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THE MACROSCOPIC APPROACH TO NUCLEAR MASSES AND DEFORMATIONS

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THE MACROSCOPIC APPROACH TO NUCLEAR MASSES AND DEFORMATIONS

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1. INTRODUCTION

The mass of a neutron is $M_N = 939.5731\ MeV/c^2$ and of a proton $M_Z = 938.2796\ MeV/c^2$. The mass of an atomic nucleus with A nucleons (N neutrons and Z protons) consists of the sum $(NM_N + ZM_Z)$, reduced by the mass associated with the binding energy between the nucleons, as required by the relativistic equivalence between mass and energy. These binding energies vary from 2.2 MeV for the deuteron to 1900 MeV for ^{256}Fm. After sixty years of atomic mass measurements, the binding energies are known today experimentally for ~1900 nuclei in their ground-state equilibrium configuration, as well as for dozens of nuclei in deformed, fission-barrier saddle point shapes, and for hundreds of interaction-barrier shapes corresponding to pairs of nuclei in contact. These binding-energy (or mass) measurements are often made with a precision corresponding to a small fraction of an MeV and, together, they represent an immense amount of information of practical relevance for many branches of nuclear physics, nuclear engineering, and astrophysics. They also represent an exacting challenge to

theoretical efforts at understanding the basic properties of the unique many-body problem presented to us by an atomic nucleus.

In the macroscopic approach to nuclear structure, one attempts to simplify the description of certain aspects of the nuclear many-body problem, with its 3A individual-particle degrees of freedom (not to mention possible quark degrees of freedom), by focusing attention on a number of suitably chosen macroscopic features. First and foremost among these are the degrees of freedom describing the shape of the nuclear surface (which, although not perfectly sharp, is known experimentally to be fairly well defined, except for very small nuclei). The subject of the present review, "The Macroscopic Approach to Nuclear Masses and Deformations", is then the description of theories, formulae, and techniques for the calculation of nuclear masses (or binding energies) in their dependence on macroscopic (shape) degrees of freedom.

The major part of the binding energy of nuclei may be accounted for by a simple "Liquid Drop" formula, consisting of a volume energy [assumed to depend quadratically on the relative neutron excess I,

defined as (N-Z)/A)], a surface energy proportional to the surface area, and the electrostatic energy of a uniform distribution of electric charge inside the nucleus. The effectiveness of this simple Liquid Drop Model treatment of nuclear ground-state energies is illustrated in Figure 1. Originally conceived more than 45 years ago (1,2) for the purpose of calculating only such ground-state masses, the model began to assume a wider range of applicability when it was recognized that the gross properties of nuclear fission could be understood in terms of the shape dependence of the surface and electrostatic energies of the nuclear drop (3). Unfortunately, however, there was a historically understandable tendency to associate the Liquid Drop Model (even in its static aspects) with a system of strongly interacting particles characterized by short mean free paths (and treated according to classical mechanics). Because of this misconception and the failure of idealized versions of the Liquid Drop Model to account for nuclear dynamics (e.g. excited nuclear states), the soundness of the Liquid Drop Model, even in its description of the gross, static aspects of nuclear binding energies, began to be

questioned when the nuclear Shell Model was found to be a good approximation to nuclear structure (4). According to this model, one could think of nuclei as consisting of weakly interacting constituents in a common potential well, with quantization of the particle orbits playing an essential role. How then could the Liquid Drop Model of nuclear binding energies be taken seriously? We shall discuss this question in a later section. Notwithstanding these reservations, refinements to the Liquid Drop Model formula for nuclear masses continued to be made. They did not, however, reduce substantially the remaining discrepancies between theory and experiment (up to about 10 MeV), which were soon recognized qualitatively as "Shell Effects", associated, indeed, with the quantization of the nucleon orbits.

Major advances in treating the shell effects took place about fifteen years ago. (Before this time the shell effect deviations had usually been treated in an ad hoc way, by use of tabulated empirical correction functions (5-8).) In Refs. (9-11) it was recognized that the main features of the shell effect deviations (see Figure 2) could be understood in terms of the bunching of the quantized nucleon levels

into bands, the bunching being governed by the symmetries of the nuclear shape in question and thus disappearing when the symmetries were destroyed by a deformation. A semi-empirical algebraic treatment of shell effects, made possible by these insights (11-14), was soon followed by quantitative calculations (requiring, however, numerical solutions of the Schrödinger equation in an appropriate potential well) (15-18). The result of these calculations was not only a dramatic reduction of the discrepancies between theoretical and experimental masses (from around 10 MeV to around 1 MeV) but also the explanation of the long-standing puzzle of the mass asymmetry of nuclear fission in terms of shell effects at the fission barrier, as well as the explanation of the existence of relatively stable, strongly deformed nuclei with axes in the ratio of about 2:1 (the fission isomers). Finally, and potentially most significant, these shell-effect calculations predicted the possible existence of an island of relatively stable nuclei beyond the known limits of the periodic table of elements.

