

CONSTRUCTION OF MASS FORMULAS DESIGNED TO BE VALID
FOR NEUTRON-RICH NUCLEI

J.W. Truran and A.G.W. Cameron,

Belfer Graduate School of Science, Yeshiva University, New York, U.S.A.
Goddard Institute for Space Studies, New York, U.S.A.

and E. Hilf,

Physikalisches Institut der Universitat Wurzburg, Wurzburg, Germany
Belfer Graduate School of Science, Yeshiva University, New York, U.S.A.

ABSTRACT

A semi-empirical atomic mass formula has been constructed aimed at providing improved estimates of the masses of neutron-rich nuclei. In addition to the four standard terms whose coefficients are determined by a least-squares fit to masses - the volume, volume symmetry, surface and Coulomb energy terms - a number of additional terms have also been included. Our criteria for the selection of appropriate coefficients for these terms have included the assumption that the shell corrections to the reference mass formula should be separable in Z and N and well behaved. This criterion has allowed us to assign reasonable coefficients both to a Wigner-type term which predominantly affects the masses of light nuclei and to a surface symmetry term. A higher order volume symmetry term has been included as prescribed by Myers and Swiatecki¹⁾, and a curvature term of negative sign has been included in order to give a reasonable fit to the Stanford determinations of nuclear Coulomb energies. Still higher order volume and surface symmetry terms have been included with reasonable but arbitrary assignments of coefficients in order to prevent nuclei with very small charges from having positive neutron binding energies out to indefinitely large neutron numbers. It was found that the liquid droplet model formula of Myers and Swiatecki could not be used in the form suggested by those authors; their determination of the nuclear symmetry effect in the nuclear interior suffers from the premature dropping of terms and hence the resulting truncated mass formula cannot be fitted to masses in a satisfactory self-consistent fashion.

1. INTRODUCTION

We have recently undertaken an extensive investigation of the dynamics of the rapid neutron capture process²⁾. These calculations are dependent in several different ways upon the estimation of masses far from the valley of beta stability. Such masses determine neutron binding energies and total beta decay energies in the neutron-rich region. Furthermore, detailed calculations of the rates of neutron capture and of beta decay require a reasonably accurate determination of the level densities in the various nuclei concerned, and it has been found that such level densities depend sensitively upon the shell corrections to the mass formula³⁾. Because of this level density dependence upon the shell corrections, one of the principal criteria that we have employed in developing a new mass formula is the requirement that the nuclear shell corrections behave reasonably along the valley of beta stability, where masses are measured, so that we might have greater confidence in the extrapolations that it is necessary to make into the neutron-rich region far off the beta-stable valley.

Since the introduction of the semi-empirical mass formula by von Weizsacker⁴⁾, many revised versions have been presented. Some obvious modifications have involved the correction of various mass formula terms to take into account the diffuse edge of the nucleus. Attempts have also been made to introduce higher order symmetry energy terms into the mass formula. These attempts have been motivated both by the obvious omission of a surface symmetry term from the original von Weizsacker expression and, more recently, by an interpretation of the product yield curve produced in the Mike thermonuclear explosion⁵⁾ as indicating that neutron binding energies decrease less rapidly in the neutron-rich region off the valley of beta stability than is predicted by conventional mass formulas. Cameron and Elkin⁶⁾ attempted to take this into account in a rough way by assuming an exponential form for the symmetry energy contribution to nuclear masses, which in effect introduced an infinite series of higher order symmetry terms. The choice of an exponential form amounted to an arbitrary choice of the relative values of the coefficients of these higher order symmetry terms. Although such a mass formula has the disadvantage of predicting that

all nuclei will have positive neutron binding energies, it does have the advantage that near the valley of beta stability the neutron capture cross sections calculated on this basis seem to give good agreement with more recent experimental yields of heavy nuclei from thermonuclear explosions⁷⁾.

The shell corrections of Cameron and Elkin⁶⁾, as well as earlier expressions derived by Cameron⁸⁾, were determined based on the assumption that the total shell corrections for each nucleus can be written as a sum of two independent shell correction functions for neutrons and protons:

$$S(Z,N) = S(Z) + S(N) \quad (1)$$

These shell corrections are intended to represent differences between real masses and a reference mass formula due to shell effects. It may therefore be expected that the shell corrections should increase rather abruptly beyond a shell closure and then decrease again, having suitable split between positive and negative values. The first backward differences between the shell corrections, which, apart from a constant, represent neutron or proton binding energies, should exhibit a variation of values which roughly sum to zero over a given shell. This is what should be considered "good behavior" of the shell corrections.

These expectations are not very satisfactorily borne out for the individual proton and neutron shell corrections determined originally by Cameron⁸⁾ or for those of Cameron and Elkin⁶⁾. In both instances, the shell corrections show very large departures from the roughly systematic distributions just described, but the proton and neutron shell corrections are anticorrelated in such a way that they sum to relatively small values along the valley of beta stability despite the fact that the individual shell corrections may be very large. It is clear that independent proton and neutron shell corrections which exhibit this unsatisfactory behavior cannot be used with any degree of reliability to predict total shell corrections off the valley of beta stability, since random combinations of two individual shell corrections can give total shell corrections off the valley of beta stability which are very large compared to those on the valley of beta stability. Therefore, one of our major objectives in developing a new mass formula

at this time is to provide one in which the individual neutron and proton shell correction functions are well behaved in the manner we have described. This is essential if we are to be justified in using the correlation between shell corrections and nuclear level density parameters found for nuclei along the valley of beta stability as a basis for calculating level densities of nuclei far off the valley. The level density correlation derived on the basis of this work is presented in Section 4.

It is clear that smaller correction terms must be added to the reference mass surface, if improved estimates of nuclear shell corrections are to be obtained. However, because the actual energies associated with these terms are quite small compared to the magnitudes of the four dominant liquid drop terms, with the masses to a considerable degree representing small differences between these larger terms, it is impossible to determine the coefficients of the smaller correction terms with any degree of reliability by fitting masses. It is therefore necessary to adopt subsidiary criteria for the determination of reasonable values of the coefficients of the smaller terms. We have used two such criteria; these have been the reasonable behavior of the neutron and proton shell corrections and the approximate reproduction of the nuclear Coulomb energy as determined by the Stanford electron scattering results. In our discussion of the construction of our final mass formula expression (Section 3), we show how the behavior of the shell corrections and Coulomb energies can be used in this manner. We will first describe, in Section 2, some difficulties we encountered in our attempts to fit the droplet model formula to masses.

2. STUDIES OF THE DROPLET MODEL FORMULA

Our preliminary attempts to construct a mass formula included a rather extensive investigation of the characteristics of the " droplet model " formula of Myers and Swiatecki¹⁾. We believe that their assumption of the independence of the proton and neutron distributions represents a realistic approach to the construction of an improved liquid drop formula. We have encountered difficulties, however, in our efforts to fit their final mass formula expression to masses.

The droplet formula contains a total of nine parameters, four of which are the coefficients of the dominant mass formula terms - the volume, volume symmetry, surface and Coulomb energy terms. The five additional coefficients specify various properties of nuclear systems: these coefficients were determined in the context of a Thomas-Fermi Model calculation. The droplet model also provides several equations relating various of these parameters. We have used the Thomas-Fermi Model formulae and droplet relations as presented by Myers and Swiatecki and attempted to determine the four remaining liquid drop coefficients by a least-squares fit to masses. The mass formula resulting from this fitting procedure contained some unsatisfactory features. Specifically, the value obtained for the volume symmetry coefficient was rather large (~ 50), the calculated Coulomb energies were not in good agreement with the Stanford scattering results and the residual proton and neutron shell corrections were not well behaved in the sense we have discussed previously. We were unable to eliminate these features without violating the basic droplet model relations.

