Application of Garvey-Kelson formula to mass extrapolation

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2020.01.13

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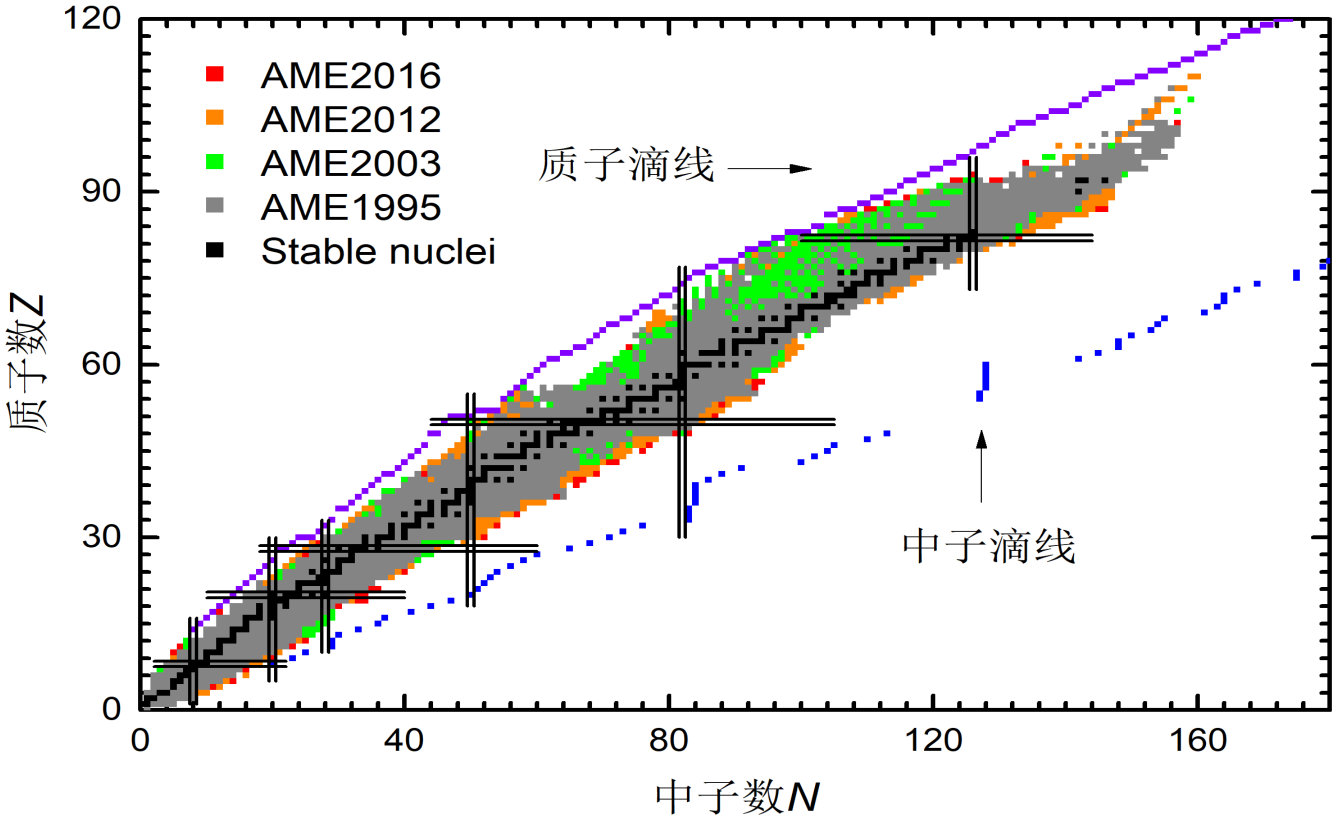
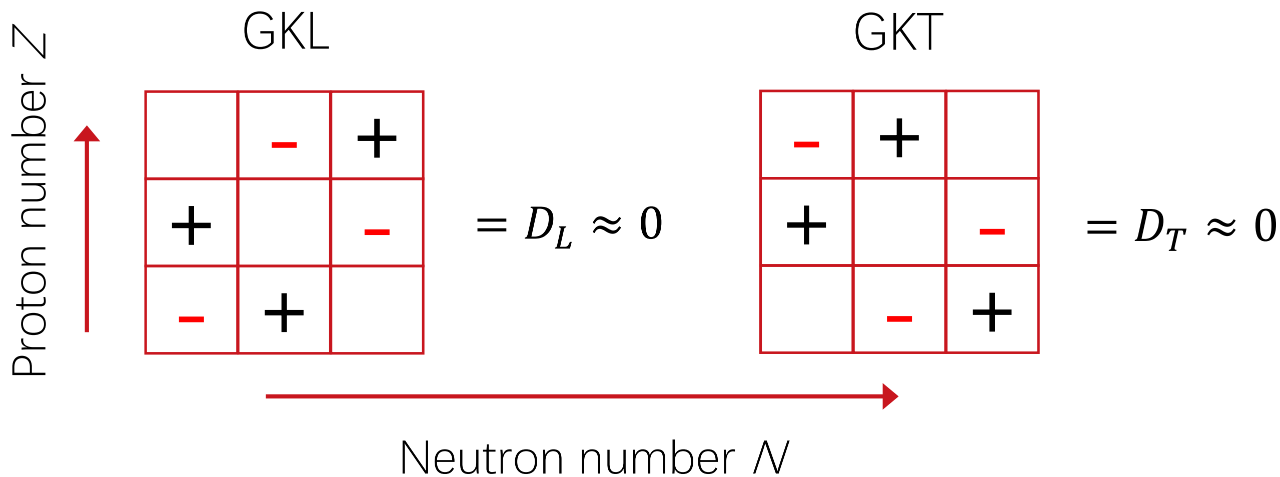
Introduction



