application in other light nuclei. It may be remarked that two other examples of large alpha-particle reduced-widths are known[5] in the same region of Ne^{20}, at $E_p=340$ ($J=1^+$) and 598 kev ($J=2^-$). In both cases, it is again the α_1 group, leading to the 3^- state of O^{16} which shows the effect.

ACKNOWLEDGMENTS

We are indebted to Dr. C. A. Barnes and Dr. R. F. Christy for many valuable comments and suggestions during the course of this work. Thanks are also due to Mr. C. Cook for his assistance during much of the experimental work.

PHYSICAL REVIEW VOLUME 106, NUMBER 6 JUNE 15, 1957

New Empirical Equation for Atomic Masses*

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(Received March 4, 1957)

A new empirical equation for atomic masses has been developed. This equation has been successfully applied to atomic masses of nuclides heavier than nickel. The form used is that of an expression for the mass defect, $\Delta M=M-A$, as a function of Z and A:

$$\Delta M(A,Z)=\alpha_0+\alpha_1A+\alpha_2Z+\alpha_3AZ+\alpha_4Z^2+\alpha_5A^2+\delta.$$

Because of the effects of nuclear shell structure a different set of coefficients is necessary for the different nuclear shell regions.

Atomic masses calculated from this equation agree with experimental mass values to within ± 0.5 millimass units in 75% of the 340 nuclides studied and agree to within ± 1.5 millimass units in 95% of the nuclides. Beta-decay energies were calculated with the new equation and checked against a total of 179 experimental values. Agreement of calculated values with experiment was better than ± 0.5 Mev in 95% of the cases and within ± 0.25 Mev in 84%.

I. INTRODUCTION

A GOOD equation for atomic masses can be a highly useful tool in many problems of nuclear physics where an accurate estimate of such quantities as nuclear binding energies, alpha- and beta-decay energies, Q values of nuclear reactions, etc. are desired. These quantities all involve differences between atomic masses. A mass equation that accurately reproduces known atomic masses is perhaps the most convenient means of estimating atomic masses of nuclides that have so far defied measurement. To facilitate calculations it is desirable that such an equation should be as simple as possible in form.

The mass equation that is probably most widely used at present is the Fermi-Weizsäcker semiempirical mass equation,[1] hereafter referred to as the FW mass equation. The form of this equation was dictated by theoretical considerations, with the numerical values of the coefficients being obtained by fitting the equation to known masses. The FW mass equation contains terms with fractional powers, and calculations with it are not simple. Metropolis and Reitwiesner have compiled a table of atomic masses using the FW mass equation,[2] thereby making calculations much easier. However, in many regions of the periodic table the FW equation deviates very markedly from experimentally measured atomic masses and becomes unsatisfactory for many calculations unless empirical corrections, which are sometimes elaborate, are made.

Recently, Green has proposed an empirical function to describe the over-all behavior of the mass surface.[3,4] Green's equation is simpler and agrees with known masses somewhat better than the FW mass equation, but the disagreement with experimental masses is still fairly large in some places, especially near "magic number" nuclei.

Much of the discrepancy between experimental masses and the Green and FW equations arises because of the latter having ignored the effects of nuclear shell structure on the mass surface. Green obtains improved agreement when he adds to his simplified equation a set of empirical functions[4,5] to correct for shell-structure effects. However, Green's equation thereby loses much of its ease of handling for calculations, while some annoying disagreements remain.

In this paper will be presented a new empirical equation developed through a new approach. The problem of nuclear shell structure was met by treating each shell region individually. (Justification for this is taken up in the next section.) The result is a simple

* This work was performed under the auspices of the U. S. Atomic Energy Commission.

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equation with different sets of coefficients for the different nuclear shell regions. The resultant extreme simplicity of form and over-all good agreement with experimental mass data more than compensate for the necessity of using more than one set of coefficients.

II. FORM OF THE EQUATION

Let the following quantities associated with a nuclide be defined:

Z = number protons,

N = number of neutrons,

A = mass number = $N+Z$,

I = neutron excess = $N-Z$.

