On the Predictive Power of Nuclear Models

G. AUDI and C. BORCEA[1]

CSNSM, IN2P3-CNRS, Laboratoire René Bernas,
Bâtiment 108, F-91405 Orsay Campus, France

One of the most important nuclear physics ingredients that is determinant in nuclear astrophysics is certainly the mass of a nucleus. For example, in the rapid neutron capture process (r-process), Goriely and Arnould [92Gor] have listed already five entries for the nuclear masses. Either directly in the position of the neutron drip line, the neutron separation energies (instrumental for determining the neutron capture cross-sections) and the Q_β (for the β-decay rates), or indirectly in the fission rates or the β-delayed processes rates.

Unfortunately it is not an information easy to get, not to say impossible, in the regions of interest for astrophysics. One could try extrapolations starting from the experimentaly known masses. But it is a quite long way to the drip lines or at least to the regions of the chart where S_n, the neutron separation energy, is of the order of 1 or 1.5 MeV. Any tentative along these lines would certainly fail.

Experiment being powerless in this respect, one would like to turn to a good theory. But there is no complete theory of the nuclear matter and of the nucleus which is ready to give all the needed informations. The way out, up to now, has been to try to marry both of them. Based on sound ideas about the nucleus many theoreticians tend to formulate simple enough equations to be calculable in large regions of the chart, and the parameters of these formulae have to fit the known masses. It is a necessary condition, but alas not a sufficient one.

As a direct consequence, strong divergences often occur between theories as discussed recently twice: by a nuclear physicist [90Hau] and by astrophysicists [92Gor] who showed the dramatic differences in the results they derive for the r-process depending on the mass formula they start with: the mass mismatch between two formulae near the drip line could vary up to 20 MeV; the neutron drip line could move up to 16 mass units further away and the resulting r-process abundances could change by more than one order of magnitude.

[1] IN2P3-Visitor, on leave from the Institute for Atomic Physics, Bucharest.

One could distinguish two types among the existing models for nuclear masses: the ones that use local relations and the ones that start from a nuclear model calculation with different ingredients of phenomenology. While for the first type, one may expect that a gradual deterioration can appear when getting to far outer masses, for the second type, in principle, every physical premise is contained so that, even if fitted to a particular sample, one should expect not too large divergences. This should be especially true for the theories that use a relatively small number of parameters.

The aim of the present contribution is to examine thoroughly the reliability of the existing models through the predictions they yield for nuclear masses. We have examined the structures they predict for the Surface of Masses, their predictive power and their divergences.

1 STRUCTURE OF THE MASS SURFACE

The experimental Surface of Masses is characterized by the very smooth behaviour of its four sheets (one for each type of parity in N and Z) manoeuvering together in a 3-dimensional space (N, Z and Mass). This smoothness is interrupted in some places by "accidents" that almost always can be associated with a relatively violent change in one or more physical parameters (e.g. shell closures, shape transitions). Unfortunately, visualizing and handling these sheets in a tridimensional space together with the constraints concerning their relative distance is not simple. A way out is to look at the "derivatives" of the surface of masses, like separation energies S_n, S_{2n}, decay energies Q_α, Q_β or pairing energies Δ_{nn}, Δ_{np} [85Bos]. These derivatives, not only exhibit the same smoothness property as the surface itself, but still more important, they enhance the physical structures. The ability of a mass formula to reproduce the general smoothness of the Surface of Masses and the clearly superposed physical structures qualifies it as a candidate for the prediction of still unknown nuclei.

For example, fig. 1 shows that the predictions of Möller and Nix [88Mol] have some oscillatory trends not present in the actual mass surface. These oscillations may deteriorate the accuracy of a prediction on a local scale but do not *a priori* imply strong deviations when going towards the drip lines. At the opposite, another model [88Sat] does reproduce quite well the masses of nuclei close to the bottom of the valley of stability but exhibits too large oscillations beyond the known masses rendering its predictions questionable in the case where far extrapolations are needed, even though it is a "global" model. More generaly, the Wigner correction terms for N=Z which are very important for predicting masses of proton rich nuclei are considered only in a few mass predictions and often, when taken into account, they do not result in a structure with the same amplitude as that displayed by the experimental masses.

