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The evaluation of Q_α based on experimental masses and other properties of atomic nuclei

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Abstract

The specially interesting experimental value, in the nuclear physic, describing the alpha decay is the decay energy Q_α. This energy is a key to understanding the series of nuclei disorders. On the basis of decay energy we may compute sequential masses and energy of unstable nuclides. Because alpha is the helium element, thus from a nucleus with N neutrons and Z protons after the alpha decay we obtain a nucleus with *N-2* and *Z-2* protons and neutrons, respectively. It is natural to compute Q_α as a difference between the mass of nuclei with N neutrons and Z protons and masses obtained after decay i.e. the mass of nuclei with N-2 neutrons and Z-2 protons and the mass of helium element. We tested this known "classical" formula based on a large collection of the newest experimental data, the so called AME2012 and NUBASE2012 data bases. We computed accurate constants in the "classical" formula. Additionally, we showed inadequacy of the "classical" model. The almost three times better model is the one based on a neutral network (named in paper MSN) but we prefer slightly better (in comparison with MSN) the nonlinear regression model (named MQT). MQT is the development of the "classical" method taking additionally into account the terms with separation energy neutrons and protons multiplied by multinomials of numbers of neutrons N and protons Z, respectively. In the paper we show how the mentioned above methods may be used to prediction of unknown values of Q_α. All computations were made in language R.

Keywords: atomic mass, data mining, energy, nucleons, R language, regression.

Oszacowanie Q_α na podstawie eksperymentalnie wyznaczonych mas i innych własności jąder atomowych

Streszczenie

Szczególnie interesującą wielkością w fizyce jądrowej jest energia rozpadu cząstki alfa. Wielkość ta umożliwia odtworzenie mas i energii jąder szybko zmieniających się w przemianach jądrowych pierwiastków. Ponieważ cząstka alfa jest jądrem atomu helu, więc z jądra o N neutronach i Z protonach otrzymujemy po przemianie jądro o *N-2* neutronach i *Z-2* protonach oraz jądro atomu helu. Dlatego naturalne jest szacowanie energii Q_α jako różnicy mas jądra przed przemianą i jądra po przemianie wraz z masą atomu helu. Jest to tzw. "klasyczny" sposób obliczania energii Q_α. Na podstawie dużego zbioru nowo uzyskanych eksperymen-

talnych wyników (bazy danych AME2012 I NUBASE2012) chcielibyśmy w tej pracy zweryfikować "klasyczny" sposób obliczania Q_α. Obliczymy dokładniej stałe występujące w "klasycznym" wzorze a potem pokażemy, że niektóre inne metody dają zdecydowanie mniejszy błąd niż wspomniana "klasyczna" metoda. W szczególności opiszemy sieci neuronowe (MSN) oraz przedstawimy preferowaną przez nas metodę MQT opartą na nieliniowej regresji. MQT może być traktowana jako rozwinięcie "klasycznej" metody poprzez uwzględnieni dodatkowo członów z energiami separacji protonów i neutronów pomnożonych przez odpowiednie wielomiany od liczby protonów i neutronów. Dodatkowo pokażemy jak te wszystkie metody służą do prognozowania nieznanych wartości Q_α. Wszystkie obliczenia wykonaliśmy w języku R.

Słowa kluczowe: „data mining", energia, język programowania R, masa atomowa, nukleony, regresja.

1. Introduction

Nuclear Physics started a little bit more than 100 years ago. Since then, scientists have accumulated a huge amount of data for a large number of nuclides. Today there are about 2830 nuclei that have been observed. It is estimated that the total number of nuclei which may be obtained by experimenters is from 6000 to 7000 [16, 2].

Thus, there exists today a huge number of experimental data on the atomic nucleus that need to be interpreted, sorted, treated in a homogeneous way, while keeping traceability of the conditions under which they were obtained.

