Mass predictions of exotic nuclei within a macro-microscopic model

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Abstract. Different Liquid Drop Model mass formulae have been studied. They include a Coulomb diffuseness correction Z^2/A term and pairing and shell energies of the Thomas-Fermi model. The influence of the selected charge radius, the curvature energy and different forms of the Wigner term has been investigated. Their coefficients have been determined by a least square fitting procedure to 2027 experimental atomic masses. The different fits lead to a surface energy coefficient of 17-18 MeV. A large equivalent rms radius ($r_0 = 1.22 - 1.24$ fm) or a shorter central radius may be used. A rms deviation of 0.54 MeV can be reached between the experimental and theoretical masses. The remaining differences come from the determination of the shell and pairing energies. Mass predictions are given for exotic nuclei.

1. Introduction

Predictions of masses of exotic nuclei close to the proton and neutron drip lines and in the superheavy element region must still be pursued and improved. Beyond the Bethe-Weizsäcker formula [1, 2] and beside the statistical Thomas-Fermi model [3] and the microscopic Hartree-Fock self-consistent mean field approaches [4], the ability and accuracy of different versions of the macro-microscopic Liquid Drop Model mass formula and nuclear radii have been studied and compared [5].

2. Different possible mass formulae

Different subsets of the following expansion of the nuclear binding energy in powers of $A^{-1/3}$ and the relative neutron excess $I = (N - Z)/A$ have been studied :

$$B = a_v \left(1 - k_v I^2\right) A - a_s \left(1 - k_s I^2\right) A^{\frac{2}{3}} - a_k \left(1 - k_k I^2\right) A^{\frac{1}{3}} - \frac{3}{5}\frac{e^2 Z^2}{R_0} + f_p \frac{Z^2}{A} - E_{pair} - E_{shell} - E_{Wigner}. \quad (1)$$

The first term is the volume energy. $I^2 A$ is the asymmetry energy of the Bethe-Weizsäcker mass formula. The second term is the surface energy. It takes into account the deficit of binding energy of the nucleons at the nuclear surface. The third term gives the curvature energy which is a correction to the surface energy resulting from the mean local curvature (see Ref. [5]). This term is considered in the TF model [3] but not in the Finite Range LDM [6]. The fourth term is the usual Coulomb energy. Different formulae may be assumed for the charge radius. The Z^2/A term is the diffuseness correction to the basic sharp radius Coulomb energy term (called also the proton form-factor correction). The shell and pairing energies of the recent Thomas-Fermi model [3, 5] have been chosen and four versions of the Wigner term have been introduced: $W_1 = |I|$, $W_2 = |N-Z| \times e^{-(A/50)^2}$, $W_3 = |N-Z| \times e^{-A/35}$ and $W_4 = e^{-80I^2}$. To obtain the coefficients of the selected expansions by a least square fitting procedure, the masses of the 2027 nuclei verifying the two conditions : N and Z higher than 7 and the one standard deviation uncertainty on the mass lower than 150 keV have been used [7].

As examples, three possible accurate possible formulae are given here.

$$B = 15.4133\left(1-1.7962I^2\right)A - 17.3079\left(1-1.7858I^2\right)A^{\frac{2}{3}} - 0.6\frac{e^2Z^2}{1.2318A^{\frac{1}{3}}} + 0.8956\frac{Z^2}{A}$$
$$-0.4838|N-Z| \times e^{-(A/50)^2} + 2.2 \times e^{-80I^2} - E_{pair} - E_{shell}. \quad (2)$$

$$B = 15.6096\left(1-1.8543I^2\right)A - 18.1132\left(1-2.0021I^2\right)A^{\frac{2}{3}} - 0.6\frac{e^2Z^2}{1.28A^{\frac{1}{3}} - 0.76 + 0.8A^{-\frac{1}{3}}}$$
$$+1.8086\frac{Z^2}{A} - 0.47|N-Z| \times e^{-(A/50)^2} + 2.4954 \times e^{-80I^2} - E_{pair} - E_{shell}. \quad (3)$$

$$B = 15.3848\left(1-1.7837I^2\right)A - 17.1947\left(1-1.8204I^2\right)A^{\frac{2}{3}} - 0.6\frac{e^2Z^2}{1.2257A^{\frac{1}{3}}}$$
$$+1.1035\frac{Z^2}{A} - 16.606|I| - E_{pair} - E_{shell}. \quad (4)$$

