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Atomic Mass Formula with Empirical Shell Terms

Masahiro UNO and Masami YAMADA*

Department of Applied Physics, Waseda University
Shinjuku-ku, Tokyo
**Science and Engineering Research Laboratory*
Waseda University, Shinjuku-ku, Tokyo

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An atomic mass formula is constructed as the sum of a gross part and empirical shell terms. The gross part is adjusted so that the shell terms may remain small and accord with the charge symmetry of nuclear forces. The shell terms show marked dips at the magic numbers 28, 50, 82 and 126, but not at 8 and 20. The standard deviation is 300 keV for even-even and odd-mass nuclei with mass number 1 to 257. For odd-odd nuclei the mass formula includes additional terms and the standard deviation is 435 keV.

§ 1. Introduction

Many authors made attempts to construct the atomic mass formula including effects of the nuclear shell structure. Among them, Cameron et al.[1)~3)] assumed purely empirical shell terms in addition to a liquid-drop formula. Myers and Swiatecki[4),5)] and Seeger[6),7)] calculated shell energies as arising from the nonuniformity of single-nucleon levels of spherical or deformed nuclei and added them to their own liquid-drop formulas. Kümmel et al.[8)] started from a formal summation of single-particle energies in each shell; by dividing it into the liquid-drop part and the shell part and applying some corrections to them, they constructed a mass formula. While these formulas include the liquid-drop part as representing the general tendency of atomic masses, there are other formulas which lack such a part. Zeldes et al.[9)] described atomic masses as a simple expression in valence nucleon numbers; the parameters in it are directly related to the matrix elements of the effective interaction. Garvey et al.[10)] proposed a kind of mass relation from another viewpoint. A detailed review of these formulas was given by Comay et al.[11)] At the present stage, each has both merits and demerits and there seems to be room for improvement.

In this paper we construct a mass formula from a somewhat different viewpoint. We start from the Yamada-Matumoto systematics of nucleon separation energies, S_p (proton separation energy) and S_n (neutron separation energy).[12)] It is summarized as follows:

A. Cases in which no odd-odd nucleus is concerned (Z: proton number, N: neutron number):

S_p(fixed-Z, even-N) increases smoothly (almost linearly) with N.

S_n(even-Z, fixed-N) increases smoothly (almost linearly) with Z.

B. Cases in which odd-odd nuclei are concerned:

B-1. The following inequality holds for those separation energies $(a, b, c, \cdots)$ as shown in Fig. 1:

$$(2b-a-c)-(2e-d-f)=(2h-g-i)-(2k-j-l)>0\,. \qquad (1)$$

This can be rewritten in terms of the masses (00), (01), $\cdots$:

$$[(11)-\tfrac{1}{4}\{(01)+(10)+(21)+(12)\}]-[\tfrac{1}{4}\{(01)+(10)+(21)+(12)\} -\tfrac{1}{4}\{(00)+(02)+(20)+(22)\}]<0\,. \qquad (2)$$

B-2. S_p(odd-Z, even-N) is not much smaller than $S_p(Z, N-1)$ and S_n(even-Z, odd-N) is not much smaller than $S_n(Z-1, N)$.

We attempt to embody this systematics in a mass formula. We are mainly concerned with even-even and odd-mass nuclei because odd-odd nuclei exhibit somewhat complicated properties due to residual neutron-proton interactions. We assume that our mass formula consists of two parts, the gross part and the shell part. Upon this shell part we impose two conditions: it should be small, and should accord with charge symmetry of nuclear forces. The gross part is adjusted so that these conditions may be satisfied. In the following two sections we construct the mass formula along this line and discuss its properties. In the last section we present a mass formula for odd-odd nuclei which is obtained from the above formula by adding two simple terms.