Any two of these four quantities are sufficient to characterize a nuclide uniquely.

Several investigators[6–12] have attempted to find a systematic behavior of atomic masses or mass differences as exemplified in various binding energies and decay energies. These quantities are plotted as functions of Z, N, A, or I to determine whether or not the behavior is systematic. The behavior of many of these quantities can be closely approximated by remarkably simple relationships. These relationships must then be satisfied by the empirical equation to be used to fit the atomic masses.

Below are the relationships adopted for the purpose of developing the form of an empirical mass equation. The relationship assumed was algebraically the simplest one consistent with the behavior of the experimental data.

(a) Parabolic relationships:
  (1) Atomic mass plotted against Z for constant A (the well-known Bohr-Wheeler parabolas).
  (2) The mass defect, $M-A$, plotted against A for constant Z.

(b) Straight-line relationships:
  (1) Z_A (most stable Z for a given A) plotted against A.
  (2) Beta-decay energy plotted against A for constant I.
  (3) Beta-decay energy plotted against N for constant Z.
  (4) Alpha-decay energy plotted against A for constant Z.
  (5) Neutron binding energy plotted against A for constant Z.
  (6) Proton binding energy plotted against A for constant Z.

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Upon consideration of these various relationships, it is possible to write a relatively simple equation for atomic masses which satisfies all of the above relationships. The equation takes the form:

$$M(U,V)=C_0+C_1U+C_2V+C_3UV+C_4U^2+C_5V^2, \quad (1)$$

where U and V are *any* two of the four quantities Z, N, A, and I. The values of the coefficients will differ, however, with different pairs of independent variables. It also becomes necessary to add a small term δ, which depends upon the odd-even character of the nuclide in question.

When one examines the systematic behavior of nuclear binding energies or decay energies, one notes decided discontinuities at "magic" proton and neutron numbers. Further, in studying the straight-line relationships mentioned above, it is noted that the slopes remain roughly constant within a nuclear shell region, but change when one goes from one shell region to another (or sometimes from one subshell region to another). This indicates that a different set of coefficients is necessary for each nuclear shell region. In obtaining coefficients for the new empirical mass equation, therefore, each nuclear shell region (or subshell region when necessary) was treated separately.

III. ATOMIC MASSES IN TERMS OF Z AND A

A nuclide is most frequently characterized by its atomic number, Z, and its mass number, A. It would seem preferable, therefore, to write the empirical mass equation in terms of Z and A. Furthermore, in order to keep the numbers small and easier to work with, one can write the equation for the mass defect, i.e., for the quantity $\Delta M=M-A$, instead of for the atomic mass, M.

The equation then can be written:

$$\Delta M(A,Z)=\alpha_0+\alpha_1A+\alpha_2Z+\alpha_3AZ+\alpha_4Z^2+\alpha_5A^2+\delta. \quad (2)$$

The value of the term δ depends on whether the nuclide in question is odd-odd, odd-even, even-odd, or even-even. It remains practically constant for a given type of nuclide throughout a given shell region. If the mass equation is written in such a manner that the δ term is separated from the other constant term [α_0 in Eq. (2)], then the same set of values for the δ term can be used even though the other terms may be rearranged so that the equation appears in a different form.

One of the conditions that was set on Eq. (2) was that it be able to reproduce Bohr-Wheeler parabolas on the mass surface. It should therefore be possible to rewrite Eq. (2) as follows:

$$\Delta M(A,Z)=\Delta M(A,Z_A)+K(Z_A-Z)^2+\delta, \quad (3a)$$

where Z_A is the most stable Z for a given A. Z_A and $\Delta M(A,Z_A)$ are functions of A alone. The only Z^2 term in Eq. (3a) has the coefficient K. The only Z^2 term in Eq. (2) has the coefficient α_4. Therefore, K must equal