The rms deviations between the theoretical and experimental masses are respectively : 0.543, 0.558 and 0.584 MeV. In the formula (2) the reduced radius r_0 is determined by the adjustment to the experimental masses. The combination of two Wigner terms allows to reach a very good accuracy. In the formula (3) the assumed radius is the radius proposed in Ref. [8]. It corresponds to a central or equivalent sharp radius. In the last formula (4) the radius $R_0 = 1.2257\ A^{1/3}$ fm has been obtained previously by an adjustment on 782 ground state charge radii [9]. So it it possible to obtain accurate mass formulae with a large constant reduced radius r_0 or with a more sophisticated central radius corresponding to a smaller value of r_0 increasing with the mass. On the other hand a constant value $r_0 = 1.16$ fm does not allow to obtain a rms deviation better than 0.72 MeV. The formula (2) is more precise for the light nuclei while the formula (4) is the most appropriate for the heaviest elements.

The difference between the theoretical masses obtained with the formula (4) and the experimental masses of the 2027 nuclei used for the adjustment of the coefficients is indicated in Figure 1 (formulas (2) and (3) lead about to the same figures). The more the colour is dark the more the accuracy is high. The errors are slightly larger for the light nuclei. The same behaviour is encountered by all the mass models. Nevertheless the error is very rarely higher than 2 MeV.

3. Predictability of the formulae

Since the last mass evaluation [7] other masses have been newly or more precisely obtained. The predictions given by the formula (4) (not readjusted) for 161 new masses are compared with the experimental data in Figure 2. The accuracy is correct in the whole mass range showing the predictability of such formulae.

Table 1. Theoretical mass excess (in MeV) predicted with the formula (3) and 2003 AME values for heavy exotic nuclei.