There are a lot of experimental data characterizing the atomic nucleus, for example, nuclear ground-state masses and radii, magnetic moments, half-lives, spins and parities of excited and ground-state, their decay modes and the relative intensities of these decays, the deformations and many others.

In papers [1, 14], the so-called AME2012 and NUBASE2012 data present the results of the most recent data that contain full information on nuclear experimental data. The tables contain values and their uncertainties for all experimentally known nucleus as a function of the mass number A, the number of protons Z or neutrons N.

The investigators believe that there must exist some dependencies between these characteristics of the atomic nucleus, which are unknown due to the poorly understood nuclear forces.

The aim of this study is to use data mining methods and artificial intelligence to attempt to discover these unknown rules. It is out of the scope of the present publication to cover all aspects of nuclear properties and nuclear data. Therefore we will focus on the disintegration of nuclei, in particular the alpha decay and its decay energy. These measurements of Q_α are very important because they allow identifying unknown nuclei formed in the reaction of synthesis and determining masses of unstable or very unstable nuclides.

2. Theory

Most of the heavy or superheavy nuclei may disintegrate by emitting an α particle, the nucleus of a helium atom. In nuclear physics the basic property of α disintegration, the so-called energy decay Q_α, has been defined by the following formula:

$$Q_\alpha(Z, N) = M(Z, N) - M(Z - 2, N - 2) - M(_2^2 He), \quad (1)$$

where Z is the atomic number, N the neutron number, and $_2^2 He$ is the helium element (α particle). For the semi-classical drop model [8], the mass of nucleus can be given by the formula:

$$M(Z, N) = a_V(Z + N) + a_S(Z + N)^{\frac{2}{3}} + a_C(Z + N)^{\frac{1}{3}} + a_T \frac{(Z - N)^2}{Z + N}, (2)$$

with absolute constants a_V, a_S, a_C and a_T which may be interpreted as phenomenological parameters. These parameters are adjusted to the known experimental masses of nuclei by minimizing the mean square error [17]. On the other hand, we can find new data bases with the last experimental results of various properties of atomic nuclei [1, 14].

In this paper we draw on the latest experimental data [1, 14] and use the advanced statistical algorithms in language R [3, 15, 12, 13] (some algorithms were made in R but on the programing platform Statistica [5]), neural of networks [4, 6, 7, 10, 11] and data mining [9] we want:

(i). Check the formula of the Q_α (1) on a large set of data.
(ii). Give the new models in order to compute Q_α and compare these models with the one from (1).
(iii). Compute the more accurate coefficients a_V, a_S, a_C and a_T.
(iv). Give the best, in our opinion, two methods to compute Q_α and show how to predict this value on he basis of other known values.

In our paper, if x denotes some values (field of data base) [1, 14] then by ∂x we denote the error of measurement x (always nonnegative), taken from the same data base. Furthermore, under the evaluation the attribute $Y = \{y_1, y_2, \cdots y_n\}$ on the basis of attributes $X_k = \{x_{k,1}, x_{k,2}, \ldots x_{k,n}\}, 1 \le k \le m, n \ge 1$, by the function $f(X_1, X_2, \ldots X_m)$ we introduce the following types of errors:

$$SE = \sqrt{\frac{\sum_{i=1}^n (y_i - f(x_{1,i}, \ldots, x_{m,i}))^2}{n}}, \quad QE = \sqrt{\frac{\sum_{i=1}^n \omega_i (y_i - f(x_{1,i}, \ldots, x_{m,i}))^2}{\sum_{i=1}^n \omega_i}},$$

where $\omega_i = \frac{1}{1 + (\partial y_i)^2}, 1 \le i \le n$. The SE error is the usual mean square error, whereas QE error takes into account the error of measure of Y and "forces" a smaller absolute error for the big values of ∂y_i.