[G. Audi, A.H. Wapstra, Nucl. Phys. A 595, 409 (1995) ;
G. Audi, A. H.Wapstra, and C. Thibault, Nucl. Phys. A 729, 337 (2003) ;
Chin. Phys. C 36, 1287 (2012) ; Chin. Phys. C, 36, 1603 (2012) ;
Chin. Phys. C 41, 030002 (2017); Chin. Phys. C 41, 030003 (2017);]

Garvey-Kelson mass relations



[G. T. Garvey and I. Kelson, Phys. Rev. Lett. **16**, 197 (1966); G. T. Garvey, W. J. Gerace, R. L. Jaffe, I. Talmi, and I. Kelson, Rev. Mod. Phys. **41**, S1 (1969)]

- Suppose that $M(N,Z) \propto \alpha N + \beta Z + \gamma NZ$.
- Apply to the description and prediction for heavy nuclei with high precision;

[Phys. Rev. C, **87**, 057304 (2013); Phys. Rev. C, **88**, 064325 (2013); Sci. China-Phys. Mech. Astron. 60, 022011 (2017)]

- For $A \geq 120$, RMSD=148 (158) keV for D_L (D_T) in AME2016.

Garvey-Kelson mass formula

- If GKL and GKT are established simultaneously, the general solution should be

$$M_{\mathrm{GKs}}(N,Z) = h_1(N) + h_2(Z) + \lambda NZ + \mu \frac{1-(-1)^{NZ}}{2}.$$

[G. T. Garvey and I. Kelson, Phys. Rev. Lett. **16**, 197 (1966); G. T. Garvey, W. J. Gerace, R. L. Jaffe, I. Talmi, and I. Kelson, Rev. Mod. Phys. **41**, S1 (1969)]

Unfortunately, RMSD~2 MeV for AME2016.

- Previous efforts:
  - Inhomogeneous terms. [Nucl. Phys. A **243**, 326 (1975)]

    e. g. $M_{\mathrm{GKs}}(N,Z) = g_1(N) + g_2(Z) + g_3(A) + g_4(E) + E_p$.

    [Z. He, M. Bao, Y. M. Zhao, and A. Arima, Phys. Rev. C **90**, 054320 (2014)]
  - Treat different regions separately. [At. Data Nucl. Data Tables **39**, 265 (1988)]

Practical method to predict atomic masses

- The GK formula does not hold globally but *"locally"* instead.
- The *"locality"* constraint is given by

$$|A_0 - A| \le R \ , |E_0 - E| \le R \ ,$$
$$A_0 \ne A \, , E_0 \ne E \ ,$$

  where R are set as proper numbers for different nuclei to be predicted.
- Determine the theoretical values by least-squares method,

$$\min_{p_v} \sum_{i=1}^{n} \left(M_{\mathrm{exp}}^{i} - M_{\mathrm{th}}^{i}\right)^2 \longrightarrow \sum_{i=1}^{n} \left(M_{\mathrm{exp}}^{i} - M_{\mathrm{th}}^{i}\right) \frac{\partial M_{\mathrm{th}}^{i}}{\partial p_v} = 0, v = 1,2 \ldots m \ .$$

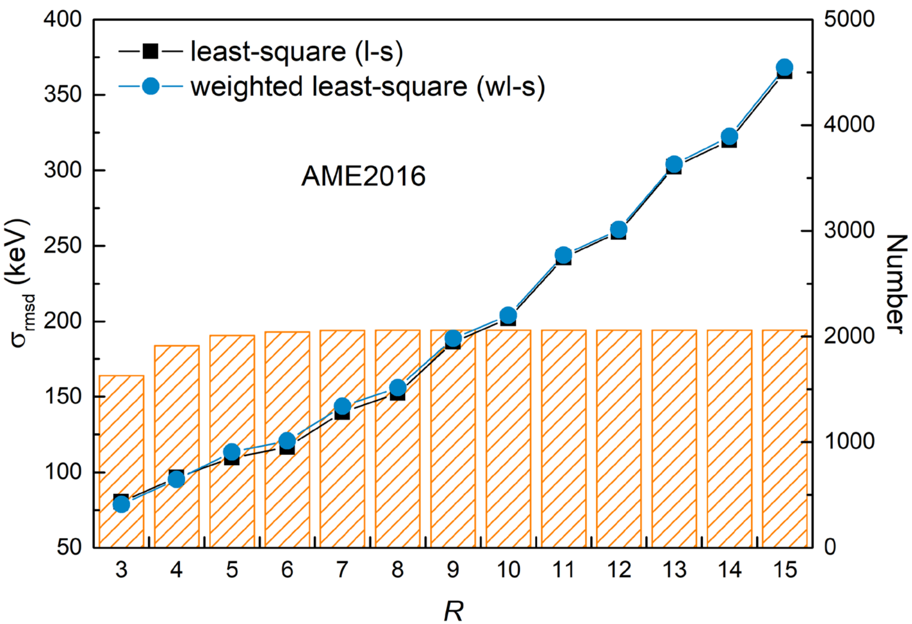
- Alternatively, determine theoretical values by introducing theoretical uncertainties σ_{th} in χ^2 fitting,

$$\min_{p_v} \sum_{i=1}^{n} \frac{\left(M_{\mathrm{exp}}^{i} - M_{\mathrm{th}}^{i}\right)^2}{{\sigma_{\mathrm{exp}}^{i}}^2 + {\sigma_{\mathrm{th}}}^2} \longrightarrow \sum_{i=1}^{n} \frac{M_{\mathrm{exp}}^{i} - M_{\mathrm{th}}^{i}}{{\sigma_{\mathrm{exp}}^{i}}^2 + {\sigma_{\mathrm{th}}}^2} \frac{\partial M_{\mathrm{th}}^{i}}{\partial p_v} = 0, v = 1,2 \ldots m \ ;$$