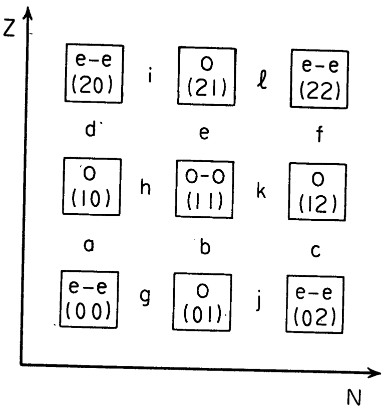


Fig. 1. An odd-odd nucleus and eight nuclei surrounding it. The letters between the nuclei stand for the proton and neutron separation energies and (10), (12), etc. represent the masses.

§ 2. Construction of mass formula

As mentioned in § 1, we first consider even-even and odd-mass nuclei. Accordingly, we pick out only the systematics A because the systematics B is mainly concerned with odd-odd nuclei. In order to embody the systematics A, we take the following form for the mass excess:

$$M_E(Z, N)=M_{Eg}(Z, N)+P_Z(N)+Q_N(Z)\,. \qquad (3)$$

Here $M_{Eg}(Z, N)$ represents the gross part which is a smooth function of Z and N; $P_Z(N)$ and $Q_N(Z)$ are proton and neutron shell terms, respectively. In order that this expression may satisfy the systematics A, the proton shell term

$P_Z(N)$ should be smooth functions of N, whereas they may not necessarily be smooth with respect to the subscript Z. Similarly, $Q_N(Z)$ should be smooth with respect to Z, but not necessarily so with respect to N. Furthermore, the derivatives of $P_Z(N)$ and $Q_N(Z)$ should be relatively small. It is easily seen that these conditions on $P_Z(N)$ and $Q_N(Z)$ are sufficient for the validity of the systematics A.

As the first step along this line, we take the simplest form for these shell terms in this paper; we assume $P_Z(N)$ and $Q_N(Z)$ to be constant parameters P_Z and Q_N neglecting their dependence on N and Z, respectively. It should be noted that there are about one hundred P_Z's and one hundred and fifty Q_N's. At this stage the parametrization of our shell terms becomes the same as that of Cameron et al.'s.[1)~3)]

We determine the values of parameters P_Z and Q_N by the method of least squares with respect to experimental masses. Moreover, we require them to satisfy the following two conditions:

(1) Gross properties of atomic masses are represented by $M_{Eg}(Z,N)$ in Eq. (3) and only the remaining mass excesses are attributed to P_Z and Q_N; accordingly, the magnitudes of P_Z and Q_N should be relatively small.

(2) In the region of light nuclei ($Z, N<20$), where the charge symmetry of nuclear forces manifests itself most clearly, the values of P_Z should be approximately equal to those of the corresponding parameters Q_N.

Special emphasis laid upon these conditions is the principal point to distinguish our formula from those of Cameron et al.[1)~3)]

Our procedure for calculating P_Z and Q_N is as follows. First, we assume a zeroth-order approximation of $M_{Eg}(Z,N)$ taking into account gross features of odd-mass data. Then, we determine the shell terms P_Z and Q_N by the method of least squares using the data on even-even as well as odd-mass nuclei. Actually, these least-squares calculations have been made by an iteration method. Next, the values of P_Z and Q_N thus obtained are examined in the light of the above-mentioned two conditions. If they do not fulfil these conditions, we change the gross part. Such trial and error procedures are repeated until no further appreciable improvement in the gross part and the shell terms is possible.

To begin with, we tested Kodama's formula[13)] as our gross part. In that case, however, the second condition was not fulfilled at all although the first one was satisfied fairly well. Consequently, we have partially modified Kodama's formula[13)] as follows (^{12}C standard, in MeV):

$$M_{Eg}(Z,N) = 7.68046A + 0.39123I + a(A)\cdot A + b(A)\cdot|I| + c(A)\cdot I^2/A + E_c(Z,N), \qquad (4)$$