Nucleus	E_{th}	E_{AME}	Nucleus	E_{th}	E_{AME}	Nucleus	E_{th}	E_{AME}
^{152}La	-49.34	-50.07	^{152}Ce	-59.26	-59.11	^{152}Lu	-33.18	-33.42
^{153}Ba	-36.48	-37.62	^{153}La	-46.02	-46.93	^{153}Ce	-54.97	-55.35
^{153}Yb	-47.09	-47.06	^{153}Hf	-26.82	-27.3	^{154}La	-41.3	-42.38
^{154}Ce	-52.25	-52.7	^{154}Lu	-39.88	-39.57	^{154}Hf	-32.87	-32.73
^{155}La	-37.71	-38.8	^{155}Ce	-47.65	-48.4	^{155}Pr	-55.37	-55.78
^{155}Nd	-62.38	-62.47	^{155}Hf	-34.18	-34.1	^{155}Ta	-24.38	-23.67
^{156}Ce	-44.6	-45.4	^{156}Pr	-51.28	-51.91	^{156}Ta	-26.2	-25.8
^{157}Ce	-39.66	-40.67	^{157}Pr	-48.29	-48.97	^{157}Nd	-56.36	-56.79
^{157}Hf	-38.54	-38.75	^{158}Pr	-43.86	-44.73	^{158}Nd	-53.94	-54.4
^{158}Ta	-31.1	-31.02	^{158} W	-23.81	-23.7	^{159}Pr	-40.68	-41.45
^{159}Nd	-49.6	-50.22	^{159}Pm	-56.5	-56.85	^{159} W	-24.99	-25.23
^{160}Nd	-46.91	-47.42	^{160}Pm	-52.73	-53.1	^{160}Sm	-60.5	-60.42
^{160}Eu	-63.14	-63.37	^{160}Re	-16.95	-16.66	^{161}Nd	-42.36	-42.96
^{161}Pm	-50.12	-50.43	^{161}Sm	-56.88	-56.98	^{161}Eu	-61.57	-61.78
^{161}Ta	-38.7	-38.73	^{161} W	-30.08	-30.41	^{162}Pm	-46.07	-46.31
^{162}Sm	-54.8	-54.75	^{162}Eu	-58.43	-58.65	^{162}Re	-22.54	-22.35
^{162}Os	-14.13	-14.5	^{163}Pm	-43.07	-43.15	^{163}sm	-50.83	-50.9
^{163}Eu	-56.47	-56.63	^{163}Gd	-61.17	-61.49	^{163}Os	-15.9	-16.12
^{164}Sm	-48.36	-48.18	^{164}Eu	-53.02	-53.1	^{164}Gd	-59.76	-59.75
^{164}Re	-27.54	-27.64	^{164}Ir	-7.55	-7.27	^{165}Eu	-50.66	-50.56
^{165}Gd	-56.41	-56.47	^{165}Tb	-60.27	-60.66	^{165}Os	-21.43	-21.65
^{165}Ir	-11.32	-11.63	^{166}Eu	-46.68	-46.6	^{166}Gd	-54.52	-54.4
^{166}Re	-31.99	-31.85	^{166}Ir	-13.32	-13.21	^{166}Pt	-4.35	-4.79
^{167}Eu	-43.65	-43.59	^{167}Gd	-50.67	-50.7	^{167}Tb	-55.69	-55.84
^{167}Re	-34.75	-34.84	^{167}Pt	-6.17	-6.54	^{168}Gd	-48.17	-48.1
^{168}Tb	-52.35	-52.5	^{168}Ir	-18.73	-18.74	^{169}Gd	-43.71	-43.9
^{169}Tb	-49.99	-50.1	^{169}Pt	-12.03	-12.38	^{169}Au	-1.71	-1.79
^{170}Tb	-46.13	-46.34	^{170}Dy	-53.49	-53.66	^{170}Ir	-23.4	-23.32
^{170}Au	-3.7	-3.61	^{171}Tb	-43.48	-43.5	^{171}Dy	-49.76	-50.11
^{171}Hg	3.57	3.5	^{172}Dy	-47.65	-47.73	^{172}Ho	-51.09	-51.4
^{172}Ir	-27.48	-27.52	^{172}Au	-9.06	-9.28	^{173}Dy	-43.62	-43.78
^{173}Ho	-49.11	-49.1	^{173}Er	-53.54	-53.65	^{173}Hg	-2.31	-2.57
^{174}Ho	-45.65	-45.5	^{174}Er	-52.09	-51.95	^{174}Au	-13.87	-14.2
^{175}Ho	-43.25	-42.8	^{175}Er	-48.73	-48.65	^{176}Er	-46.89	-46.5
^{176}Au	-18.14	-18.54	^{176}Tl	0.87	0.55	^{177}Er	-43.06	-42.8
^{177}Tm	-47.76	-47.47	^{178}Tm	-44.44	-44.12	^{178}Tl	-4.38	-4.75
^{179}Tm	-42.19	-41.6	^{179}Yb	-46.88	-46.42	^{179}Pb	2.34	2
^{180}Yb	-45.15	-44.4	^{180}Tl	-9.07	-9.4	^{181}Yb	-41.58	-40.85
^{181}Lu	-45.29	-44.74	^{182}Lu	-42.24	-41.88	^{183}Lu	-40.21	-39.52
^{184}Lu	-37.01	-36.41	^{184}Bi	1.88	1.05	^{185}Hf	-39.06	-38.36
^{185}Bi	-1.47	-2.21	^{186}Hf	-37.44	-36.43	^{187}Hf	-33.9	-32.98
^{187}Ta	-37.73	-36.77	^{188}Hf	-31.73	-30.88	^{188}Ta	-34.59	-33.81
^{189}Ta	-32.55	-31.83	^{190}Ta	-29	-28.66	^{191} W	-31.72	-31.11
^{192} W	-29.98	-29.65	^{192}Re	-32.1	-31.71	^{193}Re	-30.48	-30.3
^{194}Re	-27.15	-27.55	^{198}Ir	-25.39	-25.82	^{202}Pt	-22.66	-22.6