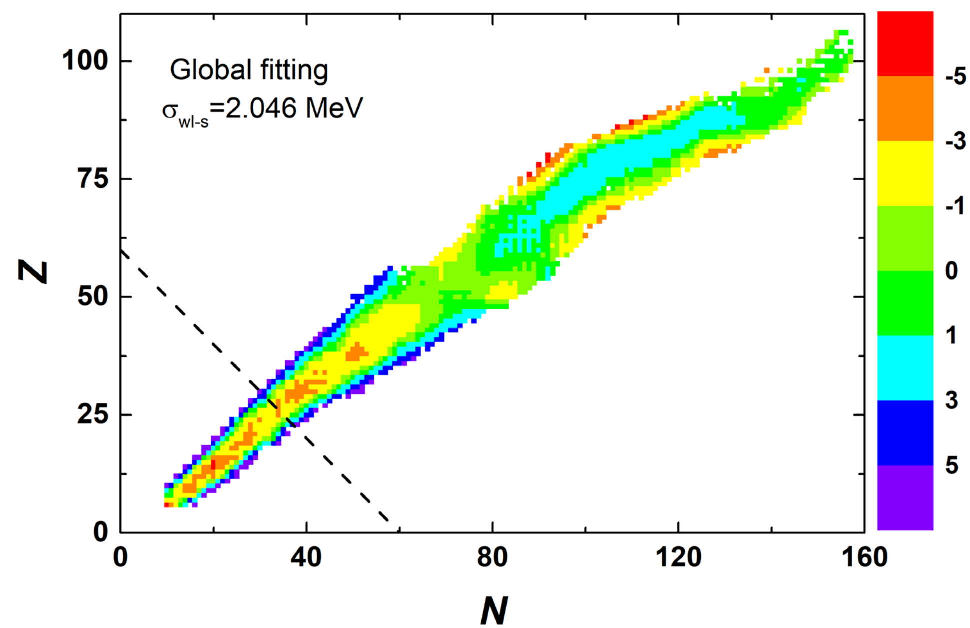
$${\sigma_{\mathrm{th}}}^2 = \frac{\sum_{i=1}^{n} \left({\sigma_{\mathrm{exp}}^{i}}^2 + {\sigma_{\mathrm{th}}}^2\right)^{-2} \left[\left(M_{\mathrm{exp}}^{i} - M_{\mathrm{th}}^{i}\right)^2 - {\sigma_{\mathrm{exp}}^{i}}^2\right]}{\sum_{i=1}^{n} \left({\sigma_{\mathrm{exp}}^{i}}^2 + {\sigma_{\mathrm{th}}}^2\right)^{-2}} .$$

*[P. Möller and J. R. Nix, At. Data Nucl. Data Tables **59**, 185 (1995)]*

Description of AME2016 Database



$$\lim_{R\to\infty} M_{\mathrm{exp}} - M_{\mathrm{wl-s}}$$



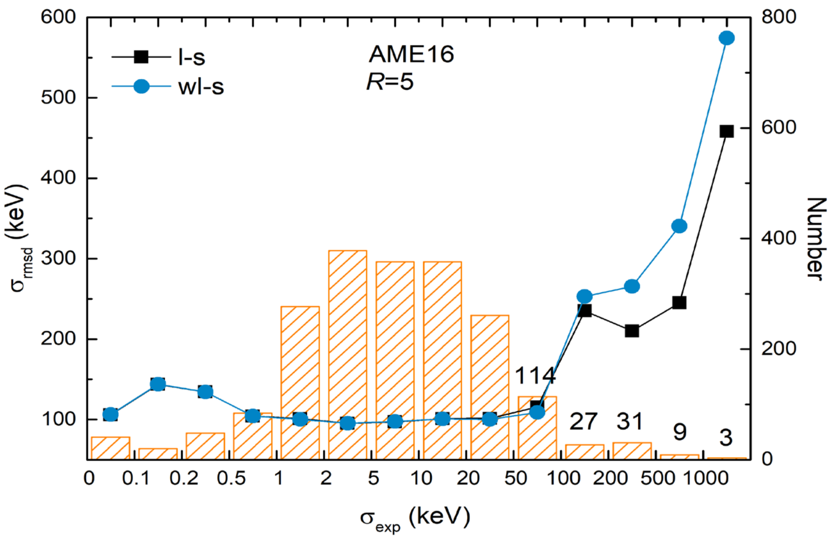
R=2 :