where

$$A = Z+N, \qquad I = N-Z,$$

$$a(A)=a_1+a_2A^{-1/3}+a_3A^{-2/3}+a_4A^{-1}, \tag{5}$$

$$b(A)=bA^{-2/3}, \tag{6}$$

$$c(A)=c_1+c_2A^{-1/3}+c_3A^{-2/3}/(1+c_4A^{-1/3}), \tag{7}$$

$$E_c(Z,N)=0.7854545\left(\frac{R}{r_0}\right)^5\left\{1+\frac{5}{6}\left(\frac{z}{R}\right)^2+\frac{1}{2}\left(\frac{z}{R}\right)^3+\frac{1}{6}\left(\frac{z}{R}\right)^4-\frac{1}{42}\left(\frac{z}{R}\right)^5\right\}\cdot\left(\frac{Z}{A}\right)^2-\frac{0.66}{r_0}\left(\frac{Z}{A}\right)^{4/3}\cdot A \tag{8}$$

with

$$R=r_0\left[\left\{\frac{A}{2}+\sqrt{\left(\frac{A}{2}\right)^2+\frac{1}{27}\left(\frac{z}{r_0}\right)^6}\right\}^{1/3}-\left\{\sqrt{\left(\frac{A}{2}\right)^2+\frac{1}{27}\left(\frac{z}{r_0}\right)^6}-\frac{A}{2}\right\}^{1/3}\right]. \tag{9}$$

Equation (8) is the Coulomb energy of the trapezoidal charge distribution as shown in Fig. 2; its last term is the approximate Coulomb exchange energy calculated on the Fermi-gas model. We use the parameter values $r_0=1.1$ fm and $z=1.5$ fm. The adjustable parameters a_i and c_i should be determined in accordance with the above-mentioned two conditions.

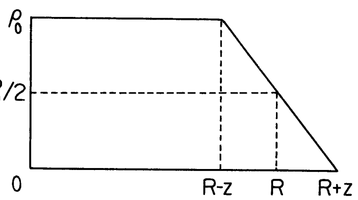


Fig. 2. The trapezoidal charge distribution. The central density ρ_0 is related to r_0 by $\rho_0=3/(4\pi r_0^3)$.

In the course of the determination of parameter values, we often obtained quite unsatisfactory results; P_Z and Q_N, as functions of Z and N respectively, oscillated with rather large amplitudes or they exhibited completely different behavior from each other in the region of light nuclei. It has become clear through analyses that this behavior of P_Z and Q_N critically depends on the location of the β-stability line, namely on the values of the symmetry-term coefficient $c(A)$. This observation has been helpful for our analysis. It should also be noted that the sum of the two shell terms (P_Z+Q_N) does not change under the substitution, $P_Z'=P_Z+D$, $Q_N'=Q_N-D$, where D is an arbitrary constant independent of Z and N. We have utilized this property, too.

We have picked out mass data with errors less than 100 keV from the mass table of Wapstra and Gove[14] and have used them with equal weight.

§ 3. Final parameter values and discussion

The final values of the shell terms, P_Z and Q_N, and the parameters of the gross part, a_i, b and c_i are tabulated in Tables I, II and III. In order to see the behavior of P_Z and Q_N as functions of Z and N respectively, we plot them in Figs. 3 and 4.

Table I. Values of proton shell term P_Z (in MeV).