The linear regression in R language is tested by commands

```
model=tryCatch(step(lm(formula[[j]], data=data1,
    weight=(data.frame(data1))$waga, na.action=na.omit),
    direction=typ), error=function(x) NA)
```

for typ=c('backward', 'forward', 'both') and formula taken from list formula. Different transformations of variables, nonlinear regression models, splines (function polymars from library polspline) were considered. Similarly the different neural networks models were considered (from packages neuralnet, nnet, RNSSN,

AMORE) but the significantly better one was Mulitilayer Perceptron with one hidden layer. The data in neural network models were randomly divided into learning, testing and validation parts with the proportion *70:15:15*.

3. Classical result

Putting $A = N + Z$ from (1) we have

$$Q_\alpha = 4a_V - M(_2^2 He) + a_S[A^{2/3} - (A - 4)^{2/3}]$$

$$+ a_C[\frac{Z^2}{A^{1/3}} - \frac{(Z - 2)^2}{(A - 4)^{1/3}}] + a_T(2Z - A)^2[\frac{1}{A} - \frac{1}{A - 4}], \quad (3)$$

We consider two models of (1) with the same coefficients a_V, a_S, a_C and a_T in formula *M(Z,N)* and *M(Z-2,N-2)* (named M2Q) as well as with, maybe, different values of constants (model M1Q). These models may be written in R as:

M1Q: Qa~I(A^(2/3))+I(Z*Z/A^(1/3))+I((Z+Z-A)^2/A)+A+I((A-4)^(2/3))
    +I((Z-2)*(Z-2)/(A-4)^(1/3))+I((Z+Z-A)^2/(A-4))
M2Q: Qa~I(A^(2/3)-(A-4)^(2/3))+I(Z*Z/A^(1/3)-(Z-2)*(Z-2)/(A-4)^(1/3))
    +I((Z+Z-A)^2*(1/A-1/(A-4))).

The computed linear regression coefficients method M2Q with SE and QE error, respectively, are:

Tab. 1. Współczynniki regresji dla metod M2QSE i M2QQE
Tab. 1. Regression coefficients of M2QSE and M2QQE methods

constants	SE	QE
$4a_v$-M($_2^2$He)	-38902,076	-36848,977
a_s	22840,074	20495,654
a_c	736,733	721,935
a_t	17135,851	17985,034

The exact analysis of behavior of Q_α leads to the following conclusions

(i). The Q_α behavior is irregular in the area of "the so called" magical numbers Z and N. These numbers are: *2,8,20,40,52,82,114,126,152*. Therefore we consider different models for the different intervals of Z and N (between sequential magical numbers) and denote this model by 'M' (the all values model is named *).

(ii). There are essentially different behaviors of Q_α dependent on parity Z and N, and therefore it should be considered as different models in cases 'Z even-N even', 'Z odd-N even', 'Z even - N odd' and 'Z odd-N odd' named by 'P (the model with all values with respect parity is named *).

The irregular behavior in the neighborhood of magical numbers effects considerations with elimination of magical numbers (named *m(0)*) elimination of magical numbers and *±2* magical numbers (*m(0,2)*) and considerations without elimination (*none*). The results are given in the following table:

Tab. 2. Błędy metod M1Q i M2Q
Tab. 2. Errors of methods M1Q and M2Q

deleted	M1Q				M2Q			
	/	P/*	*/M	P/M	*/*	P/*	*/M	P/M
SE error								
m(0,2)	1125	1119	468	401	1127	1123	623	605
m(0)	1266	1264	489	402	1273	1271	666	641
none	1284	1283	536	468	1291	1290	761	740
QE error								
m(0,2)	1228	1130	558	367	1592	1165	697	589
m(0)	1413	1376	548	411	1746	1396	699	633
none	1401	1369	538	439	1727	1368	743	696

There is no significant difference between methods M1Q and M2Q, therefore we reject M1Q in further considerations.

The conclusion on using the classical model is rather negative, the errors are worse than those for most of linear and nonlinear regression models as well as worse than for neural network models. In the later considerations model M2Q** with SE error will be denoted shortly as M2Q.