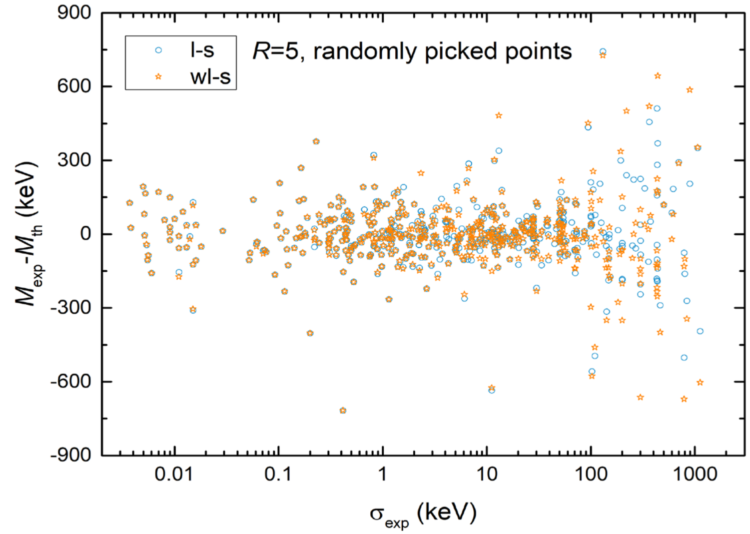
		1		
	2	3	4	
5	6	●	7	8
	9	10	11	
		12		

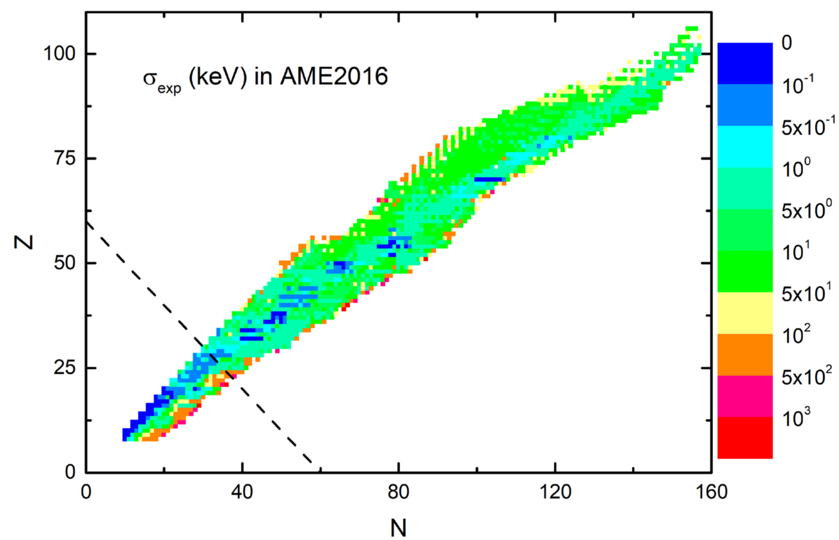
$$N_{\mathrm{para}} = 5+5+2 = 12 = N_{\mathrm{input}}$$

- R increases → Systematic deviation between theoretical and experimental masses generally increases;
- The theoretical values with minimal R is recommended (at least R=3).