Z	P_Z	Z	P_Z	Z	P_Z	Z	P_Z	Z	P_Z	Z	P_Z	Z	P_Z
0	−9.474	15	−0.588	30	−1.105	45	0.637	60	1.519	75	2.669	90	3.107
1	3.367	16	−1.759	31	0.866	46	−1.400	61	2.903	76	1.719	91	3.742
2	−2.818	17	0.315	32	−0.098	47	−0.617	62	1.798	77	2.309	92	2.292
3	2.822	18	−1.012	33	1.906	48	−2.668	63	2.937	78	1.089	93	2.742
4	0.002	19	0.966	34	0.700	49	−1.871	64	1.748	79	1.203	94	1.442
5	2.369	20	−1.168	35	2.538	50	−4.123	65	2.861	80	−0.465	95	1.621
6	−1.527	21	1.296	36	1.050	51	−2.349	66	1.714	81	−0.392	96	0.381
7	0.469	22	−0.433	37	2.717	52	−2.951	67	2.811	82	−1.648	97	0.604
8	−1.363	23	1.319	38	0.859	53	−1.335	68	1.874	83	0.343	98	−0.643
9	2.239	24	−0.665	39	2.130	54	−1.928	69	2.898	84	0.476	99	−0.438
10	−0.066	25	0.640	40	0.599	55	−0.149	70	2.007	85	2.316	100	−1.620
11	1.760	26	−1.384	41	2.199	56	−0.526	71	3.067	86	2.190	101	−1.413
12	−0.943	27	−0.156	42	0.639	57	1.202	72	2.333	87	3.681	102	−2.489
13	0.634	28	−2.314	43	1.778	58	0.790	73	3.161	88	3.177		
14	−2.084	29	−0.504	44	−0.225	59	2.509	74	2.062	89	4.253		

Table II. Values of neutron shell term Q_N (in MeV).

N	Q_N	N	Q_N	N	Q_N	N	Q_N	N	Q_N	N	Q_N	N	Q_N
0	−8.861	23	2.594	46	−0.700	69	5.336	92	1.492	115	−0.477	138	−0.752
1	3.548	24	0.184	47	0.130	70	3.938	93	2.323	116	−1.830	139	0.171
2	−3.664	25	1.033	48	−2.350	71	4.999	94	1.190	117	−1.489	140	−0.690
3	2.010	26	−1.351	49	−1.752	72	3.312	95	2.073	118	−2.841	141	−0.164
4	−0.836	27	−0.658	50	−4.440	73	4.250	96	0.889	119	−2.719	142	−0.808
5	2.050	28	−3.343	51	−2.684	74	2.235	97	1.681	120	−4.004	143	−0.139
6	−1.847	29	−1.930	52	−2.913	75	3.022	98	0.511	121	−3.728	144	−0.819
7	0.394	30	−2.721	53	−1.143	76	1.259	99	1.296	122	−5.374	145	−0.285
8	−1.761	31	−0.729	54	−1.389	77	1.936	100	0.321	123	−5.282	146	−0.670
9	1.870	32	−1.672	55	0.309	78	−0.099	101	0.970	124	−6.825	147	−0.043
10	0.139	33	0.209	56	−0.129	79	0.363	102	0.080	125	−6.870	148	−0.562
11	2.055	34	−0.887	57	1.775	80	−1.575	103	0.683	126	−7.658	149	−0.033
12	−0.501	35	1.246	58	1.341	81	−1.295	104	−0.079	127	−5.780	150	−0.526
13	1.259	36	−0.117	59	3.239	82	−3.107	105	0.514	128	−5.480	151	0.105
14	−1.590	37	1.853	60	2.291	83	−1.214	106	−0.142	129	−3.684	152	−0.520
15	−0.028	38	0.359	61	4.184	84	−1.214	107	0.470	130	−3.566	153	0.337
16	−1.511	39	2.369	62	3.149	85	0.361	108	−0.441	131	−1.901	154	0.001
17	0.192	40	0.735	63	4.959	86	0.213	109	0.313	132	−1.986	155	0.927
18	−1.105	41	2.338	64	3.875	87	1.739	110	−0.348	133	−1.115	156	0.618
19	0.935	42	0.564	65	5.341	88	1.492	111	0.373	134	−1.207	157	1.526
20	−0.785	43	1.978	66	4.213	89	2.941	112	−0.510	135	−0.614		
21	2.182	44	0.092	67	5.684	90	1.860	113	0.241	136	−0.780		
22	0.856	45	1.311	68	4.335	91	2.860	114	−0.848	137	0.016		

Table III. Values of parameters in M_{Eg} (Z, N).

a_1	−17.1157
a_2	27.4348
a_3	−14.1609
a_4	− 2.0918
b	15.0
c_1	35.8276
c_2	−87.8265
c_3	84.4186
c_4	0.730136