4. Neural networks

As mentioned in the introduction, the best obtained by us neural network was Mulitilayer Perceptron (MLP) with one hidden layer. However, taking into account the classical model and the fact that MLP is a linear combination of data we add to considerations the input values:

$$A^{\frac{2}{3}}, \; \frac{Z^2}{A^{\frac{1}{3}}}, \; \frac{(Z-N)^2}{A}, \; (A-4)^{\frac{2}{3}}, \; \frac{(Z-2)^2}{(A-4)^{\frac{1}{3}}}, \; \frac{(N-Z)^2}{A-4}$$

and additionally

$$\frac{S_p}{Z}, \; \frac{S_{2p}}{Z}, \; \frac{S_n}{N}, \; \frac{S_{2n}}{N}.$$

The SE errors are as follows:

Tab. 3. Wpływ danych wejściowych na błąd osiągany w regresyjnych sieciach neuronowych
Tab. 3. The influence of a set of dependent variables on the regression error

Attributes	MLP	Function		SE error			
		Activation	output	learning	validation	testing	all
all variables	59-11-1	Logist	Tanh	144	218	232	172
N,Z,S_p,S_{2p},S_n,S_{2n}	6-4-1	Tanh	Linear	225	218	209	221
N,Z,S_p,S_{2p}	4-5-1	Tanh	Linear	680	683	717	686
S_p,S_{2p},S_n,S_{2n}	4-5-1	Tanh	Linear	271	266	266	269
N,Z,S_n,S_{2n}	4-3-1	Tanh	Tanh	638	725	612	648
V_1	16-5-1	Tanh	Linear	193	204	224	200
V_2	11-6-1	Logist	Linear	196	197	229	201

where

$$V_1 = \{A, Z, A^{\frac{2}{3}}, \frac{Z^2}{A^{\frac{1}{2}}}, \frac{(Z-N)^2}{A}, (A-4)^{\frac{2}{3}}, \frac{(Z-2)^2}{(A-4)^{\frac{1}{3}}}, \frac{(Z+Z-A)^2}{A-4}, \frac{S_p}{Z}, \frac{S_{2p}}{Z},$$
$$\frac{S_n}{N}, \frac{S_{2n}}{N}, S_p, S_{2p}, S_n, S_{2n}\},$$
$$V_2 = \{A^{\frac{2}{3}} - (A-4)^{\frac{2}{3}}, \frac{Z^2}{A^{\frac{1}{3}}} - \frac{(Z-2)^2}{(A-4)^{\frac{1}{3}}}, (2Z-A)^2 \left(\frac{1}{A} - \frac{1}{A-4}\right), \frac{S_p}{Z},$$
$$\frac{S_{2p}}{Z}, \frac{S_n}{N}, \frac{S_{2n}}{N}, S_p, S_{2p}, S_n, S_{2n}\}$$

The results suggest that only values N, Z, S_p, S_{2p}, S_n, S_{2n} influencing Q_α and S_p, S_{2p}, S_n, S_{2n} are more valid than N,Z. Thus, we show the details of the second neural network (MLP 6-4-1) named later shortly MSN in Tables 4 and 5.

Tab. 4. Normalizacja parametrów wejściowych i wyjściowych
Tab. 4. Normalization parameters of input and output variables

Atribute	Normalization	
	a (scale)	b (shift)
N	0.007143	−0.114286
Z	0.010870	−0.108696
S_{2p}	0.000039	−0.277989
S_{2n}	0.000025	−0.005009
S_n	0.000060	−0.091422
S_p	0.000045	0.044568
Q_α	0.000038	0.630633