In these examples, deviations from the experimental surface and from the smoothness

Figure 1 : Predictions of the theory of Möller and Nix [88Mol] (solid lines) are compared to the experimental masses (points, error bars and dashed lines) in an S_{2n} representation for N=28-50. Diamonds locate the so-called "Wigner" nuclei (N=Z). Oscillations in the theoretical curves indicate lack of smoothness of the formula. Constraints to limit the variation of some parameters from one nucleus to another could certainly improve the predicted Surface of Masses. Extension of the predictions up to the drip line is highly desirable here, as for all "global" models, in order to make "far" extrapolations possible.

property do not all have the same influence on the ability to predict masses very far from stability. This analysis, while making a first selection, has to be completed by a study of the predictive power and of the divergences among the models.

2 PREDICTIVE POWER OF THE MODELS

Since the 1986 atomic mass table [88Wap] some 175 new masses have been measured and this sample can be used to test the quality of predictions made by each model. To the 10 models already presented in the "1986-1987 Atomic Mass Predictions" of Haustein [88Hau] we added the ones of Duflo [92Duf] based on doublets and triplets and the ETFSI model (extended Thomas-Fermi plus Strutinsky integral) of Pearson et al. [92Pea], both adjusted also on the 1986 experimental masses, and also the "semi-empirical shell model formula" of Liran and Zeldes [76Lir].

To calculate the deviations of the models from the experimental values, we need

Table 1 : Compensated Linear Deviation (cld) of 13 mass models calculated for 2 different sets of measured nuclear masses.

	MODEL	type	cld^a keV	nb	cld^b keV	nb	**cpr**
1	Pape and Antony	local	154	(85)	72	(3)	
2	Dussel,Caurier,Zuker	local	176	(1325)	135	(87)	
3	Möller and Nix	global	595	(1589)	632	(168)	1.06
4	Möller et al.	global	525	(1589)	593	(168)	1.13
5	Comay,Kelson,Zidon	local	149	(1628)	387	(174)	2.59
6	Satpathy and Nayak	global	298	(1589)	782	(171)	2.63
7	Tachibana et al.	global	321	(1653)	448	(175)	1.39
8	Spanier and Johansson	global	495	(884)	920	(63)	1.86
9	Jänecke and Masson	local	64	(1629)	287	(174)	4.52
10	Masson and Jänecke	local	132	(1578)	424	(168)	3.22
11	Duflo	global	288	(1381)	450	(130)	1.57
12	Liran and Zeldes	global	182	(1582)	755	(166)	4.14
13	Pearson et al.	global	543	(1489)	586	(146)	1.08

The figures in parentheses indicate the number of nuclei from the set of experimental masses for which a given theory makes predictions.

a) calculated for the set of 1655 masses of the 1986 atomic mass table [88Wap]

b) calculated for the set of 175 new masses measured since 1986

to get a feeling of the "adherence" of the theoretical mass surface to the real one. We made thus the choice of the **"compensated linear deviation"** (cld) [81Aud] $cld = \frac{1}{n}\Sigma \max\{(|m_{th} - m_{exp}| - \sigma_{exp}), 0\}$, which in a way represents the volume comprised between the theoretical surface and the experimental one.

Table 1 presents the results of calculated deviations for the 13 theories and 2 sets of experimental masses: the 1655 masses of the 1986 table [88Wap] and the set of the 175 new masses measured since 1986. There is a clear increase of the deviations for the set of new masses. Last column gives the ratios between the deviations for the two samples, which may be called **"close predictive ratios"** or **cpr**. The **cpr** for the "global" models are systematically better than for the "local" ones.

3 DIVERGENCES OF THE MODELS

Now that the predictive power of the models have been evaluated, one may consider to make an adequate statistical treatment of the predictions, provided the divergences between models are within reasonable limits (see next paragraph) and that at least [90Hau] six models give predictions for a given nuclear mass. A weighted average is being considered. The uncertainty associated with each theory's prediction in that average is taken as: $\sigma_i^{th} = cld_i \times cpr_i^2$. We observe that the dispersion among the predictions from different models increase drastically when one approaches the drip lines. However, for a relatively large region, this dispersion is in reasonable limits.