In these figures the shell effects show up clearly. Marked dips are seen at the magic numbers 28, 50, 82 and 126 but not at 8 and 20. It is also seen that P_Z and Q_N each separate clearly into two lines owing to the even-odd effect; our shell terms, P_Z+Q_N, include the usual even-odd term. Although this formula fairly well satisfies our two conditions in most mass regions, its behavior in the heaviest region is unsatisfactory; P_Z decreases with Z, and Q_N increases with N. This tendency is closely connected with the fact that

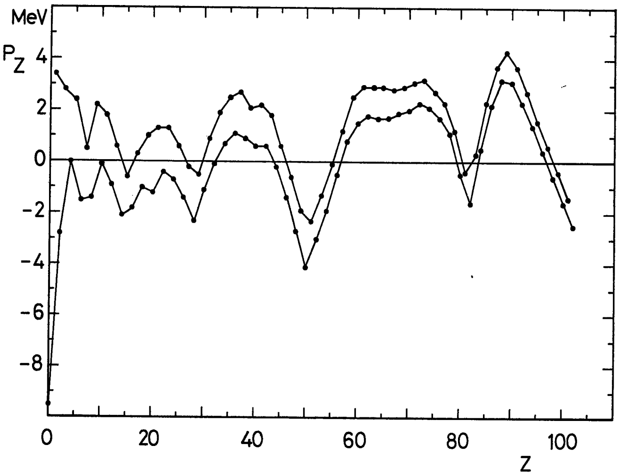
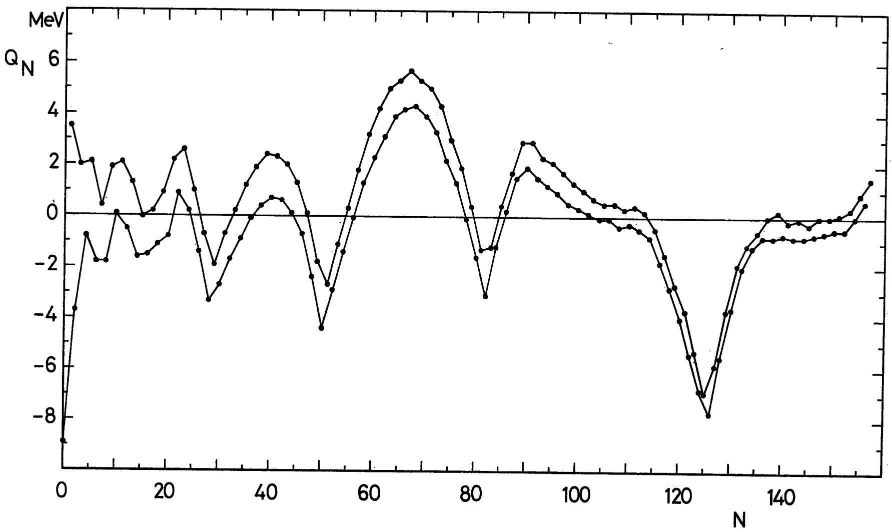


Fig. 3. The proton shell term P_Z plotted against Z.

Fig. 4. The neutron shell term Q_N plotted against N.



