shown.

Model	LSD (2003)	FRDM (1995)	TF (1996)	FRLDM (1995)	HFB21 (2010)	GHFB (2009)	DZ (1995)	KTUY (2005)	WS3.6 (2011)	WS3.3 (2010)
				Global						
$N_{\text{nucl}}(2003)$	2141	2149	2149	2149	2149	2149	2149	2149	2149	2149
$N_{\text{nucl}}(2012)$	2316	2353	2351	2353	2353	2353	2353	2353	2353	2353
rms	0.608	0.654	0.649	0.776	0.572	0.789	0.394	0.701	0.335	0.248
$\bar{\delta}$	−0.027	−0.059	0.027	0.054	0.030	−0.103	−0.032	−0.058	−0.008	−0.008
max $\|\delta\|$	4.34	3.64	4.61	4.17	3.20	3.43	3.06	2.93	1.75	1.45
				Light						
$N_{\text{nucl}}(2003)$	322	322	322	322	322	322	322	322	322	322
$N_{\text{nucl}}(2012)$	332	335	335	335	335	335	335	335	335	335
rms	1.046	1.144	1.054	1.206	0.911	1.087	0.546	0.692	0.482	0.362
$\bar{\delta}$	−0.180	−0.162	−0.012	0.173	0.035	−0.365	0.058	−0.055	0.021	0.063
max $\|\delta\|$	4.34	3.64	4.61	4.17	3.20	3.43	2.81	2.29	1.75	1.13
				Medium-I						
$N_{\text{nucl}}(2003)$	509	509	509	509	509	509	509	509	509	509
$N_{\text{nucl}}(2012)$	574	575	575	575	575	575	575	575	575	575
rms	0.650	0.664	0.701	0.630	0.578	0.748	0.406	0.783	0.357	0.277
$\bar{\delta}$	0.042	0.072	0.222	0.054	0.099	0.30	−0.097	−0.313	−0.059	−0.055
max $\|\delta\|$	2.45	2.44	2.62	2.38	1.93	2.95	1.81	2.93	1.22	1.45
				Medium-II						
$N_{\text{nucl}}(2003)$	896	897	897	897	897	897	897	897	897	897
$N_{\text{nucl}}(2012)$	961	970	970	970	970	970	970	970	970	970
rms	0.451	0.475	0.501	0.674	0.455	0.556	0.328	0.542	0.290	0.207
$\bar{\delta}$	−0.101	−0.132	−0.209	−0.221	−0.034	−0.032	−0.026	0.216	0.023	−0.006
max $\|\delta\|$	1.94	1.50	1.79	1.97	1.74	2.61	1.39	1.54	1.65	0.73
				Heavy						
$N_{\text{nucl}}(2003)$	414	421	421	421	421	421	421	421	421	421
$N_{\text{nucl}}(2012)$	449	473	471	473	473	473	473	473	473	473
rms	0.349	0.448	0.444	0.743	0.458	0.971	0.376	0.869	0.255	0.179
$\bar{\delta}$	0.156	0.006	0.302	0.530	0.073	−0.227	−0.032	−0.312	−0.033	−0.004
max $\|\delta\|$	1.43	2.00	1.75	1.92	1.60	3.23	3.06	2.38	0.87	0.88

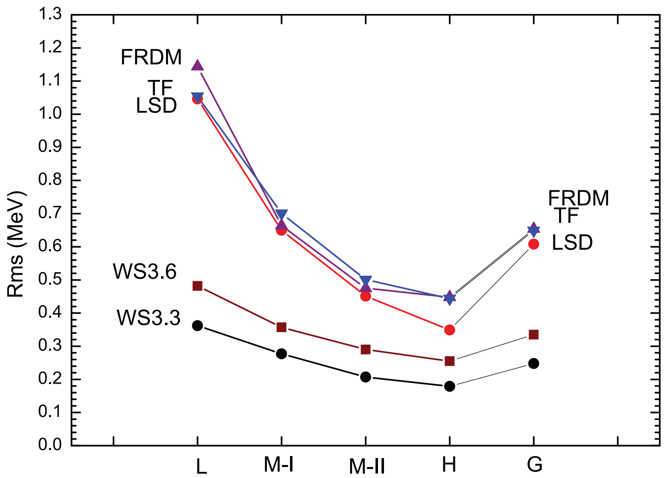

FIG. 1. (Color online) Dependence of the rms discrepancy on the region of nuclei studied for the FRDM, TF, LSD, WS3.6, and WS3.3 models.