Concurrently with this conquest of the nuclear shell effects, there followed a substantial further improvement in the treatment of the Liquid Drop Model (the so-called Droplet Model (19-31)) and the development of successful "Proximity" and "Folding" techniques for calculating the nuclear interaction between approaching nuclei (32-39), essential for a description of the energies of interaction-barrier configurations. Taking together these three contributions, Liquid-Drop, Proximity, and Shell Effects, one can today estimate theoretically the binding and deformation energies of known or hypothetical nuclei with an accuracy often approaching or even exceeding 1 MeV.

An independent advance has been the development of techniques that solve the nuclear many-body problem within a self-consistent mean-field approximation (Hartree-Fock calculations with simplified effective interactions (40)). These potentially most powerful techniques are today still somewhat limited by the computational effort that is required.

Finally, a major advance in interpolation/extrapolation methods took place around 1966 (41-46), resulting in a very elegant and generally accurate way of predicting nuclear ground-state masses from known neighboring masses (See Section 6) (47-53).

2.FRAMEWORK

The importance of the macroscopic description of nuclear deformation energies can be appreciated by viewing the problem in the context of the wider question of the macroscopic description of nuclear dynamics. In order to discuss a macroscopic dynamical problem one often needs three components in the equations of motion, corresponding to inertial, dissipative, and conservative forces, each given as a function of the macroscopic (e.g. shape) degrees of freedom (and their time derivatives) (54,55). The conservative forces follow from the potential energy (expressed as a function of shape). In the case of nuclei, the local or absolute minima in this potential-energy landscape give the ground-state masses. Saddle-point passes are related to (fission) barriers and, generally, the landscape provides the stage on which dynamical evolutions (to be treated classically <u>or</u> quantally) will be taking place.

In the context of nuclear deformation energies the problem is then to write down the potential energy V of a nucleus of arbitrary shape--a diffuse nuclear blob--consisting of A nucleons, as a function (more

precisely, a functional, $V[\Sigma]$) of its shape Σ. [The blob may be in the form of one or more deformed diffuse pieces, but the contour Σ is, by definition, a sharply defined figure. The diffuseness of the surface region of the blob may be specified by a "width" b, of the order of the range of nuclear forces. The size of the blob (not spherical, in general) may be specified by a radius R (or volume $4\pi R^3/3$).]

In a direct attack on this question one may simply attempt a solution of the many-body problem as a whole, using a suitable approximation. In the nuclear context, the mean-field Hartree-Fock approach (using simplified effective interactions) has been particularly successful in recent years and promises to provide eventually the most reliable estimates of certain features of the potential-energy landscape.

The indirect approach, which up to now has provided the main tools for accounting quantitatively for nuclear binding and deformation energies, relies on splitting the total potential energy into three parts and treating them separately. The physical reasons for the split have to do with the fact that the nuclear blob Σ is made up of elements

(nucleons) that can feel each other over finite distances by virtue of nuclear interactions (of range $\sim$b) and that inside the blob there are individual-particle wave-functions that can feel out the shape of the blob as a whole. (The eigensolution of the Schrödinger equation in a cavity is sensitive to the shape and size of the cavity as a whole). If it were not for certain specific effects of the finite range of nuclear forces and the global character of the eigenvalue problem, the total energy could be written as a sum of 'local' contributions but the finite range adds a specific 'Proximity part' and the global character of the wave functions adds a 'Global part'. Thus

$$V[\Sigma] = \text{Local part} + \text{Proximity part} + \text{Global part}.$$

The shape dependence of the Local part is made up of contributions from different points on Σ, each contribution being a function only of the local conditions at that point. The Proximity part is made up of contributions that depend also on conditions a finite distance (of order b) away from the point in question. The Global part cannot be written as a sum of local contributions--it knows about the shape as a whole and, in particular, about the symmetries of the shape.