Description of AME2016 Database

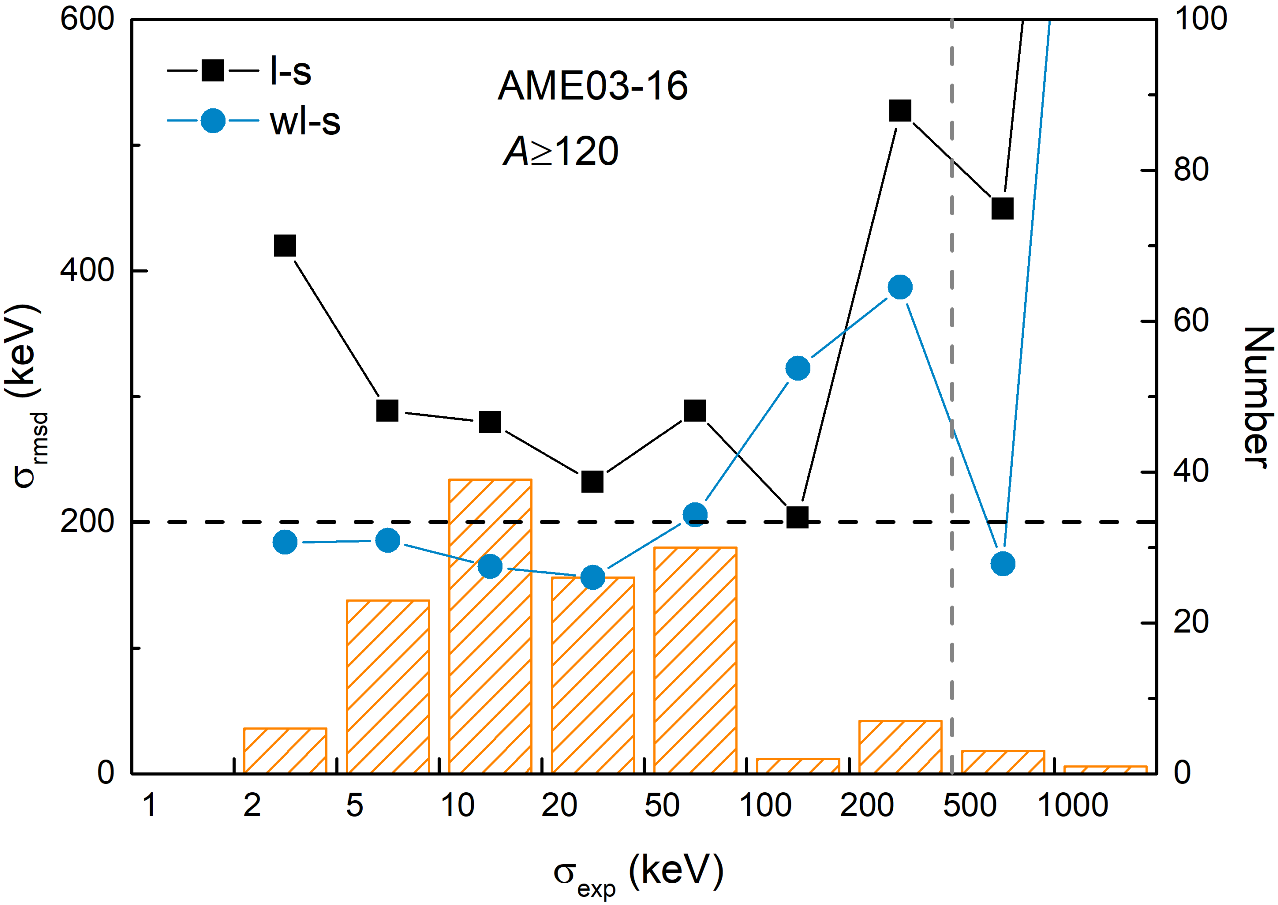




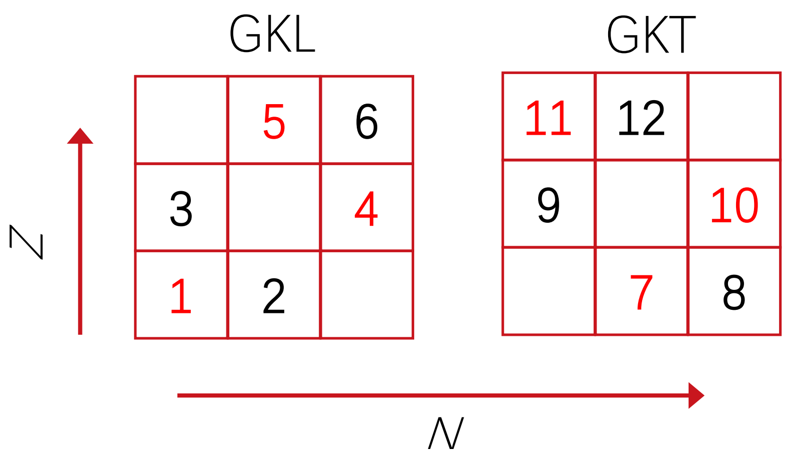


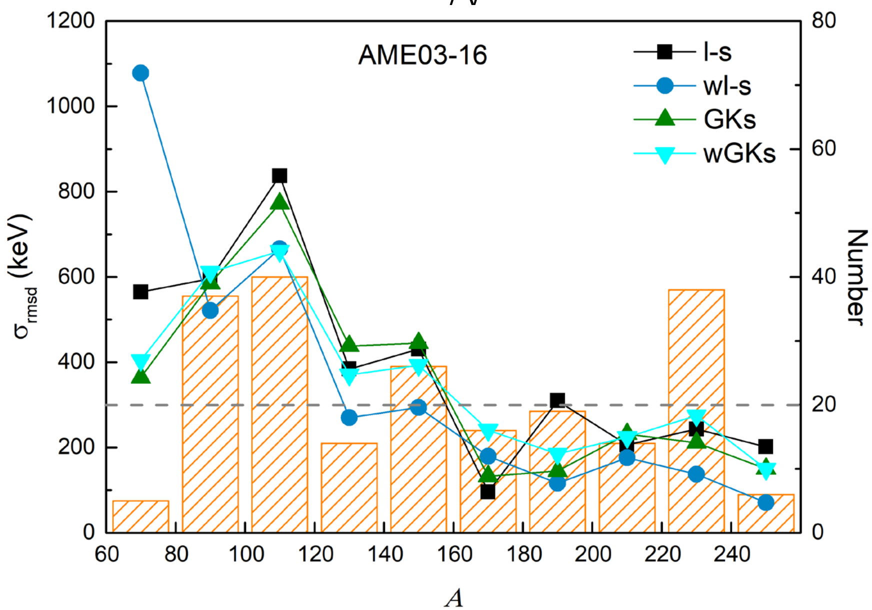
- Major differences on theoretical masses from least-square fitting and χ^2 fitting occur for nuclei with $\sigma_{\mathrm{exp}} > 50$ keV;
- Most cases are located on the border of the known region;
- Two fitting procedures may be quite different in case of extrapolation.

Extrapolation from AME2003 to AME2016



Extrapolation from AME2003 to AME2016





- GKs: take average value as final theoretical mass,

$$M_{th}(N,Z) = \sum_{i=1}^{n} M_{th}^{i}(N,Z)\,/n\ .$$

[Phys Rev C. 77. 041304 (2008)]

- wGKs: take weighted average value as final theoretical mass,

$$M_{\rm th}(N,Z) = \frac{\sum_{i=1}^{n} M_{\rm th}^{i}(N,Z)\times\omega_i}{\sum_{i=1}^{n}\omega_i}\ ,$$

$$\omega_i = 1/\sigma_i^2 = 1/({\sigma_{\rm th}^{i}}^{2} + {\sigma_{\rm exp}^{i}}^{2})\ ;$$

- $\sigma_{\rm abs} = \sum_{i=1}^{n} \frac{|M_{\rm exp}^{i}(N_i,Z_i) - M_{\rm exp}^{i}(N_i,Z_i)|}{n}\ .$

A⩾120	l-s	wl-s	ratio	GKs	wGKs	ratio
$\sigma_{\rm abs}$ (keV)	226	143	36.9%	216	218	-1%
$\sigma_{\rm rmsd}$ (keV)	300	198	33.9%	289	290	-0.5%

Mass relations based on residual neutron-proton interactions

- Total n-p interactions between the last i neutron(s) and the last j proton(s) are defined as

$$\delta V_{in-jp} = M(N,Z) - M(N-i,Z) - M(N,Z-j) + M(N-i,Z-j) \ .$$

- Empirical δV_{in-jp} formulas:

$$\delta V^{\rm cal}_{1n-1p}(N,Z) = \overline{\delta V^{\rm cal}_{1n-1p}(A)} + \Delta_{\rm sh}(N,Z) \ ,$$

$$\delta V^{\rm cal}_{2n-1p}(N,Z) = \overline{\delta V^{\rm cal}_{2n-1p}(A)} + \Delta_{\rm sh}(N,Z) + \Delta_{\rm sh}(N-1,Z) \ ,$$

$$\delta V^{\rm cal}_{1n-2p}(N,Z) = \overline{\delta V^{\rm cal}_{1n-2p}(A)} + \Delta_{\rm sh}(N,Z) + \Delta_{\rm sh}(N,Z-1) \ ,$$

where

$$\Delta_{\rm sh}(Z,N) = a_{\rm sh} + 2b_{\rm sh}|\delta_p\Omega_N(N_p - \Omega_Z) - \delta_n\Omega_Z(N_n - \Omega_N)| \qquad (3)$$