α_4. One can then write

$$\Delta M(A,Z)=\Delta M(A,Z_A)+\alpha_4(Z_A-Z)^2+\delta. \qquad (3b)$$

An expression for Z_A as a function of A can be obtained by taking the partial derivative of Eq. (2) with respect to Z, then setting this partial derivative equal to zero and solving for Z. The resultant expression is:

$$Z_A=q_1A+q_0, \qquad (4)$$

where

$$q_1=-\alpha_3/2\alpha_4 \quad \text{and} \quad q_0=-\alpha_2/2\alpha_4.$$

One can now obtain an expression for $\Delta M(A,Z_A)$ as a function of A. When Eq. (3b) is compared to Eq. (2) and coefficients of similar terms are equated, there results:

$$\Delta M(A,Z_A)=a_0+a_1A+a_2A^2, \qquad (5)$$

where

$$a_0=\alpha_0-\alpha_2^2/4\alpha_4,$$
$$a_1=\alpha_1-\alpha_2\alpha_3/2\alpha_4,$$
$$a_2=\alpha_5-\alpha_3^2/4\alpha_4.$$

The δ term in Eq. (3b) is identical to the δ term in Eq. (2). There are certain advantages in using Eq. (3b) in preference to Eq. (2). Equation (3b) entails somewhat fewer subtractions of large numbers to obtain small numbers. Equation (3b) also emphasizes the Bohr-Wheeler parabolas and is thus probably the handier expression for those interested in beta-decay energies.

IV. ANALYSIS OF THE EXPERIMENTAL DATA

In obtaining coefficients for the new mass equation by fitting to the experimental data, it was desired to take advantage of the fact that absolute errors of measured beta-decay energies are generally much less than those of measured atomic masses. By direct examination of measured beta-decay data rather than measured atomic masses, one would hope to obtain better values for those coefficients of the mass equation that are involved in the expression for beta-decay energies. The method chosen was one that allowed an easy check at all stages on how well the equation was fitting the experimental data.

Values of measured atomic masses were obtained from several sources[7,12–17] and converted into the corresponding mass defect, ΔM. Where more than one atomic mass value was found for a given nuclide, a weighted average was used. Occasionally a value was discarded when it appeared questionable or was superseded by a later measurement, but these instances were few.

Measured beta-decay energies were obtained from the Table of Isotopes[18] and a recent compilation by King.[19] Only those nuclides whose beta-decay energies were reasonably certain were considered.

Beta decays involving closed-shell nuclides showed marked deviations from the regular behavior of the other nuclides and were therefore omitted from consideration in this treatment. Further comment on these deviations is made in Sec. VII.

When Eqs. (3b) and (4) are used to calculate beta-decay energies, the term $\Delta M(A,Z_A)$ drops out. Then by analysis of measured beta-decay energies the values for α_4, q_1, and q_0 can be obtained (and also the differences between the two δ's for even-A nuclei and between the two δ's for odd-A nuclei). This was done by a series of successive approximations and least-squares fitting.

Using the values of α_4, q_1, and q_0 thus obtained, the ΔM values obtained from experimental mass data were further transformed to the corresponding values of $\Delta M(A,Z_A)$ for the various mass numbers. Equation (5) was then fitted to these points by the least-squares method to obtain values for a_0, a_1, and a_2.

The values of the δ's were determined by matching ΔM's calculated from the other terms with the measured ΔM's. Since the mass surface for even-even nuclides is always lower than those for other types, δ for even-even nuclides was arbitrarily set equal to zero and the other δ's adjusted accordingly.

From the coefficients of Eqs. (3), (4), and (5) one can readily calculate the coefficients for Eq. (2) by means of the relationships given above.

However, in calculating back and forth between the coefficients of Eq. (2) and those of Eqs. (4) and (5), small discrepancies in the ΔM values arise because of the rounding off of numbers. Therefore, the values for the α_0's and for the a_0's were so adjusted that the same set of values can be used for δ with either expression for ΔM.

The results to be given cover analysis of experimental data ranging from copper ($Z=29$) to curium ($Z=96$). It was felt that data for nuclides beyond curium were not as yet sufficiently reliable to warrant their inclusion in this study. The difficulties encountered in treating mass data below copper are discussed in Sec. VI.