We believe that these difficulties arise largely due to the premature dropping of terms in the expansion given by Myers and Swiatecki for the "bulk asymmetry" parameter, $\bar{\delta}$. In their final expression for the liquid drop energy, the volume symmetry energy is given by $J \bar{\delta}^2$ where J is the volume symmetry coefficient and the bulk asymmetry, $\bar{\delta}$, is given by

$$\bar{\delta} = \left(I + \frac{3}{8} \frac{C_1}{Q} \frac{Z^2}{A^{5/3}} \right) / \left(1 + \frac{9}{4} \frac{J}{Q} A^{-1/3} \right) \quad (2)$$

In this expression $I = (A-2Z)/A$, C_1 is the usual Coulomb energy coefficient and Q is an "effective surface stiffness" coefficient resulting from the droplet model analysis. A number of higher order terms have been omitted in this expression for $\bar{\delta}$; when we include these terms, we arrive at the final expression for $\bar{\delta}$ used in our preliminary studies:

$$\bar{\delta} = \frac{I + \frac{3C_1Z^2}{8HA^{5/3}} - \frac{C_1PZ}{8HJA^{2/3}} - \frac{3PI}{2HA^{2/3}} - \frac{3GC_1Z}{16HJA}}{1 + \frac{9J}{4Q}A^{-1/3} - \frac{3P}{2H}A^{-1/3} - \frac{9G}{4H}A^{-2/3} - \frac{9L}{4H}A^{-1/3}\bar{\epsilon} + \frac{9M}{4H}A^{-1/3}\bar{\delta}^2} \quad (3)$$

The additional parameters included in this expression are H (the "surface skin coefficient"), P (the "skin-symmetry coefficient"), G (the surface symmetry coefficient), L (the "density-symmetry coefficient"), M (the "symmetry anharmonicity coefficient") and the bulk variable $\bar{\epsilon}$ given by

$$\bar{\epsilon} = \frac{1}{K} \left(- 2a_2A^{-1/3} + L\bar{\delta}^2 + C_1 \frac{Z^2}{A^{4/3}} \right) \quad (4)$$

where K is the compressibility coefficient and a_2 is the surface energy coefficient. The relative importance of these higher order terms is illustrated below for two nuclei (Z = 30, A = 64 and Z = 84, A = 216). We have used the values quoted by Myers and Swiatecki¹⁾ for the various parameters: $C_1 = 0.717$, $H = 9.42$, $P = 17.55$, $J = 28.062$, $G = 45.4$, $Q = 16.04$, $L = 123.53$, $M = 2.673$, $K = 294.80$ and $a_2 = 18.560$ where all are in units of MeV:

$$\bar{\delta}(30,64) = \frac{0.0625 + 0.0251 - 0.0111 - 0.0436 - 0.0108}{1 + 0.986 - 0.698 - 0.675 - 7.41 \bar{\epsilon} + 0.16 \bar{\delta}^2} \sim 0.036 \quad (5)$$

$$\bar{\delta}(84,216) = \frac{0.222 + 0.0260 - 0.0139 - 0.103 - 0.00895}{1 + 0.657 - 0.465 - 0.300 - 4.94 \bar{\epsilon} + 0.107 \bar{\delta}^2} \sim 0.14$$

The added terms indicated here are clearly important. They lead to values of the bulk asymmetry, $\bar{\delta}$, which are considerably smaller than I, thus forcing the volume symmetry energy coefficient, J, to higher values in the least-squares fits to masses we described above. This sensitivity of the fitted coefficients to the details of the expansion for $\bar{\delta}$ is particularly disturbing when one notes that even the revised expression for $\bar{\delta}$ we have employed neglects some higher order corrections (see Myers and Swiatecki¹⁾, equation 2.15). We have concluded on the basis of these considerations that a reliable determination of the volume symmetry coefficient cannot be made for the droplet model in its published form. We have, nevertheless, made use of a number of the features of the droplet formula in the construction of our mass formula, as will be elaborated in the following section.

3. THE MASS FORMULA

The atomic mass formula we have arrived at in this study may be written in the form

$$\begin{aligned}
 (M-A) = & 8.07144 A - 0.78245 Z \\
 & + \beta_0 A + \beta_2 I^2 A + \beta_4 I^4 A + \beta_6 I^6 A \\
 & + \gamma_0 A^{2/3} + \gamma_2 I^2 A^{2/3} + \gamma_4 I^4 A^{2/3} \\
 & + E_{\text{Curvature}} + E_{\text{Wigner}} + E_{\text{Coulomb}} + S(Z,N) + P(Z,N)
 \end{aligned} \tag{6}$$

where $(M-A)$ is the mass excess in MeV on the ^{12}C scale of masses and $I = (A-2Z)/A$. We have included the higher order volume symmetry terms through I^6 and the surface symmetry terms through I^4 ; no reliable estimates are available for the magnitudes of still higher order terms. The curvature energy is written in the form

$$E_{\text{Curvature}} = \alpha_c A^{1/3} \tag{7}$$

where α_c is a parameter to be specified. The Wigner energy is written in the form suggested by Myers and Swiatecki⁹⁾

$$E_{\text{Wigner}} = \alpha_w \exp(-6 |I|) \tag{8}$$

where α_w is a coefficient to be determined. $S(Z,N)$ and $P(Z,N)$ are the total shell and pairing energies, respectively.

The expression for the total Coulomb energy used in this work is given by

$$E_{\text{Coulomb}} = a_1 \frac{Z^2}{A^{1/3}} + a_2 Z^2 A^{1/3} + a_3 \frac{Z^2}{A} + a_4 \frac{Z^2}{A^{4/3}} \tag{9}$$

Here, in addition to the usual Coulomb and Coulomb exchange energy terms, we have included two terms from the droplet model formula¹⁾: the term $a_2 Z^2 A^{1/3}$ is a "Coulomb redistribution" energy correction and the term $a_3 Z^2 / A$ is a Coulomb diffuseness energy contribution, which

acts to correct the pure Coulomb energy for the effects of a finite surface. The coefficients of the four terms are given by

$$\begin{aligned}
 a_1 &= 0.8640 / r_0 \\
 a_2 &= \frac{-0.0088869}{r_0} \left(0.015265 + \frac{0.250}{\beta_2} \right) \\
 a_3 &= -1.50117 / r_0^3 \\
 a_4 &= -0.65976 / r_0
 \end{aligned}
 \tag{10}$$

where r_0 is the nuclear radius parameter and β_2 is the volume symmetry coefficient. The numerics for the parameters a_2 , a_3 and a_4 have been taken from the droplet model formula¹⁾. The values for the Coulomb diffuseness coefficient (a_3) and the Coulomb exchange coefficient (a_4) are quite consistent with those obtained by Cameron and Elkin⁶⁾ for a trapezoidal density model of the nucleus.

Our determination of the various mass formula coefficients has proceeded in the following manner. It has been our experience that meaningful coefficients can be obtained by a least-squares fit to masses for only the dominant terms in the liquid drop reference formula. The coefficients of lesser terms can vary dramatically when fits are performed to restricted groups of nuclei. We have therefore chosen to determine four of the reference mass formula parameters - the volume energy coefficient (β_0), the volume symmetry energy coefficient (β_2), the surface energy coefficient (γ_0) and the nuclear radius parameter (r_0) - by a least-squares fit to experimental masses¹⁰⁾. These fits are performed for specified values of the remaining parameters (β_4 , β_6 , γ_2 , γ_4 , α_c and α_w). Having thus defined a smooth reference mass surface, the shell and pairing energies are calculated by fitting the differences between the liquid drop masses and the experimental masses. We have adopted the same procedure as used by Cameron and Elkin⁶⁾: the shell corrections are determined independently for each value of Z and N . While this approach necessitates the determination of a rather large number of adjustable constants, we believe that the shell corrections thus obtained have physical significance since they exhibit a generally smooth and understandable variation with nucleon number between closed shells.

The assumption of the independence of the neutron and proton corrections enables us to write

$$S(Z,N) + P(Z,N) = C(Z) + C(N) \quad (11)$$

where $C(Z)$ and $C(N)$ are the total shell-plus-pairing corrections for proton number Z and neutron number N

$$\begin{aligned} C(Z) &= S(Z) + P(Z) \\ C(N) &= S(N) + P(N) \end{aligned} \quad (12)$$

For each nucleus we can therefore write an expression of the form

$$(M-A)_{\text{exp.}} - (M-A)_{\text{ref.}} = C(Z) + C(N) \quad (13)$$

where $(M-A)_{\text{exp.}}$ is the experimental mass excess and $(M-A)_{\text{ref.}}$ is the reference (liquid drop) mass excess without corrections. The total shell-plus-pairing corrections for each proton and neutron number are then determined by a least-squares procedure.

With regard to the construction of a mass formula, only the total proton and neutron corrections defined above are required. We are interested as well, however, in the construction of a nuclear systematics which will enable us to make predictions of the various reaction and decay properties of neutron-rich nuclei. For this purpose, it is convenient to obtain separate shell and pairing energies. The total corrections determined as outlined above do, in fact, exhibit a pronounced odd-even oscillation. We have removed the pairing energies from the total corrections in a systematic manner, insisting on a generally smooth variation of the $S(Z)$ and $S(N)$.