Nucleus	E_{th}	E_{AME}	Nucleus	E_{th}	E_{AME}	Nucleus	E_{th}	E_{AME}
^{204}Au	-20.5	-20.75	^{205}Au	-18.8	-18.75	^{208}Hg	-13.62	-13.1
^{209}Hg	-8.54	-8.35	^{210}Hg	-5.14	-5.11	^{211}Tl	-5.61	-6.08
^{212}tl	-0.84	-1.65	^{215}Pb	5.67	4.48	^{217}Bi	9.78	8.82
^{218}Bi	14.28	13.34	^{219}Po	13.72	12.8	^{220}Po	16.51	15.47
^{220} U	22.6	23.03	^{221}At	17.4	16.81	^{221} U	24.05	24.59
^{222}At	21.58	20.8	^{222}Pa	21.27	22.12	^{222} U	24.17	24.3
^{223}At	24.39	23.46	^{226}Np	32.44	32.74	^{228}Fr	34.05	33.28
^{228}Np	33.5	33.7	^{231}Fr	43.04	42.33	^{231}Am	42.09	42.44
^{232}Fr	46.99	46.36	^{232}Np	37.42	37.36	^{232}Am	43.16	43.4
^{233}Ra	45.18	44.77	^{233}Ac	41.91	41.5	^{233}Am	43.11	43.17
^{234}Ra	47.81	47.23	^{234}Ac	45.49	45.1	^{234}Am	44.43	44.53
^{235}Ac	48.09	47.72	^{235}Am	44.62	44.66	^{235}Cm	47.98	47.91
^{235}Bk	52.44	52.7	^{236}Ac	51.75	51.51	^{236}Th	46.8	46.45
^{236}Am	46.25	46.18	^{236}Cm	47.75	47.89	^{236}Bk	53.32	53.4
^{237}Th	50.42	50.2	^{237}Am	46.79	46.57	^{237}Cm	49.36	49.28
^{237}Bk	53.04	53.1	^{237}cf	57.73	57.82	^{238}Th	52.88	52.63
^{238}Bk	54.27	54.29	^{238}Cf	57.05	57.2	^{239}Pa	53.64	53.34
^{239}Cm	51.4	51.19	^{239}Bk	54.28	54.29	^{239}Cf	58.24	58.15
^{240}Pa	57.27	56.8	^{240}Bk	55.66	55.67	^{240}Cf	57.85	58.03
^{240}Es	63.9	64.2	^{241} U	56.49	56.2	^{241}Bk	56.12	56.1
^{241}Cf	59.16	59.36	^{241}Es	63.39	63.84	^{242} U	58.8	58.62
^{242}Bk	57.91	57.74	^{242}Es	64.44	64.97	^{242}Fm	67.88	68.4
^{243}Np	59.98	59.88	^{243}Cf	60.72	60.95	^{243}Es	64.44	64.78
^{243}Fm	68.88	69.26	^{244}Np	63.5	63.2	^{244}Es	65.53	66.03
^{244}Fm	68.45	69.01	^{245}Es	65.82	66.44	^{245}Fm	69.49	70.22
^{245}Md	74.78	75.29	^{246}Es	67.39	67.9	^{246}Md	75.71	76.28
^{247}Pu	69.11	69	^{247}Am	66.85	67.15	^{247}Es	67.96	68.61
^{247}Fm	70.89	71.58	^{247}Md	75.27	76.04	^{248}Am	70.43	70.56
^{248}Bk	67.76	68.08	^{248}Es	69.79	70.3	^{248}Md	76.37	77.15
^{248}No	79.81	80.66	^{249}Am	73.26	73.1	^{249}Es	70.62	71.18
^{249}Fm	72.82	73.62	^{249}Md	76.46	77.33	^{249}No	80.9	81.82
^{250}Es	72.57	73.23	^{250}Md	77.84	78.64	^{250}No	80.58	81.52
^{251}Md	78.15	79.03	^{251}No	81.91	82.91	^{251}Lr	86.76	87.9
^{252}Cm	79.3	79.06	^{252}Bk	78.59	78.53	^{252}Md	79.67	80.63
^{252}Lr	87.72	88.84	^{253}Bk	80.96	80.93	^{253}Md	80.42	81.3
^{253}No	83.38	84.47	^{253}Lr	87.48	88.69	^{253}Rf	92.61	93.79
^{254}Bk	84.74	84.39	^{254}Md	82.89	83.51	^{254}Lr	88.69	89.85
^{254}Rf	92	93.32	^{255}Cf	84.81	84.81	^{255}Lr	88.81	90.06
^{255}Rf	93.03	94.4	^{255}Db	98.47	100.04	^{256}Cf	87.11	87.04
^{256}Es	87.01	87.19	^{256}Lr	90.89	91.87	^{256}Db	99.14	100.72
^{257}Es	89.14	89.4	^{257}Lr	91.64	92.74	^{257}Rf	94.86	95.93
^{257}Db	98.94	100.34	^{258}Es	92.54	92.7	^{258}Fm	89.92	90.43
^{258}No	90.83	91.48	^{258}Lr	93.83	94.84			