V. RESULTS

The values for the coefficients of Eqs. (2), (3), (4), and (5) obtained for the various nuclear shell and subshell regions studied are given in Tables I, II, and III. The units of all the values in these three tables are such that $\Delta M(A,Z)$ and $\Delta M(A,Z_A)$ are expressed in atomic millimass units.

To see how effective the new mass equation is in describing the mass surface, the experimental values of the mass defect, $M-A$, for the 340 nuclides included in

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TABLE I. Values of the α coefficients for Eq. (2) (ΔM in mMU).

Z	N	α_0	α_1	α_2	α_3	α_4	α_5
29–40	29–40	−155.91	13.202	−21.956	−0.9707	1.4544	0.11565
29–40	41–50	−150.06	7.359	−10.094	−0.7023	0.9473	0.10340
29–40	51–82	+96.27	3.780	−17.406	−0.5349	0.8150	0.10050
41–50	51–82	−135.41	5.342	−9.712	−0.5570	0.7432	0.09758
51–64	51–82	−133.60	6.399	−13.465	−0.4287	0.6417	0.06583
51–64	83–126	−672.82	13.059	−14.140	−0.4461	0.6492	0.05370
65–82	83–126	−83.72	3.843	−10.680	−0.4644	0.6464	0.08739
>82	127–140	−1746.56	18.067	−10.846	−0.4363	0.6133	0.05171
>82	>140	571.90	−1.407	−12.238	−0.3971	0.5706	0.08613

this study were compared with the corresponding mass defect values calculated from Eq. (2). The differences between the calculated and measured values were expressed in terms of the quantity

$$\rho = \Delta M(\text{meas.}) - \Delta M(\text{calc.}).$$

Of the ΔM's calculated for the 340 nuclides, 256, or 75%, are within ± 0.5 millimass unit of the experimental values; 295 are within ± 1.0 mMU; and 323, or 95%, are within ± 1.5 mMU.

Figure 1 is a plot of the values of ρ against mass number, A, for the new empirical mass equation. For comparison, Fig. 2 gives the corresponding ρ values for the FW semiempirical mass equation (note the different scales of the two ordinate axes). The two lines at $+1.5$ and -1.5 mMU in Figs. 1 and 2 represent the range within which fall 95% of the ρ's for the new empirical mass equation.

The 340 nuclides considered include several nuclides with closed neutron or proton shells. It was found in using Eq. (2) that the effect of closing a nucleon shell on the atomic mass of the nuclide was only of the same order of magnitude as the error in the measured mass, and in many cases was not even noticeable. However, when one adds to a nucleus with a closed shell of nucleons another nucleon of the same type, there is a marked discontinuity in the mass surface between the closed-shell nuclide and the closed-shell-plus-one-nucleon nuclide. One has now gone to a new shell region and must use a new set of coefficients in the empirical mass equation.

VI. DISCUSSION

It has been well known that light mass nuclides (with mass number less than 50 or 60) frequently show

TABLE II. Values of the term δ (in mMU).

Z	N	Even Z-even N	Odd Z-odd N	Odd Z-even N	Even Z-odd N
29–40	29–40	0	2.65	1.44	2.20
29–40	41–50	0	3.08	1.84	1.82
29–40	51–82	0	2.02	1.27	0.75
41–50	51–82	0	3.08	1.54	1.44
51–64	51–82	0	2.52	1.12	1.13
51–64	83–126	0	2.09	0.96	0.73
65–82	83–126	0	1.61	0.84	0.76
>82	127–140	0	1.66	1.01	0.88
>82	>140	0	1.33	0.71	0.50

marked deviations from the fairly smooth behavior patterns exhibited by the heavier nuclides. The fact that irregularities in the mass surface (besides the special case of a closed nucleon shell) are most pronounced in the light mass regions is not too surprising. When a nucleon is added to a nucleus, the resultant change in size affects the energy levels of the other nucleons as well. Thus, one can say that actually several nucleon energy levels are involved in the accompanying change in nuclear binding energy. Any peculiarity due to the effect on a particular energy level is more likely to be prominent in a light nucleus with few nucleons where the effect constitutes a greater percentage of the total change than in a heavy nucleus where the effect is proportionately smaller. When one examines the mass surface in the regions below mass number 60, one finds the behavior to be rather erratic. Although the general trends are similar to what is expected, the deviations from smooth behavior are such as appear to preclude a satisfactory fit of the new empirical mass equation for nuclides with less than 29 protons or 29 neutrons.