Figure 2 : Differences between the predictions of two "local" relations: Comay, Kelson and Zidon [88Com] and Jänecke and Masson [88Jan] plotted as a function of "neutrons from stability" for 5707 nuclei. The strong coherence around stability ($NFS = 0$) is due to the very good agreement of both predictions with the known masses. Divergences exceeding 10 MeV start at $NFS = +14$ on the neutron-rich side.

The averages of theoretical masses over the whole chart yielded results for 5018 nuclei of which 4227 had a dispersion below 1 MeV. These crude results will require naturally careful individual and global analysis.

Following Haustein [84Hau] we define a distance with respect to the stability line called "neutrons-from-stability": $NFS = N - Z - (0.4A^2)/(200 + A)$. A similar norm was proposed by Goriely and Arnould [92Gor] who defined a "neutron surplus", which is more precise but less convenient than Haustein's NFS. To get an overall idea about the zone where different predictions are still coherent, one may, similarly to [92Gor], compare any two theoretical predictions as a function of NFS, and also observe the deviations of a given model from the calculated "average" of predictions. Though very efficient, this method suffers however from the fact that the domains of predicted masses vary widely from one model to another. Many models do not venture to the vicinity of drip lines i.e. where we are interested to compare their predictions. This fact is in turn reflected by the size of the above set of averaged values. Anyway, as a general trend one can mention a strong divergence of "local" models among themselves and with respect to the "average" when departing from the measured masses (fig. 2). This tendency is also present but much attenuated, for those "global" models that make predictions in a large enough domain. Conclusion of the NFS analysis, confirmed by the statistical treatment above, is that going beyond

Figure 3 : Average values of theories, obtained as described in the text, are compared to the experimental masses (points, error bars and dashed lines) in an S_{2n} representation for N=28-50. The smooth character of the curves is preserved even for outer masses. Further smoothing of these averages may be considered in the production phase of our work. Extension of these predictions on the neutron-rich side is limited, due to the small number of models making predictions far enough from stability.

$|NFS| = 20$ is hazardous for the time being. This number could define the frontier separating the medium-range extrapolations from the far extrapolations.

The averaged values obtained for the medium-range predictions can be compared with the experimental masses. An example is shown in fig. 3. The smooth character of the curves is preserved even for the region of the outer masses. Of course, the medium-range extrapolated values obtained in this way are far from being perfect, but they can be considered as the best estimate presently possible for these masses. Each theory contains some truth and certainly some approximations. Being constructed quite differently from each other, one may expect that the effects of these approximations do not coincide and would be random. If this is the case, then averaging would be licit and could be considered as the best way out until drastic improvements in theories is achieved.

Towards the neutron drip line, we have seen that the above procedure fails because of the important divergences among theories. This effect can be limited if in the far extrapolations, the "local" models are not used. To compensate the resulting impoverishment in models, it would be highly desirable to have all "global" models extend their predictions up to the neutron drip line.

4 CONCLUSIONS

We have compared the behaviour of the Surface of Masses, as predicted by 13 nuclear models, with the experimental surface. We have evaluated the predictive power of these models and analysed their divergences when predicting masses far from stability. The result of these analyses showed that, based on existing models, the medium range extrapolations are reliable while extrapolations toward drip lines (far extrapolations) are to be taken with much care untill further improvements in the theories make them congruent in these regions.

Presently, the methods for close and medium-range extrapolations are defined and tested. Serial production of such predictions is the next step, but that will require much care and time. Close extrapolations will be produced very soon to be included in the next table of experimental masses. Medium-range extrapolations may be evaluated and enter a special table, if strong interest for astrophysics is expressed. Special care will be taken to ensure the continuity property of the Surface of Masses at the border between the three regions: experimental masses, close extrapolations and medium-range extrapolations.

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