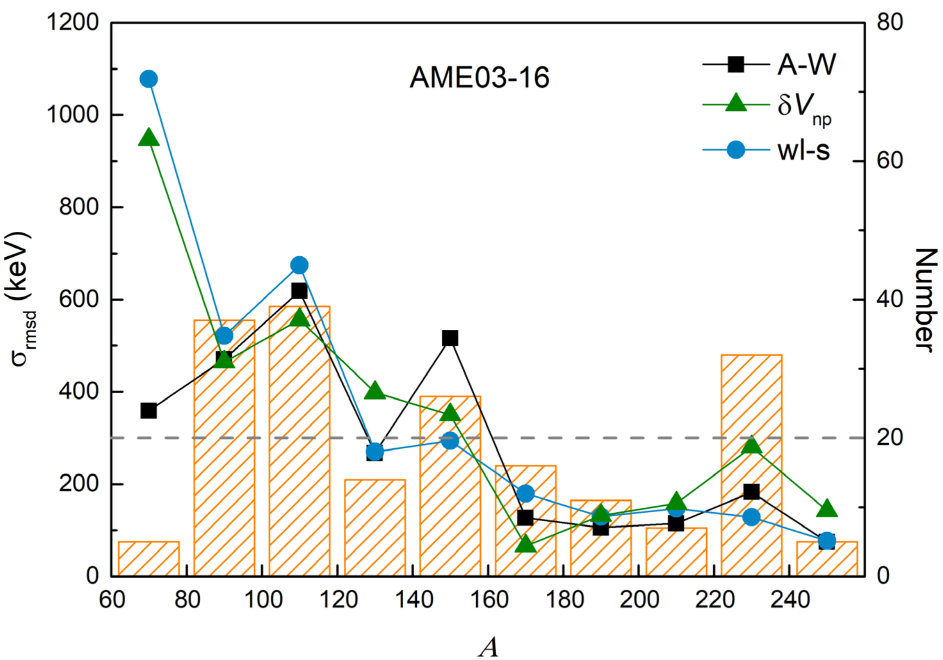
TABLE I. The parameters [in keV, see Eq. (3)] taken in this work for different mass regions. These parameters are obtained via a χ^2 fitting procedure.

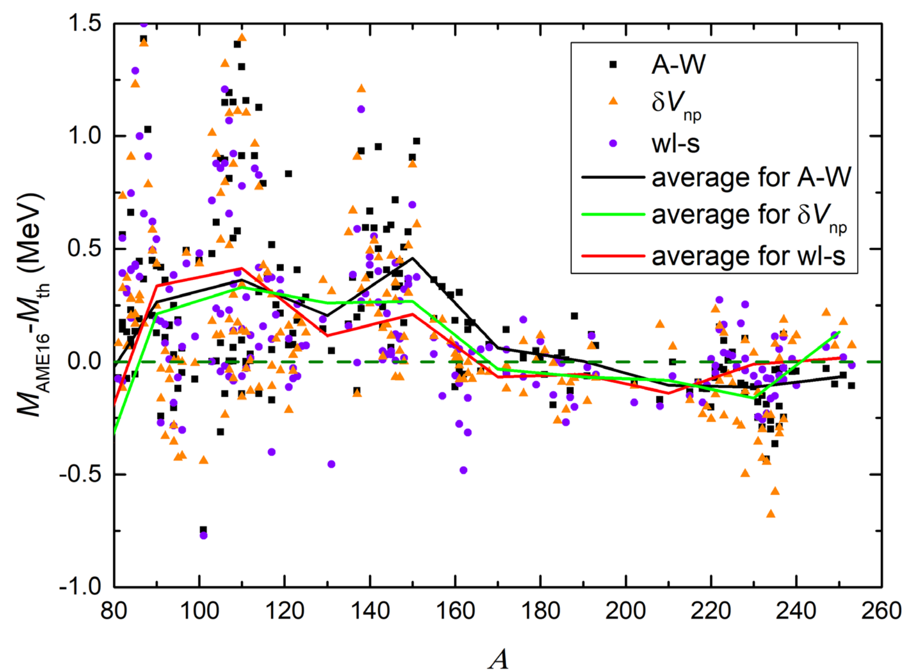
Region	Parameter	Even-A	Odd-A
$Z \in [1, 28)$, $N \in [1, 28)$	$a_{\rm sh}$	28.55	136.7
	$b_{\rm sh}$	−0.3958	−5.138
$Z \in [1, 28)$, $N \in [28, 50)$	$a_{\rm sh}$	7.372	45.74
or $Z \in [28, 50)$, $N \in [1, 28)$	$b_{\rm sh}$	−0.628	−0.1966
$Z \in [28, 50)$, $N \in [28, 50)$	$a_{\rm sh}$	141.3	−177.2
	$b_{\rm sh}$	−0.6086	0.8863
$Z \in [28, 50)$, $N \in [50, 82)$	$a_{\rm sh}$	59.26	7.282
or $Z \in [50, 82)$, $N \in [28, 50)$	$b_{\rm sh}$	−0.2223	−0.0007
$Z \in [50, 82)$, $N \in [50, 82)$	$a_{\rm sh}$	129.2	−84.88
or $Z \in [28, 50)$, $N \in [82, 126)$	$b_{\rm sh}$	−0.2666	0.1337
$Z \in [50, 82)$, $N \in [82, 126)$	$a_{\rm sh}$	60.64	107.9
or $Z \in [82, 126)$, $N \in [50, 82)$	$b_{\rm sh}$	−0.1124	−0.2617
$Z \in [82, 126)$, $N \in [82, 126)$	$a_{\rm sh}$	11.37	18.81
or $Z \in [50, 82)$, $N \in [126, 184)$	$b_{\rm sh}$	−0.1067	−0.0266
$Z \in [82, 126)$, $N \in [126, 184)$	$a_{\rm sh}$	44.67	−11.25
	$b_{\rm sh}$	−0.1697	0.0499

[H. Jiang, G. J. Fu, et. al., Phys. Rev. C. 85, 054303 (2012)]

- Take the average of 12 possible ways to derive masses.