The fission-product region extending from copper to the rare earths is of widespread interest and a fair number of good experimental data are available. The analysis of data went smoothly except in the region $Z=29$–40, $N=51$–82. In this region there were insufficient good experimental beta-decay energies available to allow use of the method described above. Instead, the coefficients of Eq. (2) were obtained directly from measured masses by a combination of interpolation and least-squares analysis. Although the resultant equation reproduces the atomic masses well enough, it is felt that the values of those coefficients involved in beta-decay energies are not as individually reliable as the corresponding values in the other regions. On the whole, agreement of the equation with experiment is quite good throughout the fission-product region. Of the 216 nuclides studied from copper to gadolinium, 71% of the calculated ΔM's agree to within ± 0.5 mMU of the experimental values and better than 95% agree to within ± 1.5 mMU.

TABLE III. Coefficients for Eqs. (4) and (5) (ΔM in mMU).

Z	N	q_1	q_0	a_0	a_1	a_2
29–40	29–40	0.3337	7.548	−238.48	5.875	−0.04632
29–40	41–50	0.3707	5.328	−176.83	3.617	−0.02677
29–40	51–82	0.3281	10.679	+3.21	−1.932	+0.01275
41–50	51–82	0.3747	6.534	−167.12	1.703	−0.006784
51–64	51–82	0.3340	10.492	−204.24	1.901	−0.005769
51–64	83–126	0.3436	10.890	−749.90	8.201	−0.02293
65–82	83–126	0.3592	8.261	−127.81	0.00699	0.00399
>82	127–140	0.3557	8.842	−1794.78	14.209	−0.02588
>82	>140	0.3480	10.724	507.67	−5.666	0.01702

In the region between gadolinium and lead there are not available many good experimental data involving atomic masses or mass differences. Most of the measured atomic masses used in the study of this region were calculated from measured mass doublets which paired a doubly or triply charged ion of the isotope whose mass was desired with a standard of a singly charged ion of an isotope whose mass was one-half or one-third that of the desired isotope.[17] This procedure results in any error in the measured mass of the standard isotope being doubled or tripled for the mass of the heavier isotope. The fit of the equation in this region, while not as good as in other mass regions, is still encouraging. Out of a total of 26 nuclides with measured atomic masses, 22 of these values agreed to within ± 2.0 mMU of the values calculated from the new mass equation. The agreement of measured beta-decay energies with those calculated from the equation is better and is almost as good as in the other mass regions studied.

Coryell,[8] in an analysis of the behavior of Z_A in this region, found it desirable to admit a break in the curve at 106 neutrons. Cameron,[20] on the basis of a study of nuclear binding energies now in progress, suggests breaks at 95 and 110 neutrons, but says that the changes are not sharp at either point. This present analysis did not show definite evidence either for or against a break at any of these neutron numbers. However, more good experimental mass data are needed in this region before any definite conclusions can be drawn concerning these possible breaks.

In the *trans*-lead region an excellent set of self-consistent atomic masses is obtainable.[12] Because of the alpha-decay data available in this region, a series of closed energy cycles can be set up tying in the masses of all the *trans*-lead nuclides to the four end-product nuclides of the different alpha-decay series. Although the absolute values of the atomic masses may be somewhat in error, the values relative to each other should be very good. Thus the shape of the mass surface, although not necessarily the position, should be well-defined in the *trans*-lead region.