As stated previously, of the ten parameters in our reference mass formula only four can be meaningfully determined, in our view, by a least-squares fit to masses. The higher order volume symmetry coefficients, the surface symmetry coefficients and the curvature and Wigner coefficients must be otherwise estimated. Preliminary studies revealed that the fitting of the reference formula to masses near the valley of beta stability is quite insensitive to three of these

parameters - the two higher order volume symmetry coefficients (β_4 and β_6) and the higher order surface symmetry coefficient (γ_4). It is important to recognize, however, that these three parameters play a significant role in determining the position of the neutron drip line. All mass formula predictions of the relative stability of superheavy nuclei are sensitive to these energy contributions. We have used the value $\beta_4 = -24.545$ predicted by the Thomas-Fermi Model parameters of Myers and Swiatecki¹⁾ in their large-A expansion for the droplet energy. For the coefficient β_6 , our choice has been influenced both by the ratio β_6/β_4 predicted by the calculations of Weiss and Cameron¹¹⁾ for infinite nuclear matter and by a consideration of the relative position of the drip line for nuclei with low proton numbers: we take $\beta_6 = 20.0$. Finally, we choose $\gamma_4 = 40.0$, again guided largely by a consideration of the position of the drip line. We emphasize that these choices are highly uncertain; to the extent that these choices are arbitrary, so is the position of the drip line predicted by our mass formula.

Our selection of coefficients for the surface symmetry energy (γ_4), the Wigner energy (α_w) and the curvature energy (α_c) terms has been guided by several characteristics of the resulting mass formula. The magnitudes of the surface symmetry energy and the Wigner energy terms strongly influence the gross variations of the proton and neutron shell corrections with mass number. The curvature energy term influences the value obtained for the nuclear radius parameter, r_0 , and thus the total Coulomb energy. The nature of these dependences and the reasons for our choices of these coefficients will be illustrated below. For the moment, we simply quote our final values: $\gamma_2 = -70.0$, $\alpha_c = -10.0$ and $\alpha_w = -11.50$.

The final coefficients enumerated above are collected in Table 1. The numerical values, as throughout this paper, are given in MeV. For these values, a least-squares fit to masses was performed for the following four coefficients: β_0 (volume energy), β_2 (volume symmetry), γ_0 (surface energy) and r_0 (nuclear radius parameter). The coefficients thus obtained are also given in Table 1. The proton and neutron shell and pairing corrections determined by the procedure defined earlier are presented in Tables 2 and 3. Note that pairing corrections are given only for even nucleon numbers; they are defined to be zero for odd values of Z and N.

The proton and neutron shell corrections are plotted as a function of nucleon number in Fig. 1. Both sets of corrections exhibit a rather smooth variation with nucleon number; the effects of shell closures at proton numbers $Z = 28, 50$ and 82 are readily apparent, as are those for neutron numbers $N = 28, 50, 82$ and 126 . Note particularly that there is no gross dependence of these two sets of shell corrections on nucleon number; that is, neither the proton or the neutron corrections show a general increase or decrease over the entire range.

We believe that this 'level' behavior of the proton and neutron shell corrections is significant. We would interpret any alternative behavior (for example an overall increase in the proton corrections together with a general decrease of the neutron corrections) as an indication that the reference formula was somehow skewed relative to the behavior of the experimental masses. This criterion, as we have discussed in our introduction, has provided a guide for our determination of the magnitudes of the Wigner energy and the surface symmetry energy. The influences of these two terms on the behavior of the proton and neutron shell corrections are illustrated in Figs. 2 and 3. The corrections shown in Fig. 2 are those obtained by setting the Wigner energy term to zero. This has resulted in a profound increase in the proton corrections in the region $Z \leq 30$ and a comparable decrease in the neutron corrections for $N \leq 40$. Note that the ordinate for this figure has been altered by a factor of three relative to Fig. 1. As we can find no alternative method for leveling these corrections in the region $Z \leq 30, N \leq 40$, we would argue in the spirit of the semi-empirical mass formula that the inclusion of a Wigner-type term is justifiable.

The shell corrections shown in Fig. 3 are those resulting from our procedures when the surface symmetry coefficient, γ_2 , is set equal to zero. This results in a severe distortion of the behavior of both the proton and the neutron shell correction functions. We should point out again that the total shell corrections, $S(Z) + S(N)$, for nuclei near the valley of beta stability are still quite well behaved, as these corrections have been fit to the experimental masses. For purposes of extrapolation, however, we believe that such a distorted behavior is entirely unsatisfactory.

The surface symmetry energy and the Wigner energy have somewhat opposing effects on the behavior of the shell correction functions, as indicated by the results in Figs. 2 and 3. The values we have taken for the coefficients of these two terms therefore represent to some extent what we have found to be a satisfactory compromise.

Our choice for the coefficient of the curvature energy term is governed by Coulomb energy considerations. Myers and Swiatecki¹⁾ determined this coefficient to be approximately 9-10 Mev. This value was obtained in the context of the Thomas-Fermi model as a difference between small quantities and is therefore, in our opinion, far less reliable than their other estimates. Keeping all other specified parameters as before (Table 1), we have constructed mass formulas for three different choices of the curvature energy coefficient: $\alpha_c = -10$, 0, and + 10. The behavior of the resulting shell corrections is not particularly sensitive to the value of this parameter, as is illustrated in Fig. 4. While some slight tipping of the proton corrections relative to the neutron corrections is evident compared to those of our adopted mass formula shown in Fig. 1, the magnitude of this effect is far less than we observed when the Wigner and surface symmetry energy terms were adjusted.

The influence of the curvature energy term on the determination of the nuclear radius parameter, r_0 , and thus on the Coulomb energy, is significant. This dependence is illustrated in Table 4, where the Coulomb energies calculated from our formula for the three values of α_c are compared to those deduced from the experimental (Stanford) charge distributions¹²⁾. The fitted mass formula coefficients for the three cases are also tabulated. For the purposes of these comparisons, the calculated Coulomb energies are given by

$$E_{\text{Coulomb}} = a_1 \frac{Z^2}{A^{1/3}} + 2 a_2 Z^2 A^{1/3} + a_3 \frac{Z^2}{A} \quad (14)$$

where a_1 , a_2 and a_3 are as given in equations (10). The Coulomb exchange energy contribution is not appropriate to these comparisons, and therefore is omitted. Further, we have adjusted the redistribution energy term to remove a contribution which is a purely nuclear effect¹⁾.

Our motivation for choosing the coefficient $\alpha_c = -10.0$ Mev is apparent from these comparisons. For this choice, the agreement of our calculated Coulomb energies with the Stanford results is extremely good. The maximum deviation is less than 2.5% and, moreover, our determinations oscillate somewhat about the accepted values. For the choice $\alpha_c = 0$, the calculated energies are all low by 2-5% while, for $\alpha_c = +10.0$, they are all low by 6-10%.

The first backward shell correction differences for protons and neutrons ($\delta S(Z)$ and $\delta S(N)$) are shown in Fig. 5 and 6 for our final mass formula. We have also indicated in these figures possible extrapolations of the shell correction differences to large proton and neutron numbers, assuming that the next closed shells occur at $Z = 114$ and $N = 184$, respectively. These differences are expected to be large and positive immediately following closed shells and to fall gradually and smoothly to large negative values immediately preceding the next closed shells, assuming the nuclei to be undeformed. This behavior is quite apparent in our corrections for neutron numbers in the range $21 \leq N \leq 28$, $29 \leq N \leq 50$ and $51 \leq N \leq 82$. The proton shell corrections similarly show shell features at proton numbers $Z = 20, 28$ and 50 ; a proton shell feature at $Z = 40$ is also evident.

For deformed nuclei, the $\delta S(Z)$ and $\delta S(N)$ are expected to be small. This is true for neutron numbers in the ranges $90 \leq N \leq 115$ and $135 \leq N \leq 150$ and for proton numbers $60 \leq Z \leq 75$. The $\delta S(Z)$ for protons in the range $90 \leq Z \leq 101$ are all negative by approximately 0.5 MeV. It is unclear to us at this time whether this feature implies that our reference mass surface is slightly skewed in this region; crude estimates based on the single-proton levels of Gustafson *et al*¹³⁾ suggest to us that this may be a real shell feature.

The shell correction differences plotted in Fig. 5 and 6 exhibit a very different character in regions of nuclear deformation than in undeformed regions. Such regions of deformation among heavier nuclei occur only when both the neutron numbers and the proton numbers are substantially removed from closed-shell values. For purposes of extrapolation into the neutron-rich regions off the valley of beta stability, it is clear that some allowance should be made for the possibility that both undeformed and deformed shell corrections may be

required for certain ranges of proton or neutron number. Based on the characteristic behavior of the shell correction differences shown in Figs. 5 and 6, we have interpolated "undeformed" shell corrections for both proton and neutron numbers associated with the rare-earth region. These corrections are presented in Table 5. We employ the following prescription for choosing the appropriate shell correction in these cases. For proton numbers in the range $60 \leq Z \leq 76$, the undeformed shell corrections should be chosen when $122 \leq N \leq 130$ or $180 \leq N \leq 188$. Similarly, for neutron numbers in the range $90 \leq N \leq 115$, the undeformed shell corrections should be used when $46 \leq Z \leq 54$. In both instances, some smoothing across the transition region may be desirable.

