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► **To cite this version:**

Guy Royer, A. Onillon, Maxime Guilbaud, A. Auzizeau. Mass predictions of exotic nuclei within a macro-microscopic model. 10th International Spring Seminar on Nuclear Physics: New quests in nuclear structure, May 2010, Vietri, Italy. pp.012010, 10.1088/1742-6596/267/1/012010. in2p3-00567946

HAL Id: in2p3-00567946

<https://in2p3.hal.science/in2p3-00567946v1>

Submitted on 22 Feb 2011

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Mass predictions of exotic nuclei within a macroscopic-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 :

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

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.

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

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

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

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 is 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			

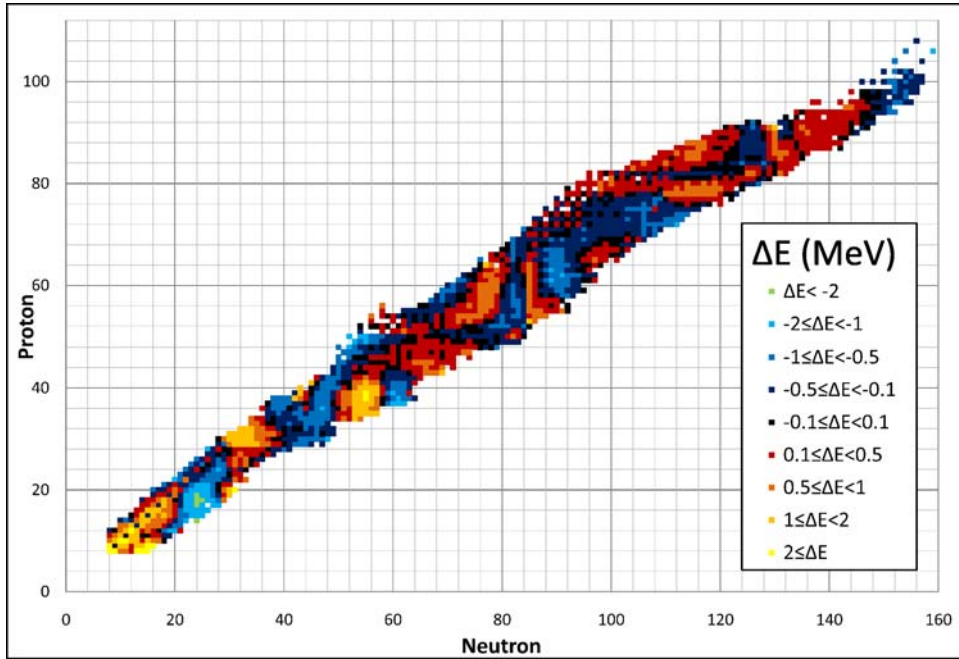


Figure 1. Difference between the theoretical masses obtained with the formula (4) and the experimental masses of the 2027 selected nuclei.

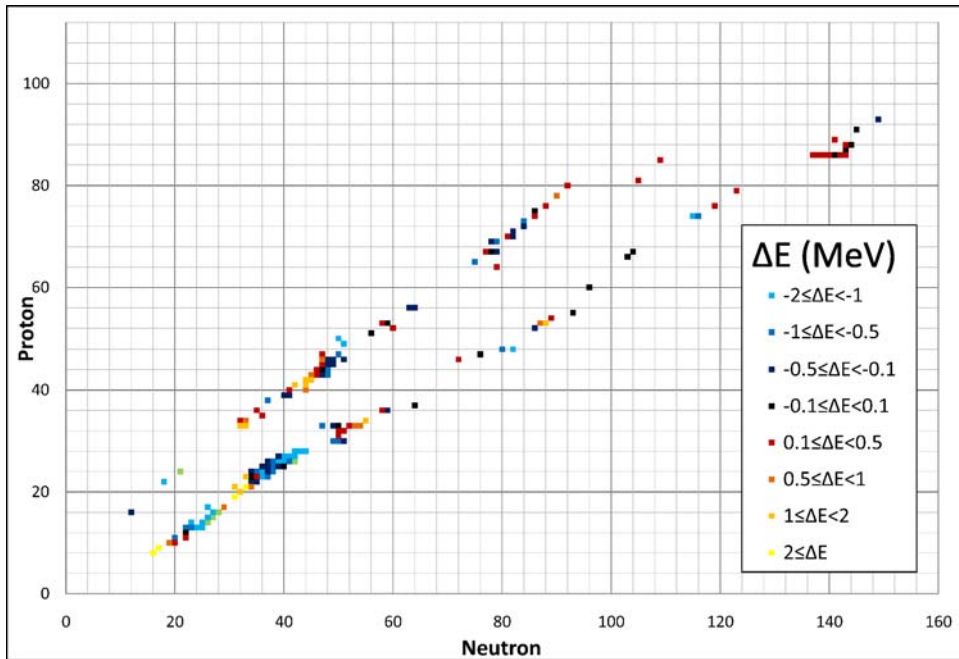


Figure 2. Difference between the theoretical masses obtained with the formula (4) and 161 new experimental masses.

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

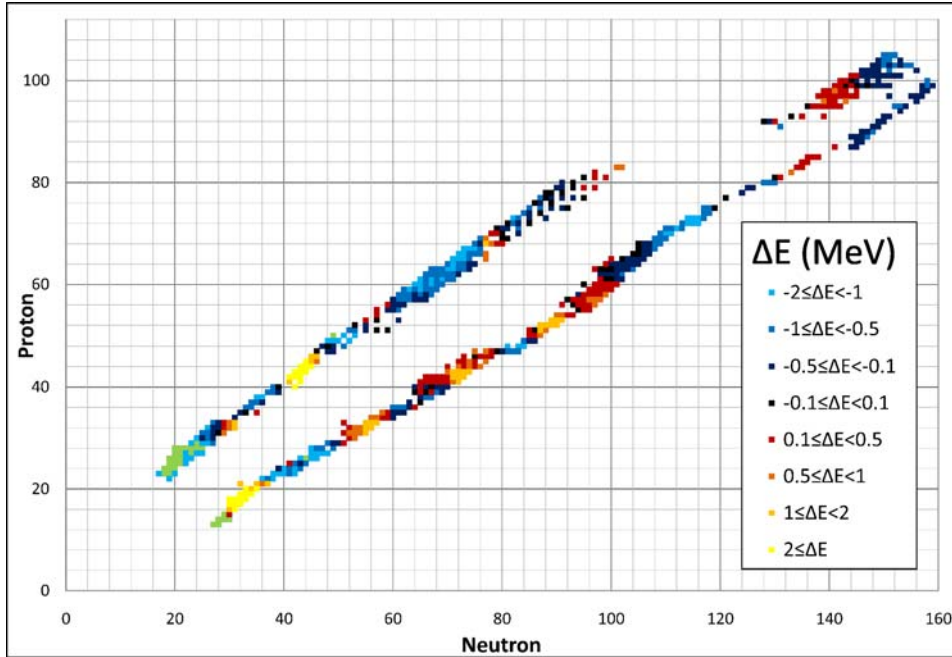


Figure 3. Difference between the theoretical masses obtained with the formula (4) and 656 extrapolated masses.

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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