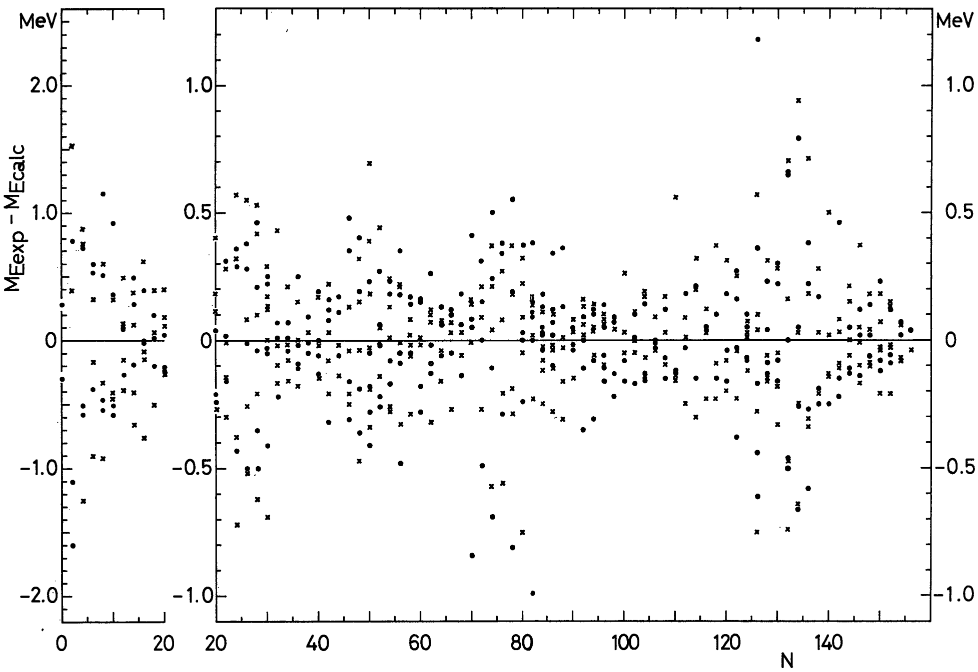


Fig. 5. The differences between the experimental and calculated masses ($M_{E\mathrm{exp}}-M_{E\mathrm{calc}}$). ●: odd-$Z$-even-$N$ nucleus, ×: even-even nucleus.

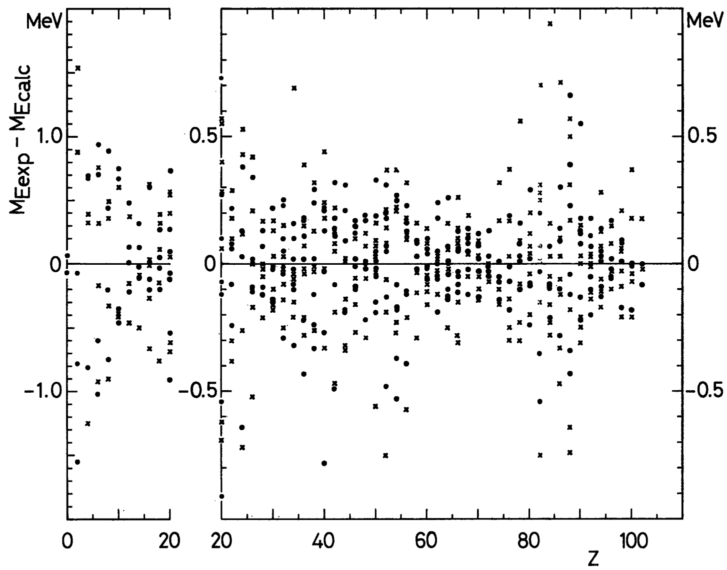


Fig. 6. The differences between the experimental and calculated masses ($M_{E\mathrm{exp}}-M_{E\mathrm{calc}}$). ●: even-$Z$-odd-$N$ nucleus, ×: even-even nucleus.

the β-stability line has not been well reproduced by most mass formulas in the heaviest region.[13),15)] It is not known at present whether this defect is due to the gross part or to the shell part. Anyway, this situation is unfavorable for predicting the masses of superheavy nuclei.

The differences between the experimental and the calculated masses are shown in Figs. 5 and 6. In Fig. 5, those of odd-Z-even-N as well as even-even nuclei are plotted against N; in Fig. 6, those of even-Z-odd-N as well as even-even nuclei are plotted against Z. These figures show that the differences are larger for magic nuclei, and smaller for nonmagic nuclei. The standard deviation is 300 keV for 857 nuclides with $1 \leq A \leq 257$, and 254 keV for 819 nuclides with $17 \leq A \leq 257$. This is somewhat smaller than that of Truran et al.[8)] (about 300 keV for $A > 20$) and larger than that of Garvey et al.[10)] (about 160 keV for $A \geq 17$). Note that the number of parameters in our formula, ≈ 250, is much smaller than that of the Garvey-Kelson formula,[10)] ≈ 450. We can expect that the deviation will be reduced by taking into account the N-dependence of $P_Z(N)$ and the Z-dependence of $Q_N(Z)$.