4. NUCLEAR LEVEL DENSITY SYSTEMATICS

One of the essential ingredients of any nuclear systematics aimed at estimating the properties of neutron-rich nuclei is the nuclear level density. Our calculations both of nuclear radiation widths and of the beta decay lifetimes for neutron-rich nuclei formed in the rapid neutron capture process require these level density estimates. It is therefore appropriate for us to consider whether the mass formula we have constructed provides a basis for a realistic level density systematics.

The formulation of the theory of nuclear level densities based upon the Fermi gas model of the nucleus^{14,15)} leads to the following expression for the nuclear level density at high excitation energies:

$$\rho(U) = \frac{\pi^{1/2} \exp(-2(aU)^{1/2})}{12 a^{1/4} U^{5/4}} \quad (15)$$

Here $\rho(U)$ is the total density of nuclear states at an excitation U above the degenerate state. The level density parameter a is predicted to obey the relation

$$a/A = \text{constant} \quad (16)$$

Gilbert and Cameron³⁾ have inferred 'experimental' values of a for a large number of nuclei by comparing the above expression for $\rho(U)$ with experimental determinations of the densities of neutron resonances.

The values of a/A thus obtained exhibited features which coincided with the positions of closed nucleon shells. They demonstrated, further, that a correlation existed between these values of a/A and the total shell corrections of the mass formula of Cameron and Elkin⁶⁾.

In the work described above, a distinction was drawn between the deformed and undeformed nuclei: two linear relationships between a/A and the shell corrections were obtained. The criterion used by Gilbert and Cameron to define deformed nuclei was rather crude; by their definition, deformed nuclei are those for which

$$\begin{aligned} 54 \leq Z \leq 78 \quad \text{and} \quad 86 \leq N \leq 122 \\ \text{or} \\ 86 \leq Z \leq 122 \quad \text{and} \quad 130 \leq N \leq 180 \end{aligned} \tag{17}$$

In a subsequent analysis of this problem, Brancazio and Cameron¹⁶⁾ demonstrated that a single relation can be obtained if a deformation energy correction is subtracted from the shell correction. They demonstrated further that this deformation energy is roughly proportional to the distance (number of neutrons or protons) to the nearest closed nucleon shell. We have determined a similar correlation between a/A and the total shell corrections calculated for the mass formula presented in this paper. A least-squares fit to the data compiled by Gilbert and Cameron gives the following relation

$$a/A = 0.139 + 0.0102 (S - 0.33D) \tag{18}$$

where S is the total shell energy and D is the 'distance' to the nearest closed nucleon shell. A plot of a/A verses $(S-0.33D)$ is presented in Fig. 7; the least-squares line is also shown in this figure. The distinction between deformed and undeformed nuclei is that due to Gilbert and Cameron (equations 17).

5. SUMMARY AND DISCUSSION

The semi-empirical atomic mass formula we have developed in this paper has two features which we find particularly satisfying: the shell-correction functions for protons and neutrons show no gross

systematic dependences on nucleon number and the calculated Coulomb energies are in excellent agreement with those deduced from the Stanford charge distributions. In order to incorporate these features, we found it necessary to introduce both a Wigner-type energy term and a curvature energy term of negative sign. Our justification for the inclusion of these terms is entirely empirical in nature, although a curvature term of positive sign is in fact predicted for the droplet model formula¹⁾. We are continuing our mass formula studies in an attempt to gain a better understanding of the nature of these energy corrections.

The correlation of the nuclear level density parameter 'a' with the total shell corrections calculated from our formula is also quite satisfactory. The deformation energy adjustment to our shell corrections predicted by the least-squares fitting procedure, $\Delta S = -0.33D$, is in excellent agreement with the deformation energy relation determined by Brancazio and Cameron¹⁶⁾, $E_{\text{deformation}} = 0.33D$. In both cases, D is the distance to the nearest closed nucleon shell. This improved level density correlation, together with the more satisfactory behavior of the shell-correction functions of our mass formula, give us greater confidence in extrapolations of these systematics into the neutron-rich regions.

There are still large uncertainties associated with such extrapolations due to the absence of reliable estimates of the coefficients of the higher order volume symmetry and surface symmetry energy terms. As we have discussed in the text, these terms play a dominant role in the determination of the position of the neutron drip line. We emphasize, in conclusion, the need for further theoretical studies of this problem.

ACKNOWLEDGMENTS

The authors wish to thank Dr. R. Jastrow for the hospitality of the Goddard Institute for Space Studies, where the computations were performed. This research was supported in part by grants from the U.S. National Science Foundation, the U.S. National Aeronautics and Space Administration, and the U.S. Atomic Energy Commission.

REFERENCES

- 1) W.D. Myers and W.J. Swiatecki, *Annals Phys.* 55, 395 (1969).
- 2) A.G.W. Cameron, M.D. Delano and J.W. Truran, *The Dynamics of the Rapid Neutron Capture Process* (these proceedings).
- 3) A. Gilbert and A.G.W. Cameron, *Can. J. Phys.* 43, 1446 (1965).
- 4) C.F. von Weizsacker, *Z. Physik* 96, 431 (1935).
- 5) A.G.W. Cameron, *Can. J. Phys.* 37, 322 (1959).
- 6) A.G.W. Cameron and R.M. Elkin, *Can. J. Phys.* 43, 1288 (1965).
- 7) J.W. Truran and A.G.W. Cameron, *Arkiv f. Fysik* 36, 509 (1968).
- 8) A.G.W. Cameron, *At. Energy Can. Ltd. Rept.* CRL-41 (1957).
- 9) W.D. Myers and W.J. Swiatecki, *Nucl. Phys.* 81, 1 (1966).
- 10) J.H.E. Mattauch, W. Thiele and A.H. Wapstra, *Nucl. Phys.* 67, 1 (1965).
- 11) R.A. Weiss and A.G.W. Cameron, *Can. J. Phys.* 47, 2171 (1969).
- 12) B.Hahn, D.G. Ravenhall and R. Hofstadter, *Phys. Rev.* 101, 1131 (1956).
- 13) C. Gustafson, I.L. Lamm, B. Nilsson and S.G. Nilsson, *Arkiv f. Fysik* 36, 613 (1968).
- 14) H.A. Bethe, *Phys. Rev.* 50, 332 (1936).
- 15) H.A. Bethe, *Rev. Mod. Phys.* 9, 69 (1937).
- 16) P.J. Brancazio and A.G.W. Cameron, *Can. J. Phys.* 47, 1029 (1969).

TABLE 1

MASS FORMULA COEFFICIENTS

<u>Specified Coefficients</u>	<u>Energy Term</u>	<u>Numerical Value</u>
β_4	$\beta_4 I^4 A$	- 24.545
β_6	$\beta_6 I^6 A$	20.0
γ_2	$\gamma_2 I^2 A^{2/3}$	- 70.0
γ_4	$\gamma_4 I^4 A^{2/3}$	40.0
α_c	$\alpha_c A^{1/3}$	- 10.0
α_w	$\alpha_w \exp(-6 I)$	- 11.50
 <u>Fitted Coefficients</u>		
β_0	$\beta_0 A$	- 17.070591
β_2	$\beta_2 I^2 A$	36.698710
γ_0	$\gamma_0 A^{2/3}$	27.184659
r_0	$(R=r_0 A^{1/3})$	1.104825

TABLE 2

SHELL CORRECTIONS

Z or N	S(Z)	S(N)	Z or N	S(Z)	S(N)
10	2.349	2.439			
11	1.936	1.829	41	1.128	0.140
12	1.596	1.419	42	1.007	0.149
13	1.061	0.746	43	0.603	-0.001
14	0.341	-0.082	44	0.013	-0.230
15	-0.040	-0.832	45	-0.635	-0.604
16	0.565	-0.960	46	-1.258	-1.010
17	1.065	-1.006	47	-1.905	-1.570
18	1.536	-1.045	48	-2.562	-2.466
19	1.972	-1.114	49	-3.266	-3.489
20	1.855	-0.900	50	-4.099	-4.552
21	2.043	-0.081	51	-3.615	-4.214
22	1.931	0.334	52	-3.171	-3.375
23	1.652	0.064	53	-2.814	-2.526
24	1.347	-0.639	54	-2.337	-1.725
25	0.973	-1.363	55	-1.778	-0.923
26	0.579	-2.138	56	-1.220	-0.164
27	0.159	-2.987	57	-0.694	0.601
28	-0.487	-4.042	58	-0.181	1.316
29	-0.192	-4.001	59	0.323	1.947
30	0.443	-3.582	60	0.624	2.482
31	0.932	-3.120	61	0.841	2.971
32	1.387	-2.677	62	0.904	3.398
33	1.810	-2.259	63	0.906	3.737
34	1.969	-1.778	64	0.930	3.979
35	2.067	-1.315	65	0.919	4.183
36	2.064	-0.944	66	0.934	4.374
37	1.825	-0.599	67	0.941	4.517
38	1.539	-0.285	68	0.978	4.605
39	1.251	-0.020	69	0.982	4.539
40	0.957	0.121	70	1.083	4.375