Tab. 5. Wagi neuronów sieci MSN
Tab. 5. Weights of neurons of MSN net

Input	Neurons			
	1	2	3	4
$\tilde{N}$	−0.1702845	2.8351736	2.5576550	−0.0256944
$\tilde{Z}$	0.6673700	−2.9450580	−1.6933664	1,2119331
$\tilde{S}_{2n}$	−0.5528986	2.4523362	2.3518647	−1.4032433
$\tilde{S}_{2p}$	−0.3981826	1.4650598	2.1776523	−0.8225645
$\tilde{S}_n$	0.1367833	0.1220575	0.4165193	0.1887259
$\tilde{S}_p$	0.1020960	−0.0471798	0.1826506	0.1586468
Shift	0.4674285	−1.0865727	−2.0792817	1.5757171
Hidden Layer	Output Q_α			
Neuron1	2.9573116			
Neuron2	0.7683365			
Neuron3	−0.8355626			
Neuron4	−1.7641578			
Shift	0.8049652			

The activation input function is a hyperbolic tangent, whereas the output activation function is identity (linear). The neutral network considered here gives SE error 230,93, whereas QE error is only 352,27. So we can draw the following conclusions:
1. All models of neural networks give SE error in the interval *(172, 221)*.
2. There is no significant improvement if we omit magical values Z and N as well values ±2 with magical values.
3. Terms which arise in formula (3) are significant for building neural networks.

5. Model MQT

Furthermore, we try MARSplines methods (with SE error between 320 and 652) and different nonlinear regression methods (with SE error greater 370) and linear regression. Considering the linear regression methods we remark that each method using values S_p, S_{2p}, S_n, S_{2n} is significantly better than the methods without those values. The significant values are Z and N, too. The better methods are considered for parity and magical intervals separately.

Finally, we return to the classical model (1) with the correction. We consider

$$Q_\alpha = M(Z,N) - M(Z-2, N-2) - M(^2_2 He) + W_1(Z)\frac{S_p}{Z} + W_2(Z)\frac{S_{2p}}{Z} + W_3(N)\frac{S_n}{N} + W_4(N)\frac{S_{2n}}{N} \quad (4)$$

where $M(Z,N)$ is given in (2),

$$W_i(x) = a_{i,1}x^2 + a_{i,2}x + a_{i,3}, \quad i = 1,2,3,4.$$

and putting $A=N+Z$ we get

$$Q_\alpha = 4a_V - M(^2_2 He) + a_S \left[A^{\frac{2}{3}} - (A-4)^{\frac{2}{3}} \right] +$$
$$a_C \left[\frac{Z^2}{A^{\frac{1}{3}}} - \frac{(Z-2)^2}{(A-4)^{\frac{1}{3}}} \right] + a_T (2Z-A)^2 \left[\frac{1}{A} - \frac{1}{A-4} \right] + \quad (5)$$
$$W_1(Z)\frac{S_p}{Z} + W_2(Z)\frac{S_{2p}}{Z} + W_3(N)\frac{S_n}{N} + W_4(N)\frac{S_{2n}}{N}$$

with values computed by linear regression:

Tab. 6. Współczynniki modelu MQT**
Tab. 6. Coefficients of model MQT**

Variables	SE	QE
$4a_v$-M($_2^2$He)	44292.524	33748.597
a_S	−29510.666	−29131.425
a_C	0	215.895
a_T	6138.214	10375.032
$a_{1,1}$	0.021	0.001
$a_{1,2}$	−1.916	0
$a_{1,3}$	34.661	0
$a_{2,1}$	−0.011	−0.005
$a_{2,2}$	0	−0.514
$a_{2,3}$	−13.208	0
$a_{3,1}$	0.002	−0.001
$a_{3,2}$	0	0.162
$a_{3,3}$	−5.179	−3.102
$a_{4,1}$	−0.001	−0.001
$a_{4,2}$	−1.096	−0.981
$a_{4,3}$	12.151	11.026

and the errors:

