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A New Finite-Range Droplet Mass Model and Equation-of-State Parameters

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The parameters in the macroscopic "droplet" part of the finite-range droplet model (FRDM) are related to the properties of the EOS. In the FRDM (1992) version, the optimization of the model parameters was not sufficiently sensitive to variations of the compressibility constant K and the density-symmetry constant L to allow their determination. In the new, more accurate FRDM-2011a adjustment of the model constants to new and more accurate experimental masses allows the determination of L together with the symmetry-energy constant J. The optimization is still not sensitive to K which is therefore fixed at $K = 240$ MeV. Our results are $J = 32.5 \pm 0.5$ MeV and $L = 70 \pm 15$ MeV and a considerably improved mass-model accuracy $\sigma = 0.5700$ MeV, with respect to AME2003 for FRDM-2011a, compared to $\sigma = 0.669$ MeV for FRDM (1992) (with respect to AME1989). These values are compatible with those obtained from other considerations.

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Several constants of the FRDM are related to the equation-of-state symmetry and compressibility parameters. Recently substantial efforts have been devoted to determining realistic values of the symmetry-energy constants experimentally [1] and theoretically [2, 3]. In the 1990's when the FRDM was developed, it was difficult to determine the compressibility K and the density-symmetry L from adjustments to known masses, but the the value 32.73 MeV was obtained for the symmetry-energy constant J [4]. Nuclear masses in the FRDM (1992) table compared to experimental data known at that time with a model $\sigma = 0.669$ MeV (see Ref. [4] for a definition of σ). Subsequently, as additional masses were measured we learned that they were well *predicted* by the model: the model reproduced 529 new masses with $\sigma = 0.462$ MeV [5–7].

In the FRDM (1992), the compressibility K and the density-symmetry L were fixed at 240 MeV and 0, respectively. Recently we have taken advantage of vastly increased computer power to improve our calculations which led to a mass model FRDM-2007b with $\sigma = 0.5964$ MeV with respect to the most recent mass evaluation AME2003 [8]. In these calculations we still retained $K = 240$ MeV and $L = 0$ [7, 9]. We now also take into account the effect of axially asymmetric deformations on the ground-state mass and redetermine the 9 macroscopic-model constants, including the density-symmetry constant L, so as to minimize the mass-model σ with respect to the AME2003 [8]. These steps, highlighted in Fig. 1, lead to FRDM-2011a with $\sigma = 0.5700$ MeV.

We review briefly these previous results in lines 1–4 of Table 1. in which we show the mass model parameters determined from adjustments to experimental data and associated model accuracy. The different lines represent results under different assumptions. Line 1 shows the parameters and accuracy of the FRDM (1992). Increased computer power allowed us to search more completely for the optimum parameter set, yielding $\sigma = 0.6614$ MeV [7]. When an optimum parameter set has been determined, the mean deviation $\mu_{\rm th}$ [4] is normally very close to zero, so to show this we give μ and σ in Table 1 to 4 decimals. The fairly large value of μ in line 1 is an indication that the parameter set was not optimally determined. Because some effects in the FRDM are calculated by expansions valid only for small deviations from spherical

Successive FRDM enhancements

Optimization ($1 \rightarrow 2$)
The search for optimum FRDM macroscopic parameters has been improved.
Accuracy improvement: 0.01 MeV

New exp. mass data base ($2 \rightarrow 3$)
We agree better with the new mass data base
Accuracy improvement: 0.04 MeV

Full 4D energy minimization ($3 \rightarrow 4$)
Search for minimum energy versus $\epsilon_2, \epsilon_3, \epsilon_4, \epsilon_6$, full 4D in steps of 0.01.
Accuracy improvement: 0.02 MeV

Axial asymmetry ($4 \rightarrow 5$)
Results in correct gs assignments in SHE regions, and mass improvements.
Accuracy improvement: 0.01 MeV

L **variation** ($5 \rightarrow 7$)
Accuracy improvement 0.02 MeV

FIG. 1. Impact of successive enhancements to FRDM(1992) with $\sigma = 0.669$ MeV, leading to FRDM-2011-a with $\sigma = 0.5700$ MeV. The line numbers in Table 1 corresponding to before and after enhancement are given in parenthesis.

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shape we no longer consider fission barriers in our adjustment [10, 11]. Their elimination yields a minor further decrease in σ, by 0.0017 MeV, to 0.6591 MeV, line 2. We showed previously [7] that although the parameters were now more tightly determined, the model extrapolated even better to the 529 new masses, with $\sigma = 0.4174$ MeV rather than $\sigma = 0.4617$ MeV with the original parameter set. Often, when model parameters are more tightly tied to a limited data set it will extrapolate more poorly to data outside the region of adjustment. That the opposite is true here is a strong indication that the various terms in the macroscopic model are realistic and that the number of parameters is not excessively large.