Extrapolation from AME2003 to AME2016



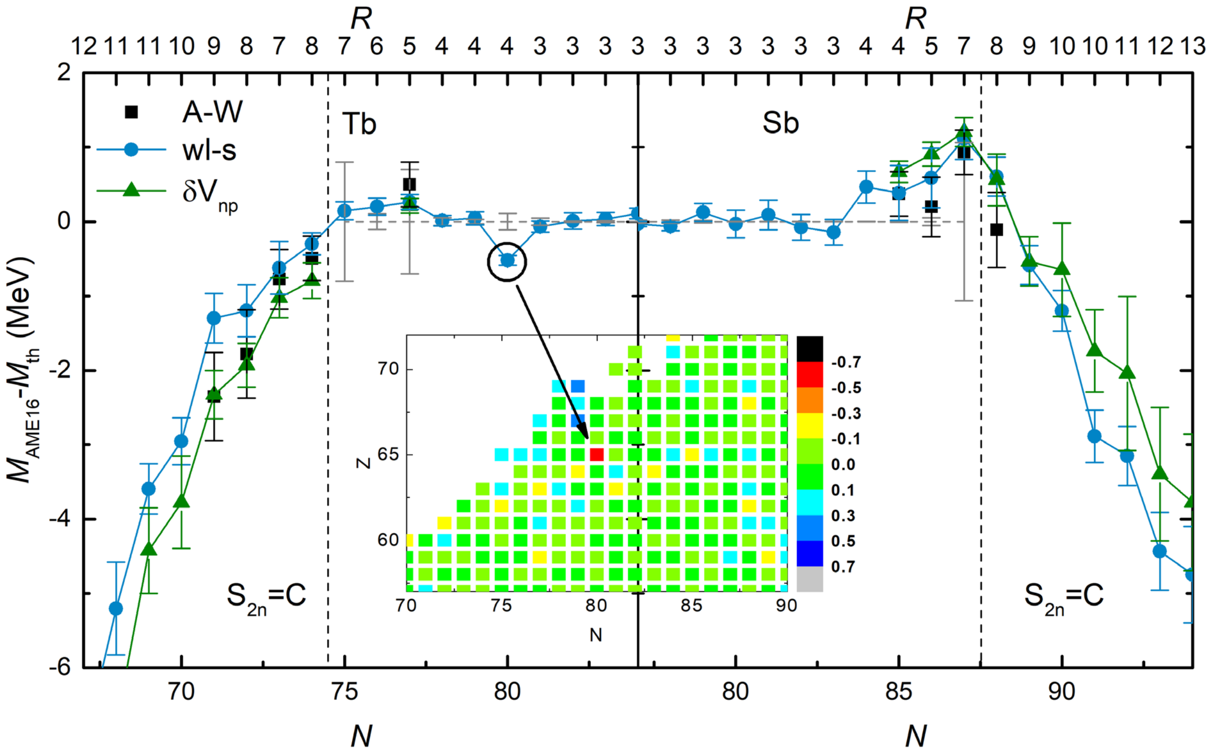


[G. Audi, A.H. Wapstra, and C. Thibault, Nucl. Phys. A 729, 337 (2003) ; H. Jiang, et. al., Phys. Rev. C. 85, 054303 (2012)]

A⩾120	A-W	δV_{np}	wl-s
σ_{abs} (keV)	208	206	147
σ_{rmsd} (keV)	291	276	204

- Underestimates at A~140: wl-s < δV_{np} < A-W ;
- Overestimates at A~230: wl-s < A-W < δV_{np} .

Extrapolation from AME2003 to AME2016



- Abnormal cases: ^{138}Sb & ^{145}Tb;
- Expansion of reference masses: keep S_{2n} invariant;
- R increases as prediction moves away from known region;
- Predictions within two or three steps are generally reliable.