TABLE 2 (continued)

SHELL CORRECTIONS

Z or N	S(Z)	S(N)	Z or N	S(Z)	S(N)
71	1.201	4.043	101	-3.499	0.727
72	1.281	3.672	102	-3.042	0.574
73	1.189	3.250	103		0.436
74	0.963	2.776	104		0.320
75	0.781	2.254	105		0.264
76	0.738	1.715	106		0.397
77	0.696	1.151	107		0.507
78	0.119	0.463	108		0.405
79	-0.619	-0.237	109		0.346
80	-1.265	-1.031	110		0.369
81	-1.898	-1.850	111		0.397
82	-2.431	-2.722	112		0.403
83	-1.326	-1.663	113		0.379
84	-0.268	-0.724	114		0.184
85	0.737	0.035	115		-0.226
86	1.451	0.786	116		-0.737
87	2.138	1.587	117		-1.305
88	2.307	2.145	118		-1.950
89	2.221	2.669	119		-2.565
90	2.041	2.680	120		-3.126
91	1.827	2.488	121		-3.721
92	1.239	2.243	122		-4.393
93	0.747	1.969	123		-5.082
94	0.214	1.778	124		-5.921
95	-0.263	1.663	125		-6.712
96	-0.778	1.487	126		-6.853
97	-1.272	1.325	127		-5.592
98	-1.800	1.148	128		-4.413
99	-2.302	0.962	129		-3.333
100	-2.846	0.843	130		-2.413

TABLE 2 (continued)

SHELL CORRECTIONS

Z or N	S(Z)	S(N)	Z or N	S(Z)	S(N)
131		-1.582	146		1.449
132		-0.966	147		1.596
133		-0.421	148		1.712
134		-0.123	149		1.851
135		0.228	150		1.949
136		0.543	151		2.044
137		0.874	152		2.155
138		1.059	153		2.307
139		1.181	154		2.621
140		1.186	155		3.096
141		1.029			
142		1.029			
143		1.153			
144		1.227			
145		1.330			

TABLE 3
PAIRING CORRECTIONS

Z or N	P(Z)	P(N)	Z or N	P(Z)	P(N)
10	-2.200	-2.400			
12	-2.120	-2.358	72	-0.714	-1.254
14	-1.981	-2.057	74	-0.799	-1.310
16	-1.491	-1.462	76	-0.840	-1.171
18	-1.450	-1.592	78	-0.726	-1.092
20	-1.701	-1.528	80	-0.815	-1.062
22	-1.344	-1.470	82	-0.715	-0.713
24	-1.349	-1.310	84	-0.788	-0.822
26	-1.397	-1.316	86	-0.793	-0.843
28	-1.311	-1.265	88	-0.663	-0.968
30	-1.161	-1.279	90	-0.705	-1.117
32	-1.201	-1.256	92	-0.711	-0.999
34	-1.449	-1.285	94	-0.561	-0.877
36	-1.331	-1.440	96	-0.694	-0.844
38	-1.272	-1.517	98	-0.683	-0.889
40	-1.198	-1.486	100	-0.501	-0.729
42	-1.340	-1.456	102	-0.491	-0.706
44	-1.407	-1.471	104		-0.623
46	-1.287	-1.336	106		-0.511
48	-1.334	-1.341	108		-0.773
50	-1.307	-1.278	110		-0.662
52	-1.128	-0.821	112		-0.808
54	-1.152	-0.814	114		-0.889
56	-1.139	-1.095	116		-0.930
58	-1.138	-1.147	118		-0.771
60	-1.115	-1.295	120		-0.751
62	-1.070	-1.281	122		-0.835
64	-1.096	-1.245	124		-0.658
66	-1.123	-1.197	126		-0.607
68	-0.901	-1.227	128		-0.657
70	-0.933	-1.291	130		-0.695

TABLE 3 (continued)

PAIRING CORRECTIONS

Z or N	P(Z)	P(N)	Z or N	P(Z)	P(N)
132		-0.457	152		-0.654
134		-0.345	154		-0.557
136		-0.452			
138		-0.648			
140		-0.681			
142		-0.416			
144		-0.545			
146		-0.482			
148		-0.481			
150		-0.611			

TABLE 4

COULOMB ENERGY COMPARISONS

NUCLEUS	E (Stanford) (MeV)	E (Calculated) - E (Stanford) / E. (Stanford)		
		$\alpha_c = 10$	$\alpha_c = 0$	$\alpha_c = -10$ *
$_{20}\text{Ca}^{40}$	78	-0.0676	-0.0204	0.0243
$_{23}\text{V}^{51}$	100	-0.0998	-0.0520	-0.0062
$_{27}\text{Co}^{59}$	130	-0.0841	-0.0343	0.0137
$_{49}\text{In}^{115}$	360	-0.1060	-0.0538	-0.0024
$_{51}\text{Sb}^{122}$	380	-0.0990	-0.0461	0.0059
$_{79}\text{Au}^{197}$	790	-0.1053	-0.0512	0.0023
$_{83}\text{Bi}^{209}$	840	-0.0886	-0.0333	0.0214

FITTED COEFFICIENTS

Volume Energy	-15.021	-16.046	-17.071
Volume Symmetry Energy	34.025	35.371	36.699
Surface Energy	14.877	21.024	27.185
Nuclear Radius Parameter	1.2517	1.1739	1.1048

* Adopted value:
this mass formula

TABLE 5

UNDEFORMED SHELL CORRECTIONS

<u>PROTONS</u>		<u>NEUTRONS</u>	
Z	S (Z)	N	S (N)
60	0.773	90	3.123
61	1.174	91	3.513
62	1.532	92	3.845
63	1.853	93	4.118
64	2.135	94	4.338
65	2.373	95	4.504
66	2.568	96	4.617
67	2.721	97	4.678
68	2.829	98	4.688
69	2.871	99	4.646
70	2.844	100	4.554
71	2.749	101	4.429
72	2.586	102	4.279
73	2.453	103	4.101
74	2.045	104	3.892
75	1.667	105	3.655
76	1.219	106	3.391
		107	3.100
		108	2.782
		109	2.438
		110	2.066
		111	1.667
		112	1.241
		113	0.788
		114	0.309
		115	-0.200