In the FRDM (1992) mass calculation the potential energy was calculated on a coarse two-dimensional grid in the quadrupole ϵ_2 and hexadecapole ϵ_4 shape parameters with spacings 0.05 and 0.04, respectively. The ground-state (gs) deformations were then determined by interpolation. With the gs values of ϵ_2 and ϵ_4 fixed, the octupole ϵ_3 and hexacontatetrapole ϵ_6 deformation parameters were varied separately and the lowest energy obtained was identified as the ground-state mass. We now vary all four (ϵ_2,ϵ_3,ϵ_4,ϵ_6) in a full four-dimensional space with a spacing of 0.01 for each variable to determine the ground-state shape and shell correction. The optimum macroscopic model constants are in line 4 of Table 1 yielding a mass table with $\sigma = 0.5964$ MeV with respect to AME2003. About half the improvement from 0.6688 MeV (top line) to 0.5964 MeV comes from a more accurate calculation, the other half is the consequence of the new experimental mass data set, in which many incorrect masses in the old data set have been removed or corrected and new mass data added. In a separate calculation [12, 13] we have recently calculated the effect of axial asymmetry on nuclear masses and include here this enhancement which improves the accuracy by 0.01 MeV (Table 1, line 4). This improvement may seem minor, but has a major impact for the limited number of nuclei where axial asymmetry occurs, deviations between experiment and calculations are reduced by up to 0.8 MeV, and ground-state shapes and level structure better predicted [12, 13]. Squeezing the σ of the mass deviation is not the only item of importance; we also look closely at several other properties, in particular how well the model can predict properties of unknown nuclei.

In a final step we again vary the macroscopic model parameters but also, for the first time, release L to vary freely. This results in the mass table FRDM-2011a, line 7 in Table 1. We reach $\sigma = 0.5700$ MeV. The improvement due to the variation of L is 2.9%. In Fig. 2 we show the difference between experimental data [14] and this new calculated mass table. The improvement due to L variation may not seem striking, but when the mass model σ is as low as in this case experience has taught us that it is quite difficult to obtain further improvements so the effect is significant. Because the density-symmetry effect is a higher-order effect [15] we *cannot* obtain a large effect on the mass model accuracy by L variation. Rather

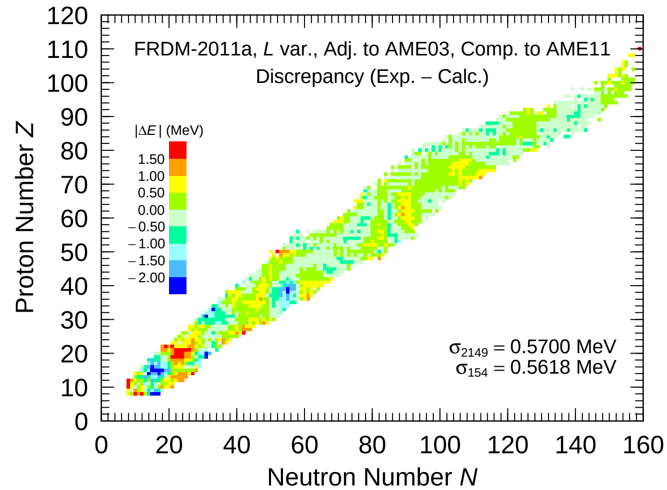

FIG. 2. Differences between measured and calculated masses corresponding to line 7 in Table 1.

the issue is: can we at all determine the effect when it is fairly small? We make the case we can, but previously, in a less accurate mass model we could not.

We show the robustness of the results including the determination of L by calculating the mass model accuracy for newly measured masses that were not taken into account in our adjustment of model parameters. Recently the interim AME2011 experimental mass evaluation [14] was released. It contains 154 new masses relative to AME2003 that we did not use in our adjustment. In line 8 of Table 1 we see that the accuracy of FRDM-2011a for these nuclei is 0.5618 MeV, that is no divergence is observed although we apply the model to nuclei outside the region of adjustment. The table FRDM-2011b, which was also adjusted to AME2003, but with L fixed at zero "extrapolates" less well to this new region, the accuracy is only $\sigma = 0.6212$ MeV, line 6 in Table 1. Very importantly, if the improvement in accuracy that we obtained when L was varied were due to "just an additional parameter", then the mass table obtained after L variation would extrapolate very poorly compared to the $L = 0$ mass table. This is not the case.