§ 4. Formula for odd-odd nuclei

In constructing our mass formula we have excluded odd-odd nuclei because their masses behave somewhat irregularly due to residual neutron-proton interactions. On the average, the distance between the mass surfaces of odd-odd and odd-mass nuclei is smaller than that between the mass surfaces of odd-mass and even-even ones.

In order to see this situation, we first calculate the left-hand side of in-

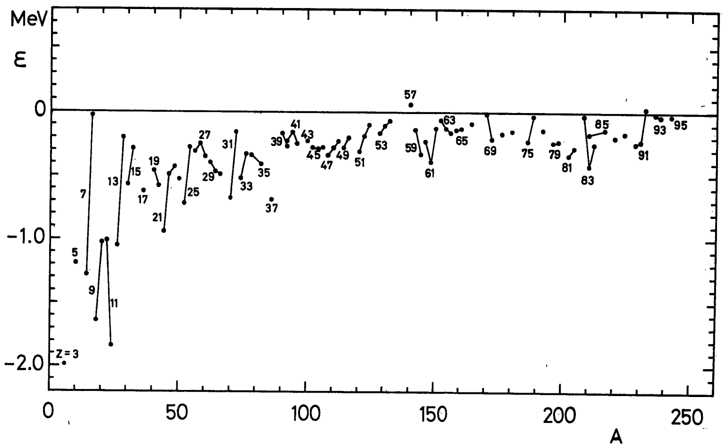


Fig. 7. The left-hand side of inequality (2) (referred to as ε) calculated with experimental mass data for all the nuclei concerned. Isotopes are connected by solid lines and are labeled by Z.

equality (2) (referred to as ε) using experimental mass data for all the nuclei concerned, and plot it in Fig. 7. This figure shows that inequality (2) actually holds for almost all odd-odd nuclei with only few possible exceptions, for which the ε's are nearly equal to zero.

Second, we calculate the mass excesses of odd-odd nuclei using the formula obtained in the previous sections, and subtract them from the experimental ones. Only the experimental data with errors less than 100 keV are used. The quantities thus obtained are essentially the semitheoretical values of ε and are plotted

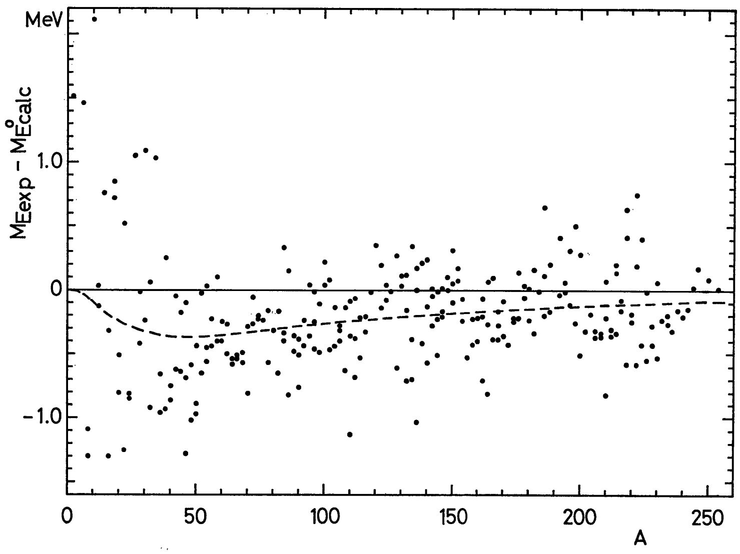


Fig. 8. The differences between the experimental and calculated masses ($M_{E\mathrm{exp}}-M^0_{E\mathrm{calc}}$) for odd-odd nuclei, where $M^0_{E\mathrm{calc}}$ are calculated from the formula in §§ 2 and 3. These differences are essentially the semitheoretical values of ε. The dashed line is $\varepsilon_0(A)$.