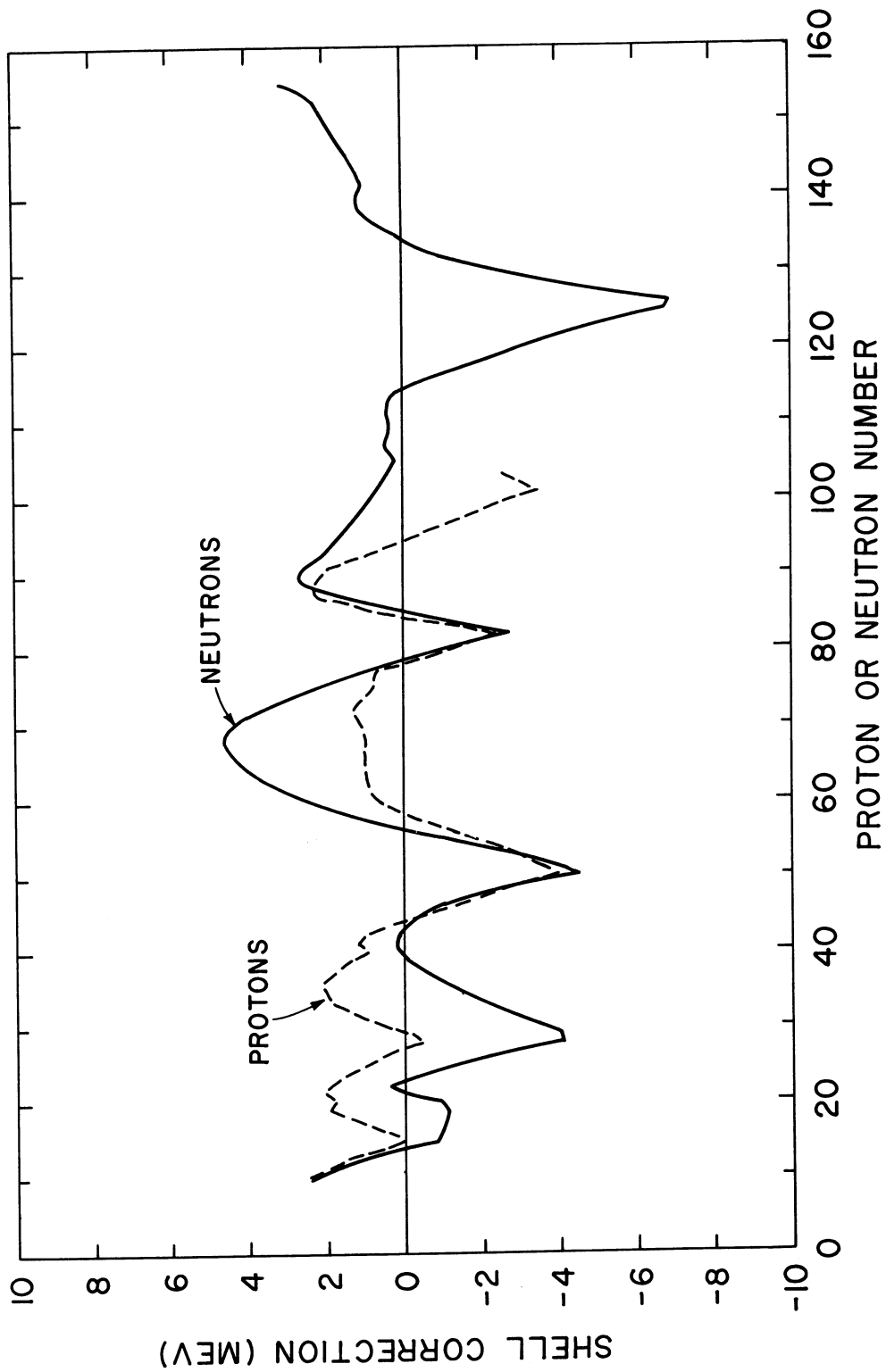


Fig. 1
Proton and neutron shell corrections for
the adopted mass formula.

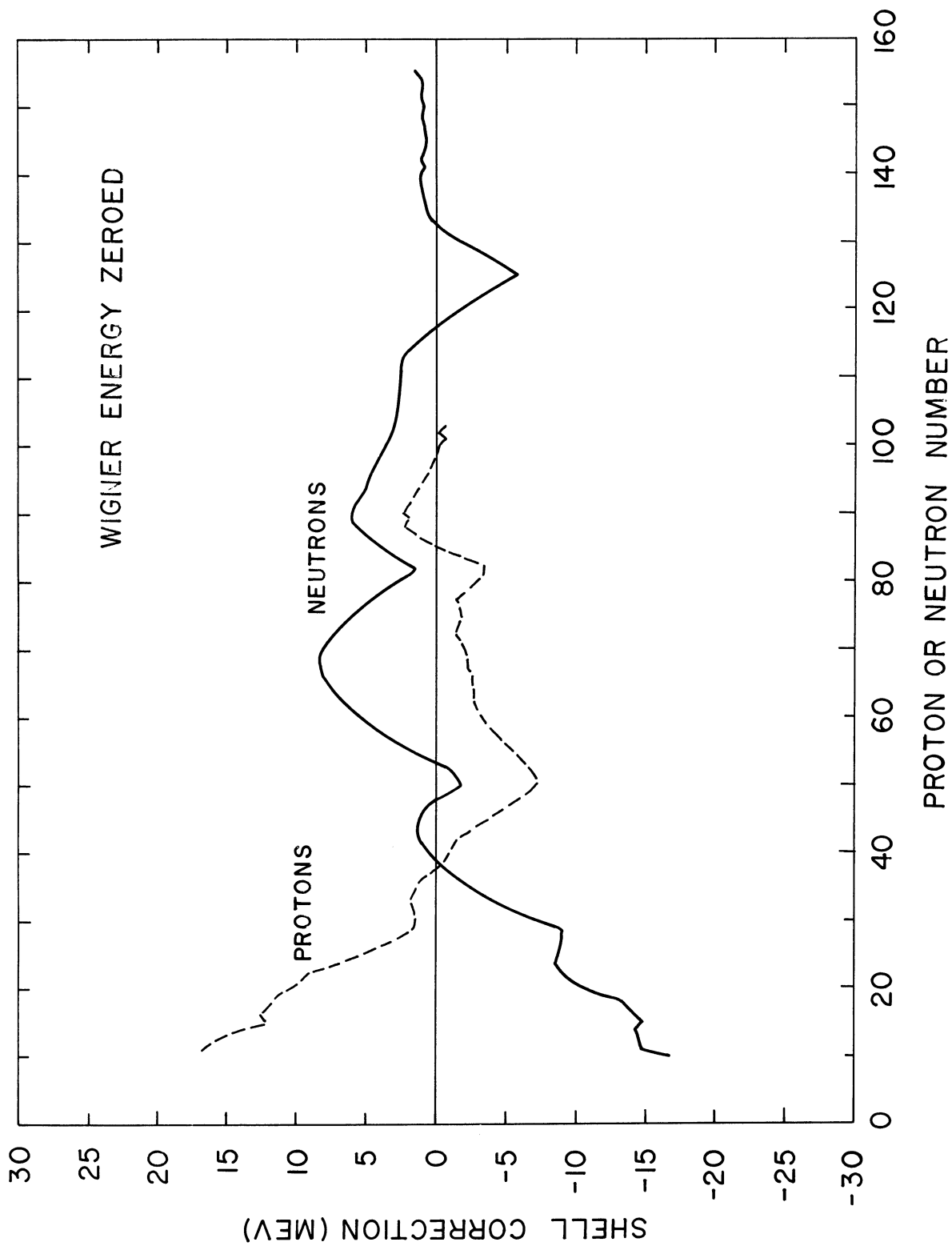


Fig. 2

Proton and neutron shell corrections
calculated for the choice: $\alpha_w = 0$.