Tab. 6. Współczynniki modelu MQT**
Tab. 6. Coefficients of model MQT**

Deleted	*/*	P/*	*/M	P/M
SE error				
m(0,2)	296	265	197	143
m(0)	339	306	215	148
none	346	316	216	154
QE error				
m(0,2)	458	321	242	133
m(0)	519	390	259	141
none	579	431	259	145

It is better than in the models mentioned in the two previous sections. We have not a place to display the coefficients of the best method MQT (MQTPM- include parity of N and Z and intervals between magic numbers). We only show that in the case of odd $Z \in (82,114]$ and odd $N \in (126,152]$ we obtain the formulae with

$$W_1(Z) = -0.085 * Z^2 + 7.299 * Z, \; W_2(Z) = -0.911 * Z,$$
$$W_3(N) = 2.847 * N^2 - 773.907 * N + 52500.544,$$
$$W_4(N) = -1.183 * N^2 + 321.723 * N - 21922.900, \quad (6)$$
$$4a_V - M(_2^2 He) = 1483379.76, \quad a_S = -2156032.69,$$
$$a_C = -9058.73, \quad a_T = 302192.65.$$

In further considerations model MQTPM will be referred to as MQT.

6. The quality of models

For the residuals in the obtained models we compute correlation and adjacent correlation, values of Fish statistics,VIF coefficients, Durbin-Watson's test, Breusch-Godfrey's test, Goldfeld-Quandt's test, studentized Breusch-Pagan's test, Harrison-McCabe's test and Harvey-Collier's test for the evaluation of quality of fit. Additionally, we investigate the normality of residuals by Shapiro-Wilk's test, Lilliefors (Kolmogorov-Smirnov) test, Anderson-Darling's test, Shapiro-Francia's test and Cramer-von Misses test. The tests mentioned above may be found in libraries: stats, car,

perturb, lmtest, nortest, lawstat of language R. All the results for all methods are good except for, may be, the big values of VIF coefficients for some variables. However, the omitting of some independent variables (indicated by factor methods) does not give a significantly better model. Furthermore, there are big correlation coefficients between the dependent variables (even for all variables). The dependence of these variables is physically obvious. Factor analysis shows the validation Z, *MASS, N, S_{2p}, S_p, MASS-EXCESS, S_{2n}, S_n* in order to compute Q_α but the great role is played by values S_{2p}, S_p, S_{2n}, S_n of the elements with *N'=N-2, Z'=Z-2*. This suggests the correctness of classical methods M1Q, M2Q and method MQT. The mentioned analysis shows that variables *MASS* and *MASS-EXCESS* play a great role in areas of extremely big and small N or Z. The small numbers of observations in these areas suggest unstable behaviour of regressions methods, which in consequence needs the bigger values of variables. The illustration of error behaviour of methods M2Q, MSN and MQT is presented in Figures 1 and 2.
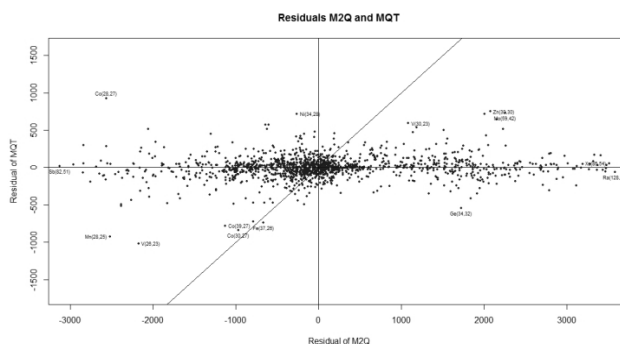
Rys. 1. Reszty metod M2Q i MQT
Fig. 1. Residuals of methods M2Q and MQT
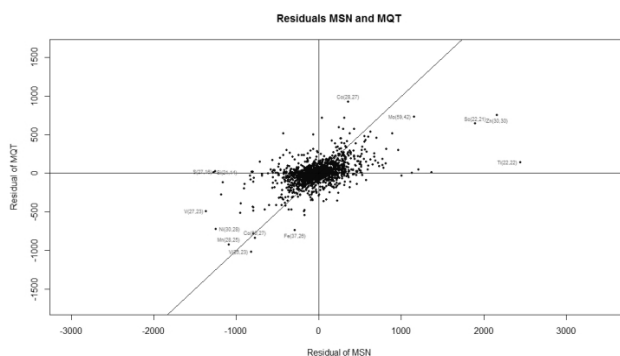
Rys. 2. Reszty metod MSN i MQT
Fig. 2. Residuals of methods MSN and MQT