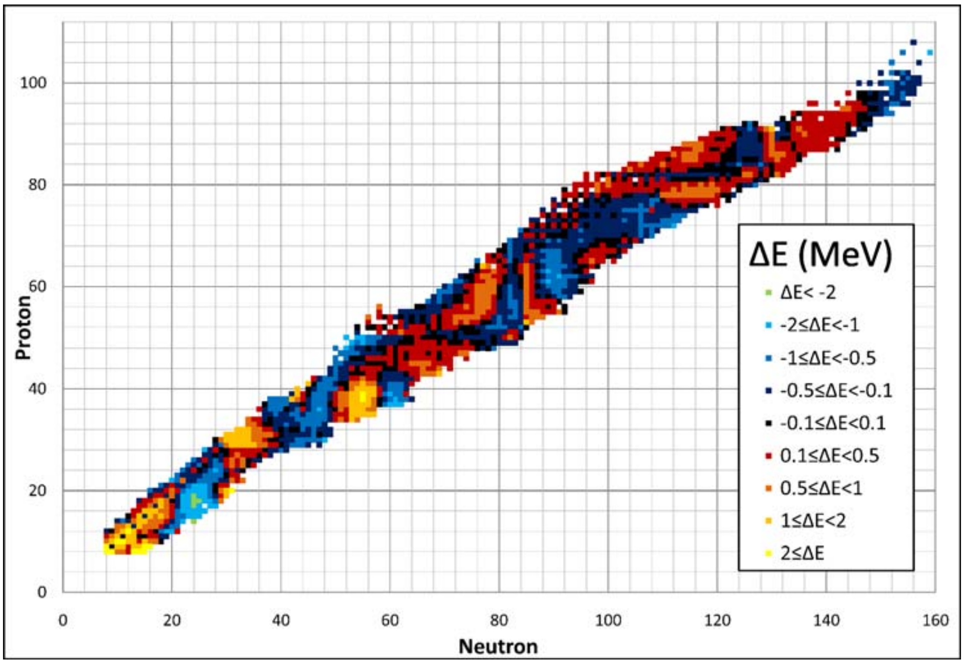

Figure 1. Difference between the theoretical masses obtained with the formula (4) and the experimental masses of the 2027 selected nuclei.