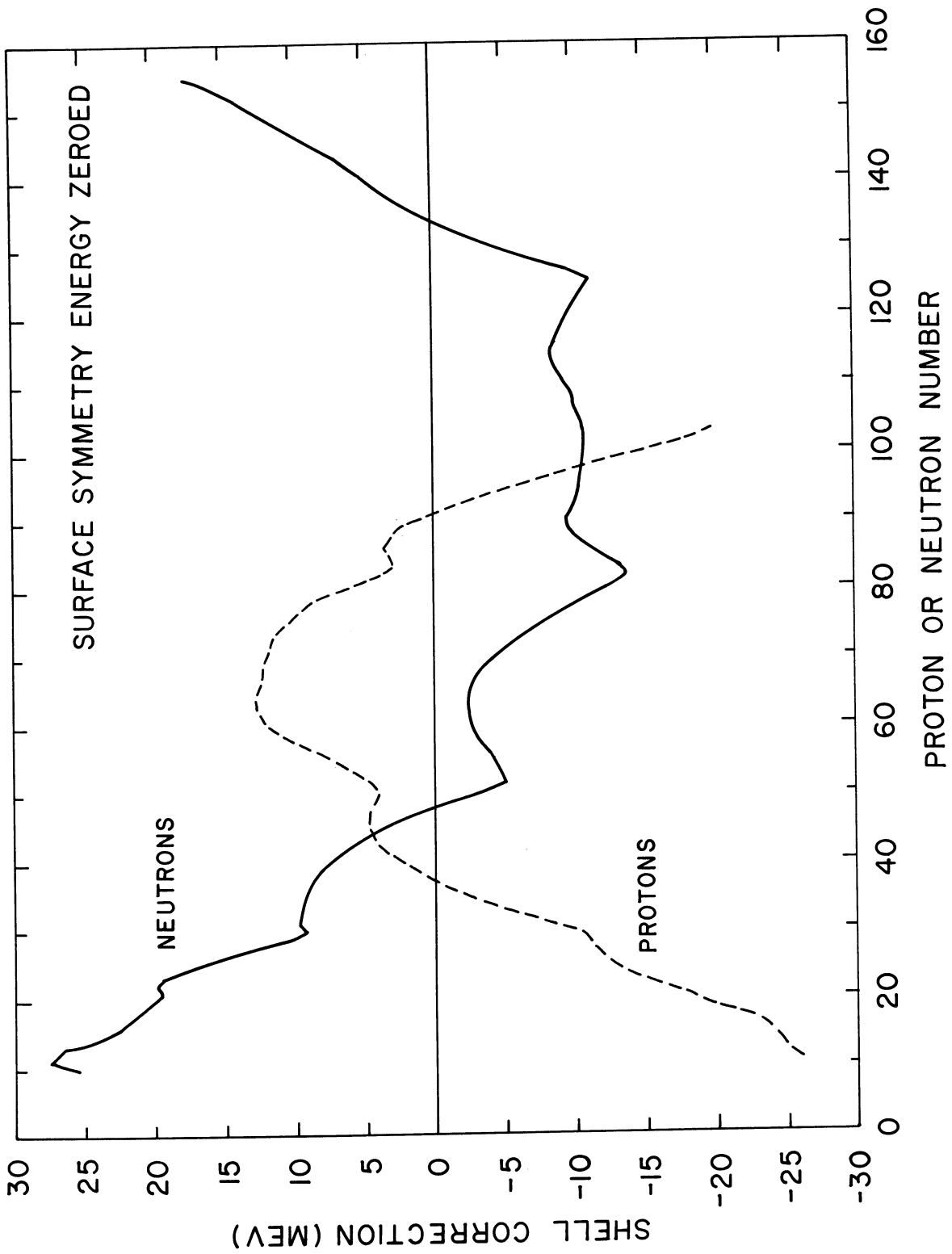


Fig. 3
Proton and neutron shell corrections
calculated for the choice: $\gamma_2 = 0$.

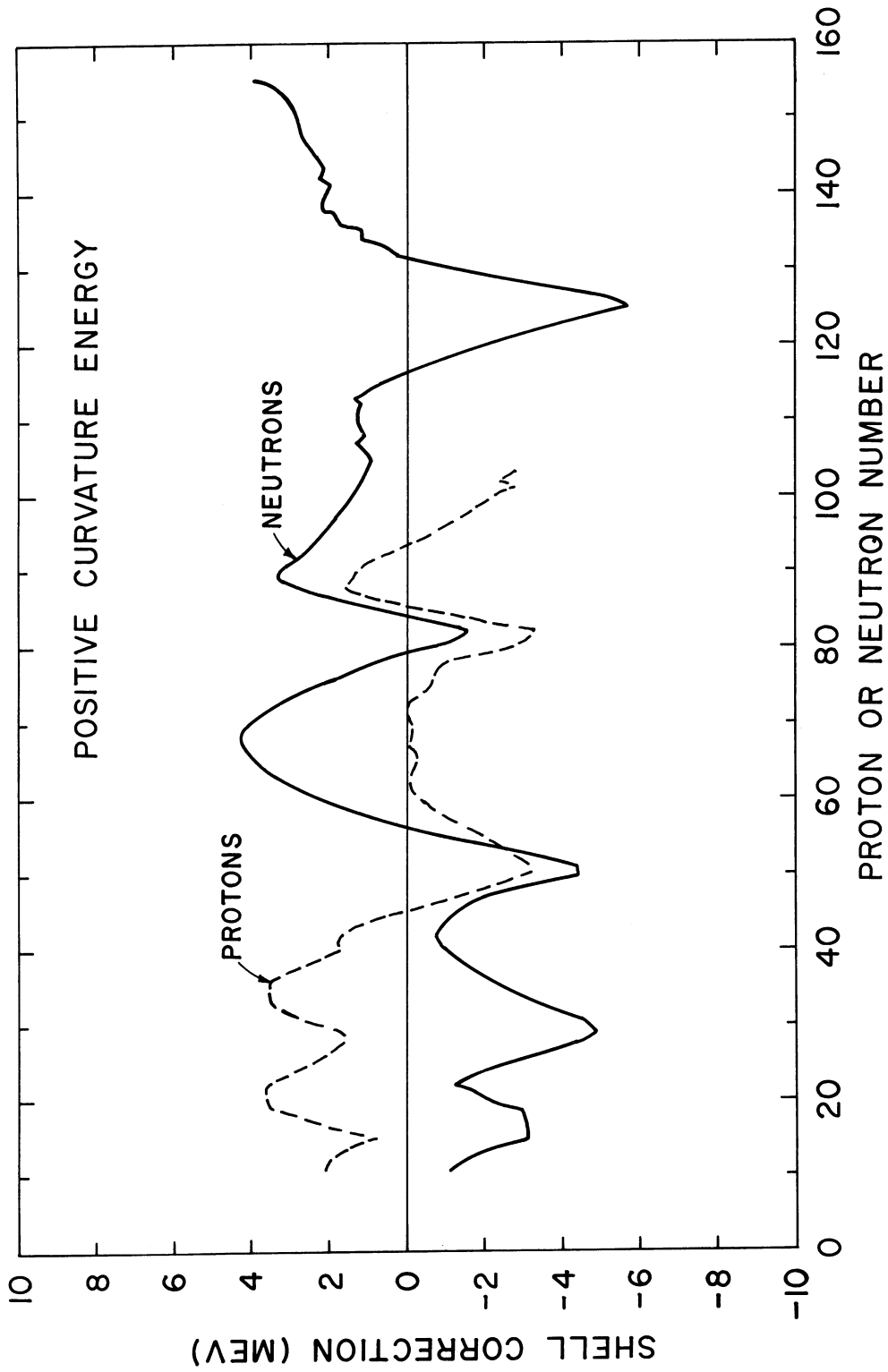


Fig. 4

Proton and neutron shell corrections
calculated for the choice: $\alpha_c = +10$ MeV.

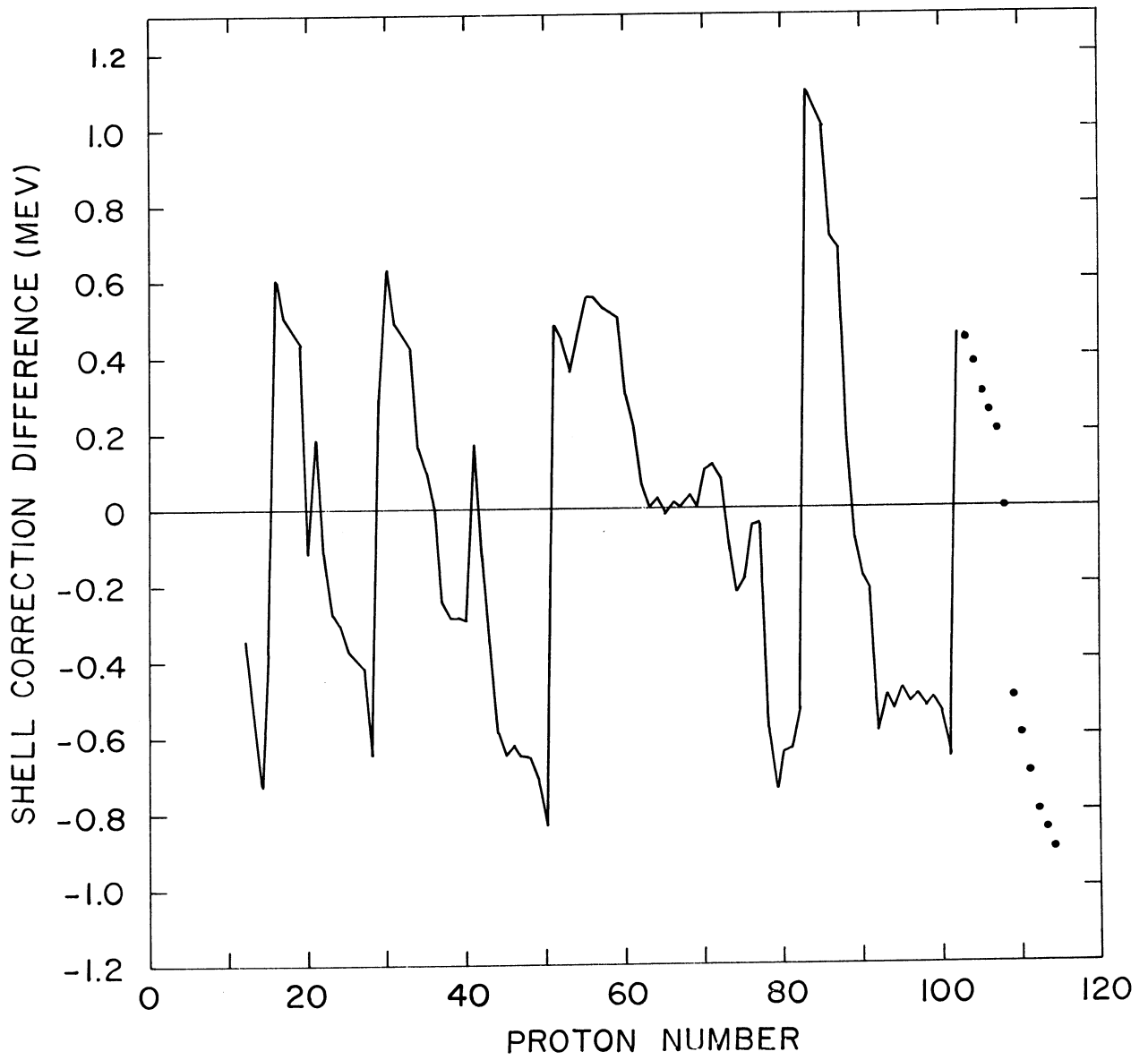


Fig. 5
Shell-correction differences for protons
plotted as a function of proton number.