in Fig. 8. Although the majority of data points lie below zero in agreement with inequality (2), not a few points lie above zero. In consideration of Fig. 7, this disagreement seems to be due to inaccuracy of our formula. The dashed line in Fig. 8 is the average curve, which is approximated as*)

$$\varepsilon_0(A) = -\left[\frac{11719.21}{(A+31.4113)^2} - \frac{1321495}{(A+48.1170)^3}\right]. \tag{10}$$

*) According to the shell model, the interaction energy between the last proton and neutron is, on the average, proportional to A^{-1}. This mass-number dependence is not much different from that of $\varepsilon_0(A)$ as given by Eq. (10) as far as heavy nuclei ($A>60$) are concerned. While it is an interesting problem to discuss the deviation of ε from the average curve $\varepsilon_0(A)$ in connection with nuclear models, the semitheoretical values of ε shown in Fig. 8 are not sufficiently accurate for this purpose.

Thus, we recommend to calculate the mass excesses of odd-odd nuclei by adding $\varepsilon_0(A)$ to the mass formula (3):

$$M_E(Z,N) = M_{Eg}(Z,N) + P_Z + Q_N - \left[\frac{11719.21}{(A+31.4113)^2} - \frac{1321495}{(A+48.1170)^3}\right]. \quad (11)$$

The standard deviation of 246 odd-odd mass data ($2 \leq A \leq 254$) from Eq. (11) is 435 keV.

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References

1) A. G. W. Cameron, Can. J. Phys. **35** (1957), 1021.
2) A. G. W. Cameron and R. M. Elkin, Can. J. Phys. **43** (1965), 1288.
3) J. W. Truran, A. G. W. Cameron and E. Hilf, *Proceedings of the International Conference on the Properties of Nuclei Far from the Region of Beta-Stability, Leysin, 1970* [report, CERN 70-30 (1970)], Vol. 1, p. 275.
4) W. D. Myers and W. J. Swiatecki, Nucl. Phys. **81** (1966), 1.
5) W. D. Myers and W. J. Swiatecki, Ark. Fys. **36** (1967), 343.
6) P. A. Seeger, *Proceedings of the Third International Conference on Atomic Masses, Winnipeg, 1967*, p. 85.
7) P. A. Seeger, *Proceedings of the International Conference on the Properties of Nuclei Far from the Region of Beta-Stability, Leysin, 1970* [report, CERN 70-30 (1970)], Vol. 1, p. 217.
8) H. Kümmel, J. H. E. Mattauch, W. Thiele and A. H. Wapstra, Nucl. Phys. **81** (1966), 129; **A107** (1968), 695.
9) N. Zeldes, A. Grill and A. Simievic, Kgl. Danske Videnskab. Selskab, Mat-fys. Skr. **3** (1967), no. 5.
10) G. T. Garvey, W. J. Gerace, R. L. Jaffe, I. Talmi and I. Kelson, Rev. Mod. Phys. **41** (1969), S1.
11) E. Comay, S. Liran, J. Wagman and N. Zeldes, *Proceedings of the International Conference on the Properties of Nuclei Far from the Region of Beta-Stability, Leysin, 1970* [report, CERN 70-30 (1970)], vol. 1, p. 165.
12) M. Yamada and Z. Matumoto, J. Phys. Soc. Japan **16** (1961), 1497.
13) T. Kodama, Prog. Theor. Phys. **45** (1971), 1112.
14) A. H. Wapstra and N. B. Gove, Nuclear Data Tables **A9** (1971), 265.
15) M. Yamada, Prog. Theor. Phys. **32** (1964), 512.