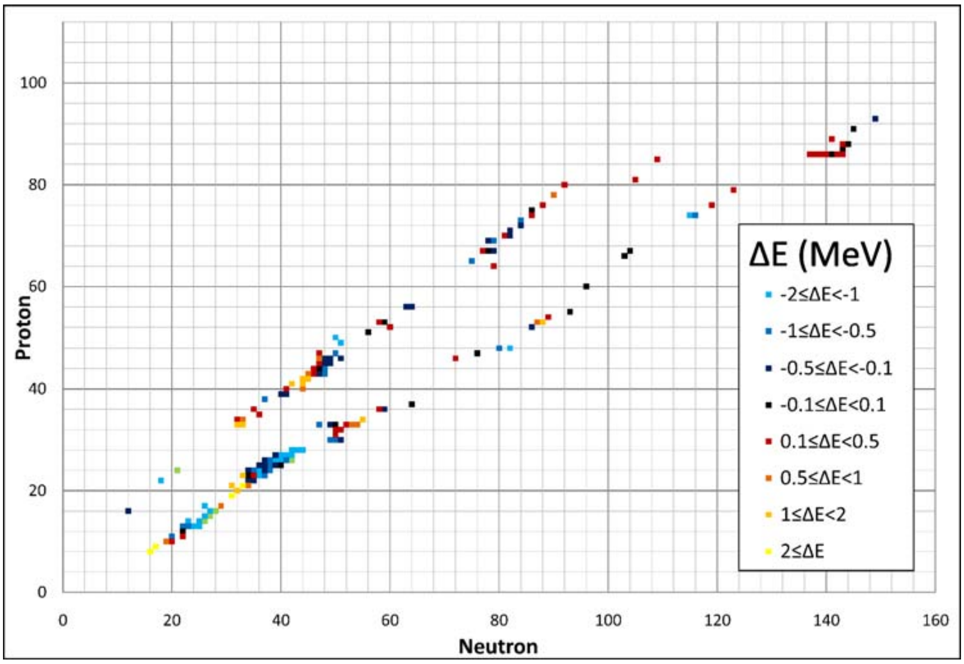

Figure 2. Difference between the theoretical masses obtained with the formula (4) and 161 new experimental masses.

4. Mass of exotic nuclei

Finally, the predictions given by the formula (4) for 656 other nuclei for which the mass is still unknown are compared in Figure 3 to the extrapolations given in Ref. [7] with an

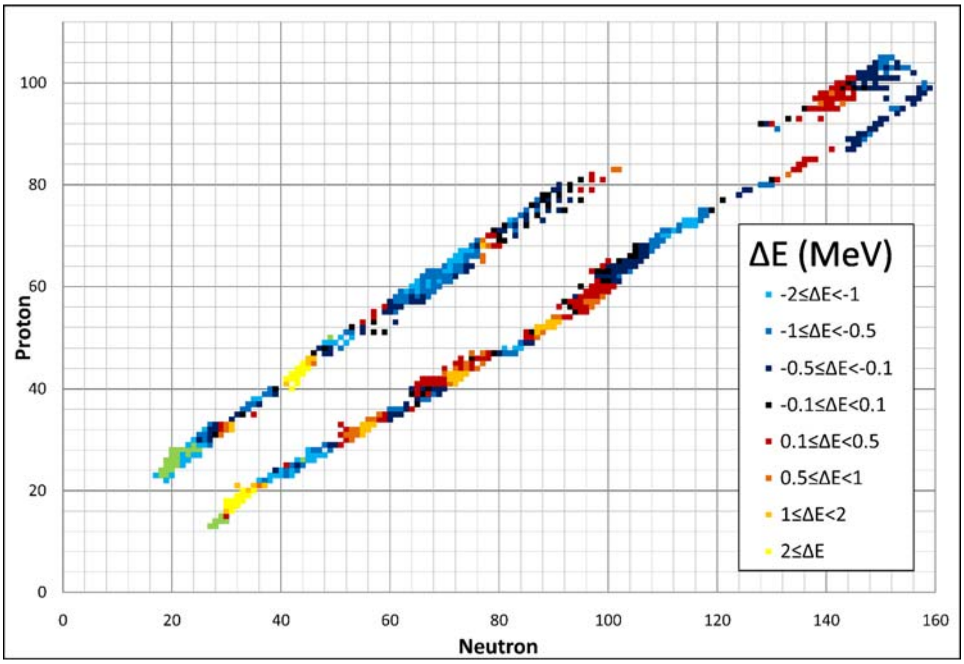

Figure 3. Difference between the theoretical masses obtained with the formula (4) and 656 extrapolated masses.

assumed uncertainty often higher than 500 keV. Without readjustment the formula (4) leads to $\sigma = 0.748$ MeV for the 2844 nuclei.

The theoretical mass excesses predicted with the formula (3) (which uses the radius adopted in our generalized liquid drop model) and 2003 AME values are given and compared in the table for heavy elements.

5. Conclusion

The coefficients of different macro-microscopic Liquid Drop Model mass formulae have been determined by an adjustment to 2027 experimental atomic masses. A rms deviation of 0.54 MeV can be reached. The remaining small differences come probably mainly from the determination of the shell and pairing energies (Strutinsky procedure and Thomas-Fermi model [3]). A large constant coefficient $r_0 = 1.22 - 1.23$ fm or a small value increasing with the mass can be used. Extrapolations are compared to 161 new experimental masses and to 656 mass evaluations of exotic nuclei. The different fits lead always to a surface energy coefficient of around 17-18 MeV.

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