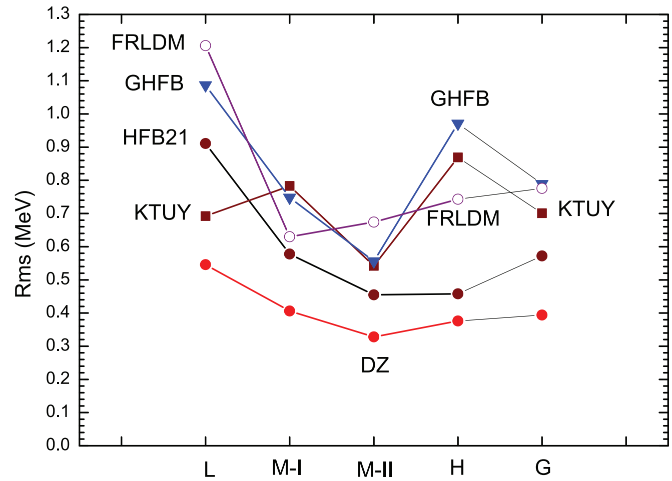

FIG. 2. (Color online) Same as in Fig. 1, but for the FRLDM, GHFB, HFB21, KTUY, and DZ models.

calculated and evaluated masses in 2003, N_{nucl} (2003), and 2012, N_{nucl} (2012), are also shown. They give information on how many new masses are involved in the description. The table also gives the rms of the discrepancies, rms, the average value of the discrepancies, $\bar{\delta}$, and the maximum of the absolute values of the discrepancies, max $|\delta|$. For each model, the year of its publication is also shown.

One can see in the table that for each region of the nuclear chart, the rms changes quite strongly from one model to another. For example, for the light-nuclei region, the rms changes from 0.362 (WS3.3) to 1.206 MeV (FRLDM). However, the rms also strongly varies with the change of region for a given model. For example, the rms changes from 0.448 (heavy) to 1.144 MeV (light) for the FRDM approach. Also the average discrepancy $\bar{\delta}$ strongly depends on the model (e.g., it changes from −0.004 for WS3.3 to 0.530 MeV for FRLDM in the heavy region) and also on the change of region for a given model (e.g., it changes from −0.221 in the medium-II to 0.530 MeV in the heavy region for the FRLDM model). A strong variation of max $|\delta|$ is observed too: from 0.73 (WS3.3; medium-II) to 4.61 MeV (TF; light and medium-II regions).

The dependence of the rms discrepancy on the model and on the region of nuclei studied is illustrated in Figs. 1 and 2. One can see in Fig. 1 that the dependence of the rms on the region of nuclei is very strong, especially for the FRDM, TF, and LSD models. For these three approaches, not only the dependence, but also the values of the rms are very close to each other for all the regions investigated. This reflects the fact that the natures of these macroscopic-microscopic models are very similar. The dependences of the rms of the WS3.3 and WS3.6 models are also similar to each other, also reflecting the similarity of their natures. Their values, however, are much smaller than those for the FRDM, TF, and LSD models. It is worthwhile noting that the rms of all these five models systematically decreases with increasing mass of the nuclei. In other words, the quality of the description of masses systematically increases when one passes from lighter to heavier nuclei. This might be interpreted to mean that the assumption of a good mean field, on which all the models are based, is better fulfilled for heavier nuclei.

Similar behavior is observed in Fig. 2 for the HFB21 and DZ approaches. However, the results for the FRLDM, GHFB, and KTUY models show different trends. Here, it is interesting to note that the HFB21 and GHFB models, although using the same approach (HFB), show a difference in the dependence of the rms on the region of nuclei. This is probably the effect of the difference in the effective forces used. This illustrates the sensitivity of the dependence of the rms on the region of nuclei described to the details of a particular model.

IV. SUMMARY

To summarize our study, one can say the following: Ten different theoretical models are quantitatively tested for their accuracy in the description of nuclear masses. A recent evaluation of experimental masses [25] is used for these tests. The accuracy is studied in five regions of the nuclear chart: light (335 nuclei), medium-I (575), medium-II (970), heavy (473), and global (2353) regions. Much attention is given to the dependence of the accuracy of a given model on the region of nuclei described.

The following conclusions may be drawn from the study:

(i) A strong dependence of the accuracy of the description of the mass on the region of nuclei considered is obtained for each model.

(ii) For most of the models, the accuracy improves when passing from lighter nuclei to heavier ones. This might be interpreted as due to a better fulfillment of the condition of a good mean field, on which all the models are based.

(iii) The difference between the accuracies (rms) of different models varies from one region to another. It is largest for the light-nuclei region (from 0.362 for WS3.3 to 1.206 MeV for FRLDM) and smallest for the medium-II region (from 0.207 for WS3.3 to 0.701 MeV for KTUY).

(iv) The dependence of the accuracy of a model on the region of nuclides studied closely reflects its nature. Models of similar natures show similar dependences, while those of different natures, differ much in this property.

(v) In all regions considered, the best accuracy is obtained by the WS3.3 model.

(vi) For the first time purely microscopic, self-consistent models of the Hartree-Fock Bogoliubov series (here HFB21) show about equal or even better accuracy than the widely used macroscopic-microscopic models (e.g., FRDM, TF, or LSD models).

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