The study of the experimental mass surface was carried only as far as curium-244 ($Z=96$, $N=148$). It was felt that decay data for nuclides beyond curium were not as yet sufficiently reliable to warrant their inclusion in this study. It was found desirable on empirical grounds to make a break in the mass surface at 140 neutrons, although there was no *a priori* expectation of a neutron subshell at 140. Alpha-decay systematics, however, do show a definite change in slope around 140 neutrons. The point of change is not well defined, but best results were obtained by assuming a break at $N=140$. This agrees with Cameron's[20] suggestion of a break at $N=140$. As Cameron suggests, the nucleon numbers such as 95, 110, and 140 (he suggests a break at 152 also) do not correspond to expected nucleon subshells but may be connected with changes in the nucleon interaction outside the closed shells.

The fit of the new-mass equation to the experimental masses is exceptionally good in the *trans*-lead regions. Of a total of 98 nuclides from bismuth to curium studied, 96 of the mass values calculated from the new equation agree to within ± 0.5 mMU of the experimental mass values.

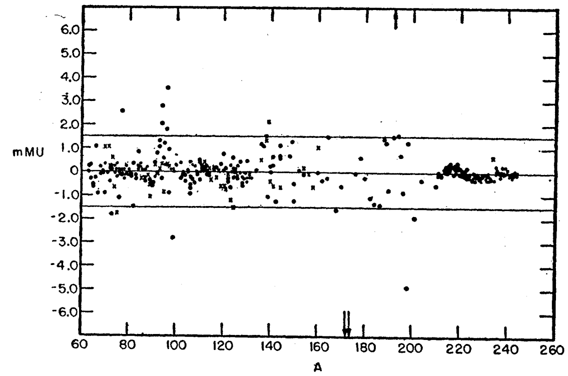

FIG. 1. The values in mMU of $\rho = \Delta M(\text{meas.}) - \Delta M(\text{calc.})$ for the new empirical mass equation plotted *vs* mass number, A. An × represents a "closed shell" nuclide. Lines at $+1.5$ and -1.5 mMU represent the range within which fall 95% of the ρ's.

VII. CALCULATION OF BETA-DECAY ENERGIES

Because those coefficients of the empirical mass equation that are involved in beta-decay energies were obtained by direct analysis of experimental beta-decay data, the empirical mass equation should be a useful tool for the estimation of unknown beta-decay energies. Expressions for beta-decay energies may be derived from either Eq. (3b) or Eq. (2). For positive beta decay (positron emission or electron capture), one has:

$$Q_{\beta^+} = 2\alpha_4(Z - Z_A - 0.5) + (\delta_1 - \delta_2), \tag{6a}$$

or

$$Q_{\beta^+} = (\alpha_2 + \alpha_3 A + 2\alpha_4 Z) - \alpha_4 + (\delta_1 - \delta_2), \tag{6b}$$

and for negative beta decay (negative beta emission)

$$Q_{\beta^-} = 2\alpha_4(Z_A - Z - 0.5) + (\delta_1 - \delta_2), \tag{7a}$$

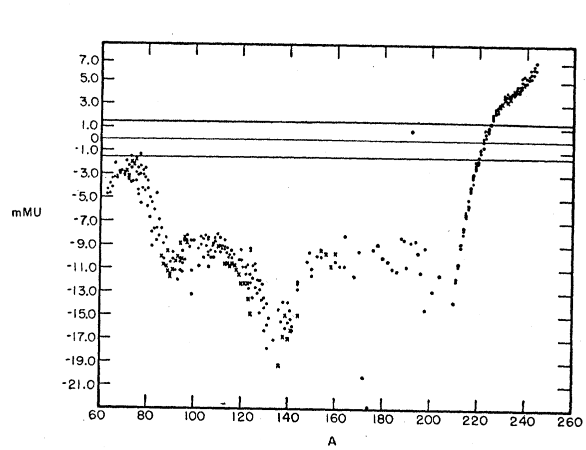

FIG. 2. The values in mMU of $\rho = \Delta M(\text{meas.}) - \Delta M(\text{calc.})$ for the FW semiempirical mass equation plotted *vs* mass number, A. An × represents a "closed shell" nuclide. Lines at $+1.5$ and -1.5 mMU represent the range within which fall 95% of the corresponding ρ values for the new empirical mass equation.