From Table 1, lines 1-10 we estimate the uncertainty in the values of J and L from the values obtained under different constraints, such as different experimental data sets and the increasing refinement of the theory, as discussed above. The parameter J varies only in a narrow range, from 32.11 MeV to 32.98 MeV, and L, in its two determinations varies by 15 MeV. The best estimates are in line 7. Therefore we conclude that best values for J and L, with error bars are $J = 32.5 \pm 0.5$ MeV and $L = 70 \pm 15$ MeV, using the same estimate for the lower bound for L as was obtained for the upper bound. These are uncertainties related to the experimental data. Uncertainties due to issues of model formulation are in the category of "systematic" errors and in practice challenging to estimate. Very briefly we can say that the earlier FRDM (1992) has over 20 years compared extremely

Line No	Model	A/C	a_1 (MeV)	a_2 (MeV)	J (MeV)	Q (MeV)	L (MeV)	a_0 (MeV)	$c_{\rm a}$ (MeV)	C (MeV)	γ	$\mu_{\rm th}$ (MeV)	$\sigma_{{\rm th};\mu=0}$ (MeV)
1	(92)	1/1	16.247	22.92	32.73	29.21	0	0.00	0.436	60	0.831	0.0156	0.6688
2	(92)-b	1/1	16.286	23.37	32.34	30.51	0	−5.21	0.468	179	1.027	0.0000	0.6591
3	(06)-a	2/2	16.274	23.27	32.19	30.64	0	−5.00	0.450	169	1.000	0.0000	0.6140
4	(07)-b	2/2	16.231	22.96	32.11	30.83	0	−3.33	0.460	119	0.907	0.0000	0.5964
5	(11)-b	2/2	16.231	22.95	32.10	30.78	0	−3.14	0.456	113	0.896	0.0001	0.5863
6	(11)-b	2/3										−0.0850	0.6212
7	**(11)-a**	**2/2**	**16.147**	**22.44**	**32.51**	**28.54**	**70.84**	**−2.96**	**0.531**	**150**	**0.880**	**−0.0004**	**0.5700**
8	**(11)-a**	**2/3**										**−0.0516**	**0.5618**
9	(11)-c	1/1	16.251	23.10	32.31	30.49	0	−3.43	0.471	123	0.935	−0.0003	0.6300
10	(11)-d	1/1	16.142	22.39	32.98	27.58	85.95	−2.64	0.548	138	0.853	0.0000	0.6092
11	HFB21	2/2	16.035		30.00		46.58					−0.0603	0.5587
12	HFB21	2/3										0.1959	0.6504
13	(FY1970)	2/2	15.949	21.10	31.37	32.49	0	1.76	0.543	78	0.589	−0.0001	0.6909
14	(FY1970)	2/2	15.935	21.01	31.37	31.96	39.03	2.30	0.543	106	0.668	−0.0003	0.6876

TABLE I. FRDM (1992) and successive enhancements. Adjustments have been performed for 9 macroscopic constants, i.e, the volume-energy (a_1), the surface-energy (a_2), the symmetry energy (J), the effective surface-stiffness (Q), the density-symmetry (L), the A^0 (a_0), the charge-asymmetry ($c_{\rm a}$), the preexponential compressibility term (C) and the exponential compressibility-term range (γ) constants. The second column indicates a model designation and the third is which data set (denoted "1", "2", or "3") the model was "Adjusted and Compared (A/C)" to. The last two columns are the mean deviation (with sign) $\mu_{\rm th}$ and the model $\sigma_{{\rm th};\mu=0}$, both defined in Ref. [4], with respect to the data set specified in the "C" column. In column three, the data sets "1", "2", and "3" stand for the Audi 1989 mass evaluation [16], the Audi 2003 mass evaluation [8], and masses that are in the 2011 evaluation [14] but not in the 1989 evaluation, respectively. There are 154 such new nuclei in data set "3" in the region we consider ($Z \geq 8$, $N \geq 8$). The model constants are given in the middle section. The top line gives the original model constants [4]. When no values are given, the set on the line just above is used. The value "0" in the L column indicates L was fixed at zero. See the text for additional discussions.

well to new measurements both towards the drip lines and towards the superheavy region [5, 7, 17], which is compatible with a low systematic error. Can the model become more accurate? It has been suggested that the residual error is due to the presence of specific types of chaotic motion [18, 19]. However, we note that in Fig. 2 some type of correlated behavior in the error stands out, in particular large and correlated errors in the region of light nuclei. It has been our experience previously that straightforward remedies for such correlated errors can sometimes be identified [4, 12]. However, some deviations are outside the model. At $N = 56$ some nuclei near $Z = 40$ are underbound by up to 2 MeV. Further away from $Z = 40$ deviations are near zero. It is a well-known experimental observation that the $N = 56$ subshell widens near $Z = 40$ leading to more bound nuclei than obtained in theoretical calculations. There is no mechanism in our model that can widen $N = 56$ near $Z = 40$ in a global approach. But it might be described by an additional term or "force" in the single-particle potential, for example a tensor force [20].