In less formal language the Local part is, essentially, the Liquid Drop or Droplet contribution to nuclear masses (it is typically of the order of hundreds of MeV). The Proximity part or Proximity Potential shows up most strikingly in the attraction (of range $\sim$b) between the surfaces of two approaching nuclei (it is typically of the order of tens of MeV). The Global part, in particular as it is sensitive to symmetries, contains the Shell Effects (typically of the order of a few MeV). (The Coulomb energy, which may range from tens to hundreds of MeV, is also part of the Global contribution, but it is not specifically sensitive to the symmetries of the shape.)

We shall now describe the techniques used to treat these three parts of the nuclear potential energy.

3. LOCAL PART

For any "saturating" system, such as a nucleus or a drop of water, the main deviations from bulk behavior are confined to a surface layer (of width $\sim b$, say) that is small compared to the size of the system ($b/R \ll 1$). A <u>Leptodermous Potential Energy Theorem</u> may then be derived (32,54), according to which the local part of the potential energy can be written as the following expansion in powers of b/R:

		Relative Order	
$V = c_1 (4/3)\pi R^3$	Volume energy	1	A
$+ c_2 \oint d\sigma$	Surface energy	b/R	$A^{2/3}$
$+ c_3 \oint K \, d\sigma$	Curvature energy	$(b/R)^2$	$A^{1/3}$
$+ c_4 \oint \Gamma \, d\sigma$	Higher order curvature corrections	$(b/R)^3$	A^0
$+ c_4' \oint K^2 \, d\sigma$			
+ corrections that go to zero as $A \to \infty$			A^{-n} .

(1)

In the above, the integrals are over the surface Σ defining the shape of the system, K is the total curvature and Γ the Gaussian curvature at a point on the surface ($K = R_1^{-1} + R_2^{-1}$, $\Gamma = R_1^{-1}R_2^{-1}$, where R_1, R_2 are the principal radii of curvature at the point in question).

The coefficients $c_1 \ldots c'_4$ are constants, independent of the shape and size of the system, which are, in general, functions of the bulk density and composition (neutron excess). With respect to the leading volume-energy term, the constants are of the relative order 1, b, b^2, b^3, b^3, which implies energy contributions of order A, $A^{2/3}$, $A^{1/3}$, A^o, A^o.

The derivation of Equation (1) may be found in Blocki et al. (32); the important point to stress is that it does not rest on assumptions that the particles constituting the system are classical objects with short mean free paths. The crucial assumption is that the deviations from bulk behavior should be confined to a (relatively thin) surface layer, an assumption that is found to be satisfied quite accurately also for systems of quantized, weakly interacting (or even noninteracting) particles (56,22,54).

In particular, it is now well established that, when the nuclear problem of quantized individual-particle orbits in a common potential is treated by the statistical (nuclear) Thomas-Fermi method, the resulting energy reduces, in the appropriate limit of large systems

with relatively thin surfaces, to a volume energy, a surface energy and curvature corrections, as predicted by Equation (1) (57-59,19).

It follows that the structure of the Liquid-Drop formula, Equation (1), is not an ad hoc parametrization, but a well-defined approximation exploiting the smallness of the expansion parameter (b/R), and accurate to within the nonlocal effects to be described in Sections (4) and (5).

Apart from the electrostatic energy, the standard Liquid Drop mass formula follows from Equation (1) by writing $R = r_0 A^{1/3}$ (r_0 = nuclear radius constant, about 1.18 fm), and assuming the volume- and surface-energy coefficients c_1, c_2 to depend quadratically on the relative neutron excess I. Thus

$$V = -a_1(1 - \kappa I^2)A + a_2(1 - \kappa_s I^2)A^{2/3}B_s + \text{higher order terms}, \qquad (2)$$

where a_1 and a_2 are new constants (with the dimensions of energy), κ is the "symmetry energy coefficient", and κ_s is the "surface symmetry energy coefficient". The quantity B_s, a dimensionless functional of the shape Σ, is the surface area of Σ divided by $4\pi R^2$. (Thus $B_s = 1$ for the spherical shape.) In older treatments, the poorly determined coefficient κ_s was usually set equal to zero. A

somewhat more reasonable choice is to put $\kappa_s = \kappa$. If this is done (13), then Equation (2) predicts that, if the measured nuclear binding energies per particle, (V/A), are corrected for the neutron excess, shell effects and the electrostatic energy, and are then plotted against $A^{-1/3}$, a straight line should result, with $-a_1$ as the intercept and a_2 as the slope. How well this expectation is borne out is shown in Figure 3 taken from (13).