Comparison with various models

For AME03-16

For AME12-16

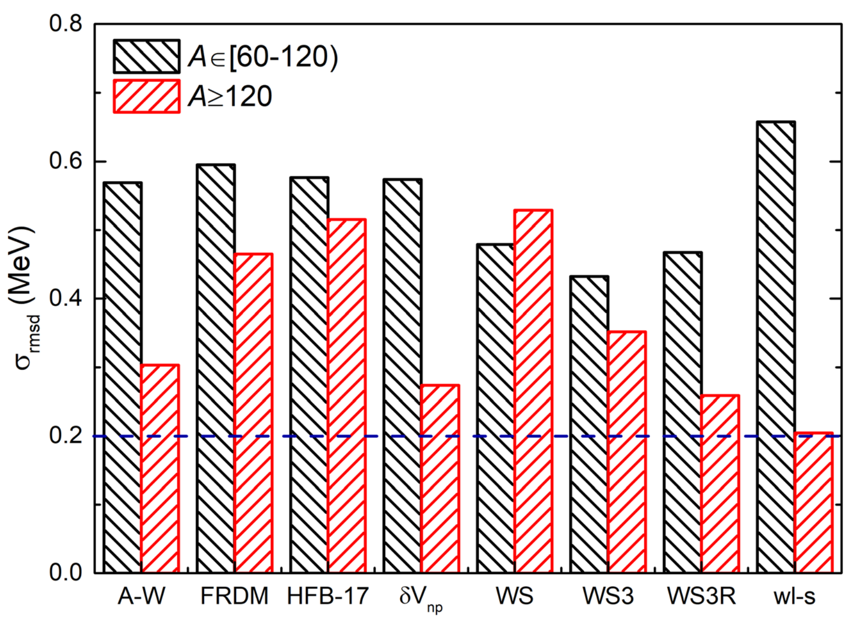


TABLE I: Predicted mass excesses and their uncertainties (in keV) predicted by Audi-Wapstra (A-W) extrapolation [19], by Bao *et al.* [17], by Jiang *et al.* [29], WS4+RBF [9], WS4+RBFoe [30] and this work, respectively, for the nuclei with $A \geqslant 120$, from the AME2012 database [19] to the AME2016 database [20]. The last row present the RMSD (in keV) of the 21 calculated masses in this Table with and without consideration of ^{138}Sb, given outside and inside the bracket, respectively.

Element	AME2016	A-W	Bao *et al.*	Jiang *et al.*	WS4+RBF	WS4+RBFoe	this work
^{121}Rh	-56250 ± 619	-56430 ± 298	-56390 ± 190	-56325 ± 144	-55859	-56113	-56325 ± 149
^{123}Pd	-60430 ± 789	-60417 ± 196	-60322 ± 199	-60531 ± 192	-60391	-60151	-60276 ± 128
^{129}Cd	-63058 ± 17	-63509 ± 196	-63569 ± 124	-63638 ± 96	-63646	-63508	-63338 ± 194
^{131}Cd	-55219 ± 102	-55331 ± 196	-54984 ± 159	-55822 ± 170	-55385	-55390	-54954 ± 363
^{138}Sb	-54220 ± 1064	-54539 ± 298	-54521 ± 157	-54552 ± 117	-54493	-54572	-54653 ± 65
^{141}I	-59927 ± 16	-59904 ± 196	-59951 ± 135	-59930 ± 100	-59882	-59832	-59943 ± 78
^{149}Ba	-53120 ± 438	-53021 ± 196	-53171 ± 149	-52947 ± 395	-53069	-52986	-53153 ± 154
^{150}La	-56130 ± 435	-56383 ± 196	-56432 ± 136	-56337 ± 174	-56299	-56538	-56450 ± 144
^{151}La	-53310 ± 435	-53729 ± 196	-53472 ± 224	-53275 ± 153	-53701	-53564	-53238 ± 121
^{137}Eu	-60146 ± 4	-60119 ± 196	-60100 ± 94	-59998 ± 94	-60147	-60001	-60145 ± 96
^{190}Ti	-24372 ± 8	-24379 ± 50	-24416 ± 83	-24410 ± 56	-24431	-24328	-24376 ± 111
^{215}Pb	4342 ± 52	4416 ± 101	4466 ± 114	4499 ± 66	4328	4296	4456 ± 68
^{194}Bi	-16029 ± 6	-16036 ± 51	-15958 ± 85	-15957 ± 56	-16167	-16004	-15957 ± 62
^{198}At	-6715 ± 6	-6721 ± 51	-6659 ± 87	-6636 ± 60	-6872	-6696	-6715 ± 69
^{197}Fr	10254 ± 54		10488 ± 145	10441 ± 117	10282	10197	10334 ± 60
^{198}Fr	9574 ± 32		9613 ± 105	9597 ± 90	9184	9523	9514 ± 84
^{202}Fr	3096 ± 7	3092 ± 51	3140 ± 91	3123 ± 69	2876	3126	3030 ± 51
^{232}Fr	46073 ± 14	45986 ± 155	45984 ± 114	46091 ± 71	46030	46146	45941 ± 57
^{233}Fr	48920 ± 20	49034 ± 298	48894 ± 132	48907 ± 107	49062	48966	48898 ± 48
^{201}Ra	11937 ± 20	11841 ± 106	11950 ± 94	12033 ± 100	11820	11981	11970 ± 73
^{205}Ac	14107 ± 51		13940 ± 105	14049 ± 119	13973	13980	14032 ± 62
^{206}Ac	13479 ± 50	13462 ± 71	13446 ± 103	13392 ± 94	13250	13432	13376 ± 82
^{215}U	24923 ± 88		24917 ± 154	25184 ± 128	25212	25034	24817 ± 62
^{216}U	23066 ± 28		23191 ± 123	23283 ± 130	23118	23235	23072 ± 56
^{221}U	24520 ± 51	24483 ± 102	24498 ± 111	24468 ± 88	24546	24485	24541 ± 107
^{222}U	24273 ± 52	24222 ± 101	24204 ± 98	24292 ± 89	24321	24257	24235 ± 105
^{219}Np	29457 ± 88	29277 ± 196		29606 ± 249	29316	29391	29115 ± 154
^{229}Am	42150 ± 87		41891 ± 199	41912 ± 170	42148	42128	42168 ± 170
^{259}No	94079 ± 7	94111 ± 100	94107 ± 93		93995	93986	94121 ± 60
RMSD (keV)		175 (164)	169 (160)	216 (209)	215 (212)	189 (177)	158 (130)

- wl-s yields smallest σ_{rmsd} compared with various models in the market, in both cases of AME03-16 and AME12-16, for $A \geq 120$.

Summary

- The processing of experimental errors in local mass relations may need to be reconsidered;
- A new method to predict atomic masses based on the GK relations is constructed by considering experimental uncertainties;
- Its predictive power is exemplified in comparison with other previous models for $A \geq 120$.
- Unsolved problems:
  - How far can we predict;
  - Application to the prediction of α-decay energies for superheavy nuclei.

Thank you！