In lines 11 and 12 we compare to HFB21 [21] another global mass model based on self-consistent treatment and optimization of a Skyrme interaction, with additional phenomenological "macroscopic-type" terms. In contrast to this work J is not determined from mass model variations but fixed at $J = 30$ MeV based on other considerations. While the HFB21 agrees well with the mass data in AME2003 to which it was adjusted ($\sigma = 0.5587$ MeV), the model extrapolates somewhat less well to the new region of 154 nuclei with $\sigma = 0.6504$ MeV there.

It is only recently that we have been able to investigate how sensitive our results are to the choice of single-particle spin-orbit and diffuseness parameters, line 13, see Ref. [17] for details. We have carried out a full-fledged nuclear mass calculation based on the single-particle parameters that were selected in 1970 when the folded-Yukawa single-particle model was introduced [22] and obtain $\sigma = 0.6909$ MeV. A variation of L, line 14, lowers σ to 0.6876 MeV, a decrease by only 0.47%. Whereas the random errors in this mass model are too large to allow the determination of L, the accuracy of FRDM-2011a is sufficient to allow this determination. An earlier study, similar to the one here, but based on a Thomas-Fermi model, the earlier, less refined microscopic corrections [4], and the earlier experimental data base [16] obtained $K = 234$ MeV, $J = 32.65$ MeV, and $L = 49.9$ MeV [23, 24].

In investigations of other types of experimental data, for example multifragmentation in heavy-ion collisions, Pigmy dipole resonances, neutron skin thicknesses, and global optical potentials have been used to derive values for the J and L constants [25]. The constraints obtained from these data are $J = 31{\pm}4$ MeV and $L = 60{\pm}23$ MeV, which are compatible with the values obtained from the present mass analysis. In another study [26] a somewhat lower value of L was obtained, but not much below our admittedly rough estimate of the one-σ limit.

The symmetry-energy constants J and L have often been extracted from Skyrme Hartree-Fock (SHF) and

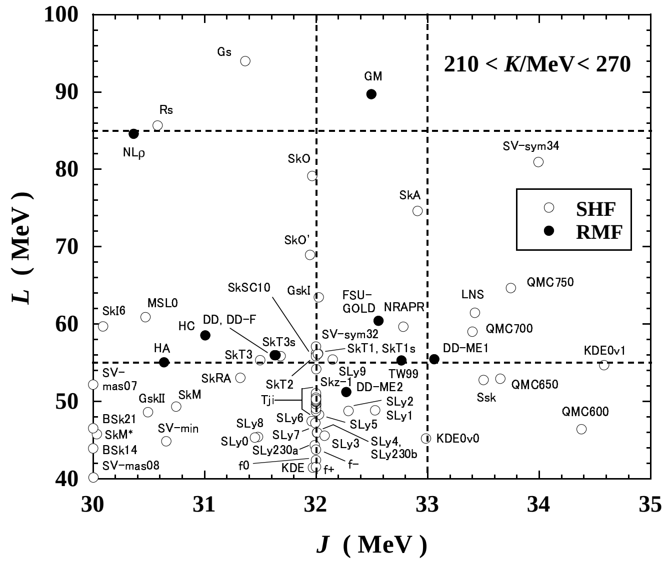

FIG. 3. Calculated symmetry parameters J and L in a selection of different SHF (white circles) and RMF (black circles) models. The dashed lines indicate the one-σ limits in our determination.

relativistic-mean-field (RMF) models [2, 3]. Fig. 3 shows J and L values determined from a number of different Skyrme and RMF energy densities [27]. From the investigation in Ref. [27] we display results for a parameter region extending about two σ from our preferred values and for which the compressibility is in the realistic range $K = 240 \pm 30$ MeV [28, 29]. Only 8 sets of constants are within or close to the one-σ boundaries in Fig. 3. We suggest that the limits of J and L from our mass study be considered in evaluating existing and future effective SHF and RMF energy-density functionals.

In summary we have obtained a new mass table FRDM-2011a, with $\sigma = 0.5700$ MeV, $J = 32.5 \pm 0.5$ MeV and $L = 70 \pm 15$ MeV. When associated quantities (for example ground-state spins, β-decay half-lives) have been calculated, estimated in 2012, the results will be posted on our web site [30] and simultaneously submitted to an appropriate journal.

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