A refinement of the Liquid Drop Model may be achieved by retaining in Equation (1) higher order terms in the small expansion parameters $A^{-1/3}$ and I^2. This is indicated in Figure 4. A theory of nuclear binding energies retaining only terms of order A corresponds to the study of standard nuclear matter. Including the terms of order $A^{2/3}$ (surface energy) and I^2A (volume symmetry energy) corresponds to the Liquid Drop Model. Retention of the terms in $A^{1/3}$, $I^2A^{2/3}$ and I^4A defines the nuclear "Droplet Model" (19,24,30). It turns out that in order to work consistently to this order, it is necessary to include in the theory degrees of freedom corresponding to compressibility and polarizability (i.e. deviations of the neutron and

proton densities from uniform values in the bulk) as well as a "neutron-skin" degree of freedom (i.e. the introduction of separate neutron and proton effective surfaces Σ_n, Σ_p). The Droplet Model thus becomes very much richer than the Liquid Drop Model and establishes contact with many nuclear phenomena such as details of nuclear RMS radii, charge distributions, isotope shifts, and Giant Dipole resonances. Regarding nuclear ground-state binding energies, the Droplet Model Formula is still a closed algebraic expression.

Another extension of the Liquid Drop Model can be found in the work of Weiss and Cameron (60,61) who consider a large number of higher order terms in the symmetry energy. Truran, Cameron and Hilf (62) use these higher-order terms in an actual fit to masses. Similar factors enter in the work of Baym, Bethe and Pethick (63) and Mackie and Baym (64) who are concerned mainly with formulating a binding energy expression that goes over correctly into an equation of state for pure neutron matter when the neutron excess is increased.

Whether the Liquid Drop or Droplet Model formulae are used for the specifically nuclear part of the binding energy, a term representing

the electrostatic interaction of the protons must be added. (Although the electrostatic energy is, strictly speaking, an example of a Global contribution, it is more logical to discuss it along with the Liquid Drop or Droplet Model Formula.) In the simplest approximation the electrostatic energy is taken to be that of a uniform distribution of charge Ze inside the sharp surface Σ. Closed expressions for this energy are available for slightly distorted spheres, spheroids of any eccentricity, slightly distorted spheroids, and some other special cases (65-67,36). In general, however, the Coulomb energy must be calculated by numerical quadratures (68,69). Corrections to the electrostatic energy for the diffuseness of the charge distribution and for the anti-correlation of the protons (due to the exclusion principle) are easily estimated. Their inclusion in a mass formula is trivial since, to lowest order in b/R, they turn out to be constants independent of shape (14,30).

4. PROXIMITY PART

It may come as a surprise that the Leptodermous expansion, Equation (1), even if carried to an infinite order in the small parameter $\varepsilon = A^{-1/3}$, is bound to miss an important piece of even the smooth part of the nuclear energy (quite apart from the oscillating Global shell effects). This has to do with the circumstance that, in a system made up of particles interacting through finite-range forces, the interaction energy contains, in general, a part that "knows about" the conditions at two finitely separated points (for example, two surface elements of appproaching nuclei, or the front and back sides of a single nucleus). This part cannot be reduced to a sum of local contributions, each a function of local conditions on the surface Σ, and this invalidates the assumption underlying the local Leptodermous Potential Energy Theorem. The mathematical feature of this elusive contribution that evades even an <u>infinite</u> power expansion is its <u>non-analiticity</u>, which means that the contribution in question cannot be expanded in a Taylor series. (A typical example of such a term is $\exp(-A^{1/3})$ i.e. $\exp(-1/\varepsilon)$. See p. 454 in Reference (32).) This

type of contribution may be only a fraction of an MeV for a single undeformed nucleus, but it reaches 20-30 MeV for two nuclei near contact and is of decisive importance for the discussion of such configuratons. It is also of considerable importance for the fission saddle-point configurations of the lighter nuclei, in the shape of two pieces connected by a small neck.