As it is shown, the residuals of M2Q lie "higher" than those of MQT, which confirms that the method M2Q is significantly worse. The second figure shows that the method MSN is not significantly worse than MQT. The worst cases (Co(28,27), Sc(22,21), Sn(82,50), Sn(81,50), Ti(22,22), Mo(59,42), Ti(28,22)) suggest connection with the magical numbers N or Z.

7. Prediction of unknown values Q_α

Example 1.

Let us consider the element Fr (N=139, Z=87). It is easy to check that $S_{2n}=10421.32$, $S_{2p}=14911.64$, $S_n=4514$, $S_p=6471.99$ whereas Q_α is not obtained in experiments.

M2Q: Because in this case $A=N+Z=226$ and

$$A^{2/3} - (A-4)^{2/3} = 0.4391,$$
$$\frac{Z^2}{A^{1/3}} - \frac{(Z-2)^2}{(A-4)^{1/3}} = 49.3922,$$
$$(2Z-A)^2 \left(\frac{1}{A} - \frac{1}{A-4}\right) = -0.2156,$$

thus we have

Q_α = -38902.076 + 22840.074 * 0.4391 + 736.733 * 49.3933
- 17135.851 * 0.2156 = 3822.39.

MSN: We normalize all values such that for example

$$\widetilde{N} = 0.00714 * N - 0.11428 = 0.879$$

and similarly

$$\widetilde{Z} = 0.837, \widetilde{S}_{2n} = 0.133, \widetilde{S}_{2p} = 0.365, \widetilde{S}_n = 0.181, \widetilde{S}_p = 0.335.$$

Taking into account the weights of neurons and activation function (tanh) we get

$\text{neu}_1 = \tanh(0.7162) = 0.6146, \quad \text{neu}_3 = \tanh(-0.0039) = -0.0039,$

$\text{neu}_2 = \tanh(-0.1924) = -0.1901, \text{neu}_4 = \tanh(2.1674) = 0.9741,$

$\widetilde{Q}_\alpha = 0.6146 * 2.957 - 0.1901 * 0.768 - 0.0039 * (-0.836)$
$+ 0.9741 * (-1.764) + 0.805 = 0.76118,$

and renormalisation Q_α procedure ends computation. We have

$$Q_\alpha = \frac{0.76118 - 0.63063}{0.0000375\,03} = 3481.143.$$

MQT: From (6) we obtain $W_1(Z)=-5.325$, $W_2(Z)=-79.331$, $W_3(N)=-60.314$, $W_4(N)=-54.192$ and $Q_\alpha=4081.434$.

The unknown values Q_α are computed as above and summarized in the following table:

Tab. 8. Przewidywanie nieznanych wartości Q_α
Tab. 8. Prediction of unknown values Q_α.

N	Z	El	M2Q	MSN	MQTPM
34	23	V	-10856.6	-10014.9	-9441.1
87	55	Cs	-4047.6	-2058.2	-1276.2
132	83	Bi	2939.1	5031.2	5453.9
139	87	Fr	3822.4	3481.2	4081.5
143	89	Ac	4188.2	3001.7	3451.0

As a conclusion we note the similarity of the results of MSN and MQT methods and differences (for elements Bi and Cs) with the method M2Q, but it is still an open question which values better approximate true value Q_α.

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