[20] A. G. W. Cameron (private communication).

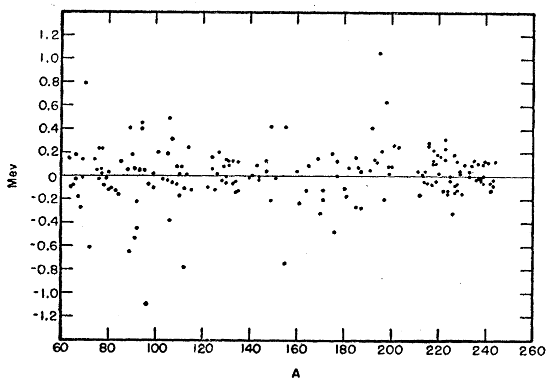

FIG. 3. The values in Mev of Q_β(meas.)$-Q_\beta$(calc.) plotted *vs* mass number, A, using the new empirical mass equation to calculate Q_β.

or

$$Q_{\beta^-}=-(\alpha_2+\alpha_3A+2\alpha_4Z)-\alpha_4+(\delta_1-\delta_2). \quad (7b)$$

The values for Z_A can be calculated from Eq. (4).

To test the applicability of the new mass equation for the calculation of beta-decay energies, Eqs. (6) and (7) were used to calculate beta-decay energies and these calculated values were compared with corresponding experimental values. Figure 3 shows a plot of the differences between measured and calculated values of beta-decay energies, Q_β(meas.)$-Q_\beta$(calc.), against mass number. Of a total of 179 cases considered, 150 or 84% agreed to within ± 0.25 Mev, and 170 or 95% agreed to within ± 0.50 Mev.

Beta decays which involved a nuclide with a closed proton or neutron shell were not included in this study. It was noted previously that the effect of closing a nucleon shell on the mass of a nuclide was small enough as to be hardly noticeable when one is considering atomic masses. However, when beta-decay energies are considered, the effect of closing a nucleon shell is large enough to cause irregularities in the beta-decay energies. This is because the absolute errors in experimental beta-decay energies are much less than the absolute errors in experimental atomic masses. For this reason beta decays involving closed-shell nuclides were excluded from consideration in the analysis of beta-decay energies.

VIII. SUMMARY

A purely empirical equation has been developed for atomic masses of nuclides with Z and N greater than 28. Both the form of the equation and its coefficients were derived from a study of the behavior of the various systematics of atomic masses and mass differences as manifested by binding energies and decay energies.

This new equation has been able to reproduce experimental atomic masses to better than 1.5 mMU for 95% of the 340 nuclides studied. This represents a considerable improvement over the agreement with experimental masses attained with the FW mass equation. The new equation is of an algebraic form that lends itself readily to calculations. It is encourag'ng to note in Fig. 1 that where good experimental mass data are most plentiful the fit of the new mass equation is best.

Comparison of beta-decay energies calculated from the new equation with experimental values indicates that the new equation could be useful in the estimation of unknown beta-decay energies.

J. Riddell, using the new empirical mass equation and an I.B.M. machine, has calculated and tabulated several thousand atomic masses, decay energies, and binding energies. This tabulation is available as a Chalk River Project.[21]

IX. ACKNOWLEDGMENTS

The author would like to express his appreciation to P. C. Stevenson, H. G. Hicks, W. E. Nervik, and J. B. Niday for their continued interest, suggestions, and participation in helpful discussions.

The author also wishes to thank J. L. Brady and R. C. Carpenter of the Computer Group at this laboratory for their generous help with many of the necessary calculations.

[21] J. Riddell, *A Table of Levy's Empirical Atomic Masses*, Chalk River Project Report CRP-654. This report may be obtained from the Scientific Document Distribution Office, Atomic Energy of Canada, Limited, Chalk River, Ontario, Canada.