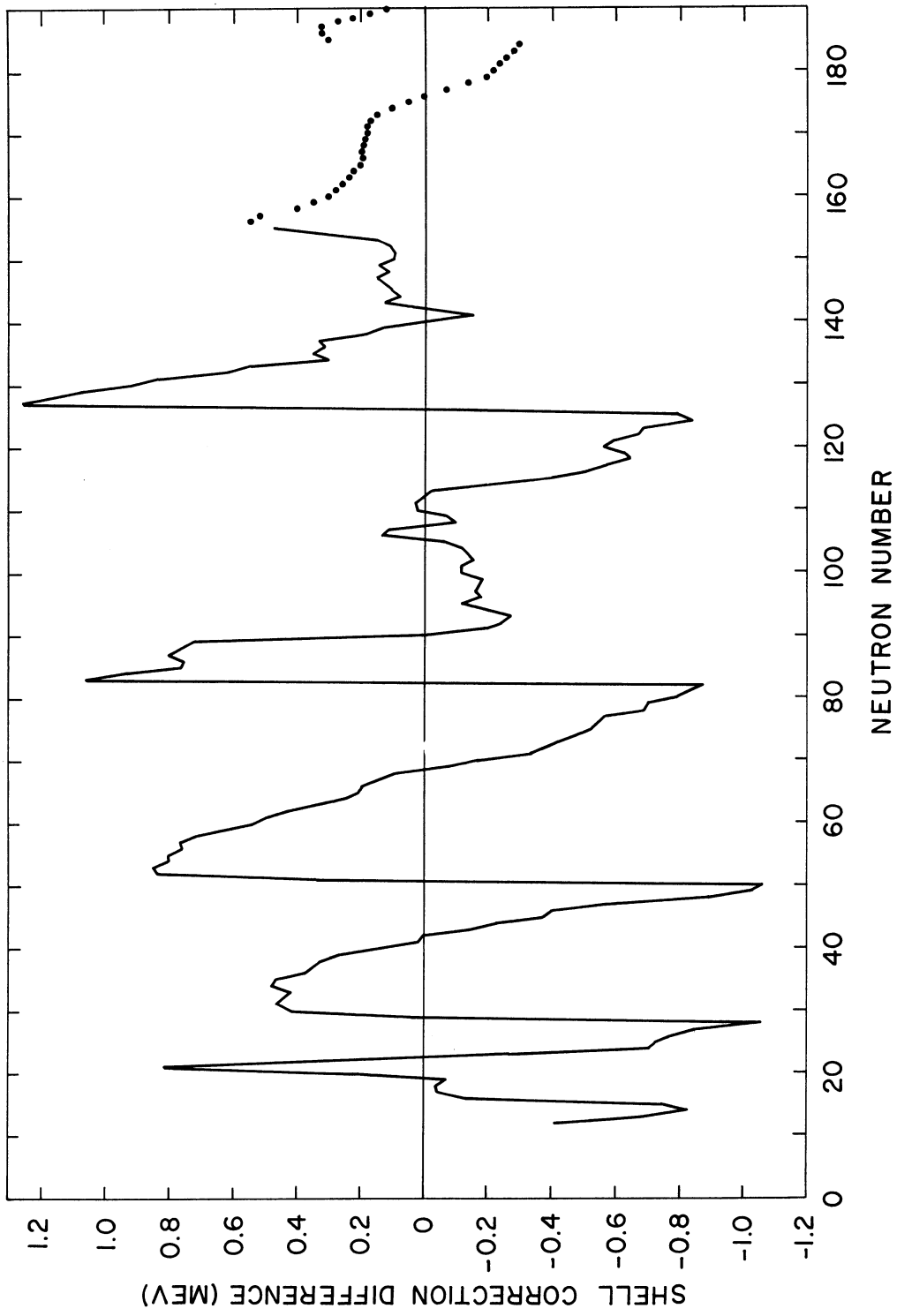


Fig. 6
Shell-correction differences for neutrons
plotted as a function of neutron number.

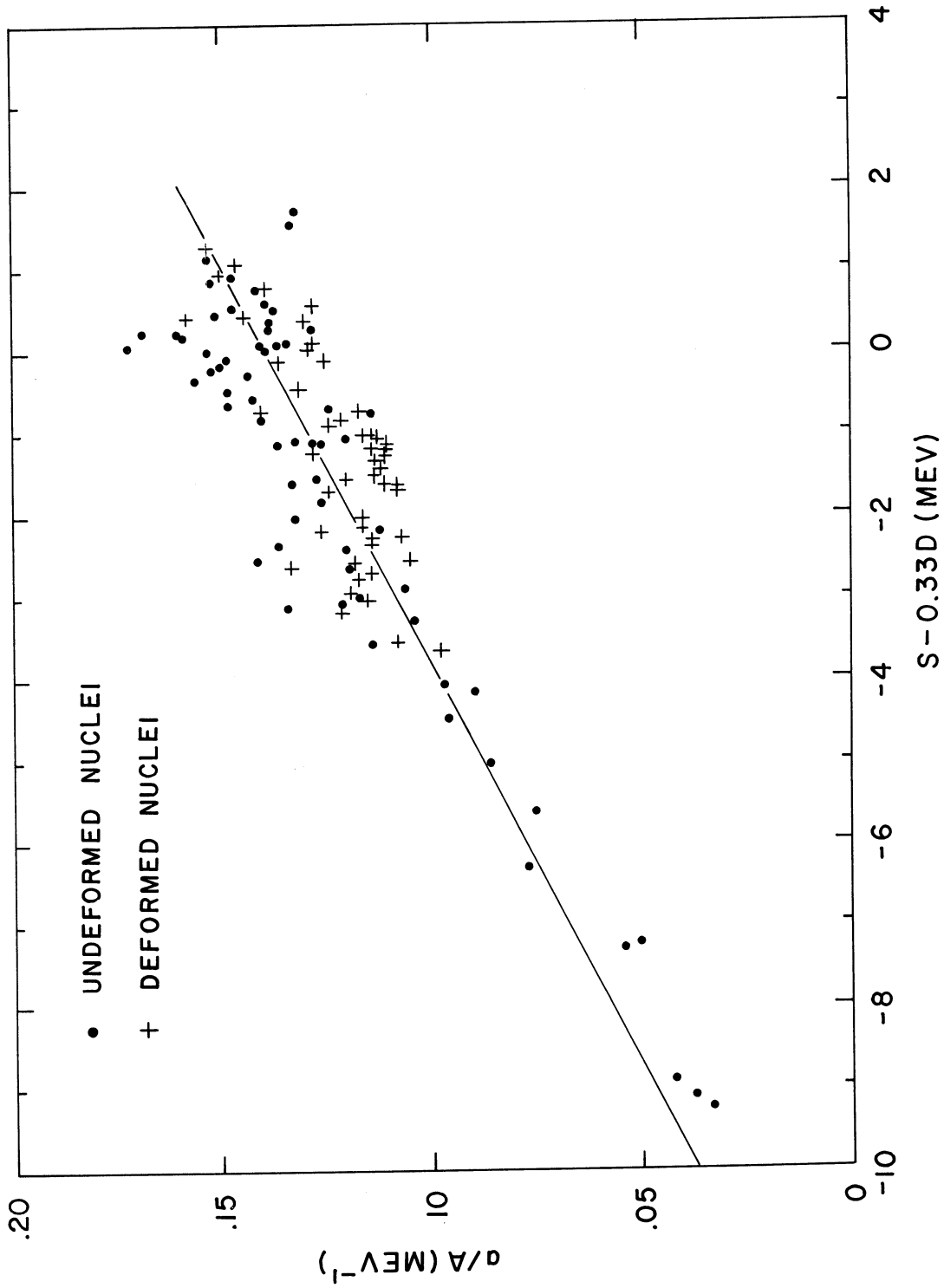


Fig. 7
 a/A as a function of the total shell energy
as fitted by equation (18).