Krappe, Nix & Sierk (34) have developed a method of calculating potential energies that, in addition to the Local part, generates also a Proximity Part. It consists of folding an effective short-range interaction (of Yukawa type, exp (-x)/x, or, more recently, a special mixture of a Yukawa and an exponential) into a sharp (or diffuse) density distribution representing the nuclear shape. A particularly elegant version of this method (36) uses the special two-parameter folding function $C(1 - 2x^{-1}) \exp(-x)$, where $x = r_{12}/a$ and r_{12} is the separation between two points. This effective interaction has the property of leaving the volume energy unaffected (its average in uniform matter is zero) and it also has the desirable property (required by nuclear saturation) that the interaction energy between

two semi-infinite slabs should be stationary when the slabs are in contact. By adjusting the parameters C and a it is then possible to reproduce the empirical surface energy, as well as to give a useful approximation to the interaction energy between two nuclei. As in the case of the Coulomb energy, closed formulae for the folding energy may be derived in several cases but, in general, numerical quadratures are required.

A less comprehensive but algebraic method of treating the Proximity contribution in certain cases was developed by Blocki et al. (32,33), where one can also find references to the earlier literature. It rests on the seemingly trivial observation that the interaction energy between two curved (nuclear) surfaces with least separation s may be approximately written as

$$V_p(s) \approx \iint e(D)\, dx\, dy \quad , \tag{3}$$

where e(D) is the interaction energy per unit area between two flat, parallel surfaces at separation D, and the integral is over the transverse dimensions of the gap between the curved surfaces, the gap

being specified by the function D(x,y). A change of variables (p. 430, (32)) leads to

$$V_p = 2\pi\bar{R}\int_{D=s}^{\infty} e(D)dD \quad , \tag{4}$$

where $\bar{R} = (R_x R_y)^{1/2}$, R_x and R_y being the radii of curvature (evaluated at the point of least separation) of the surface obtained by plotting D versus x and y. Differentiation with respect to s gives the "Proximity Force Theorem":

$$F(s) \equiv -(\partial V_p/\partial s) = 2\pi\bar{R}\, e(s) \quad , \tag{5}$$

i.e.

"The force between two gently <u>curved</u> surfaces as a function of the separation degree of freedom <u>s</u> is proportional to the interaction potential per unit area, e(s), between two <u>flat</u> surfaces, the constant of proportionality being 2π times the reciprocal of the square root of the Gaussian curvature of the gap width function at the point of least separation between the surfaces."

The theorem reduces the calculation of the force (or potential energy) for approaching nuclei to the calculation of the geometrical

quantity R (which, for two spherical nuclei with radii R_1 and R_2, turns out to be equal to the reduced radius, $R_1R_2/(R_1+R_2)$) and a universal function e(s) that has been calculated and tabulated, together with its integral, for nuclear surfaces described by the nuclear Thomas-Fermi approximation (32).

It is a trival matter to estimate the nuclear interaction energy V_p between two approaching nuclei using the simple cubic-exponential approximation given in References (32) for the dimensionless quantity $\Phi(\zeta)$, where

$$\Phi(\zeta) \equiv \int_{\zeta}^{\infty} \frac{e(D)}{2\gamma} \frac{dD}{b} . \tag{6}$$

In this expression $\zeta = s/b$, γ is the surface-energy coefficient, and b is the surface width (~1 fm). Equation (6) can be used to rewrite Equation (4) in the standard form,

$$V_p(\zeta) = 4\pi \gamma \, b \, \bar{R} \, \Phi(\zeta) . \tag{7}$$

5. GLOBAL PART (SHELL EFFECTS)

We mentioned in Section 3 that the Local, Liquid Drop or Droplet Model behavior of the potential energy is a very general property of thin-skinned systems but that, in the nuclear context, it may also be regarded as the result of applying the Thomas-Fermi method to the nuclear many-body problem of (weakly) interacting quantized particles in a common potential. The Thomas-Fermi method is based on the statistical assumption that, for a large system, the density of states in phase space (coordinate space plus momentum space) is, on the average, one per h^3, where h is Planck's constant. It follows at once that, on the average, the energy ε_n of the nth eigenvalue of the solution of the Schrödinger equation in a large, deep potential cavity is proportional to $n^{2/3}$, the total energy E $(=\sum_1^{n_{max}} \varepsilon_n)$ is proportional to $n_{max}^{5/3}$, where n_{max} is the total number of sequentially filled eigenvalues, and the level density $g(\varepsilon_n)$ (number of eigenvalues, dn, per interval of energy $d\varepsilon_n$) is proportional to $\varepsilon_n^{1/2}$.

Thus

$$\varepsilon_n \propto n^{2/3} \tag{8}$$

$$E = \sum_1^{n_{max}} \varepsilon_n \propto n_{max}^{5/3} \tag{9}$$

$$g(\varepsilon_n) = \frac{dn}{d\varepsilon_n} \propto \varepsilon_n^{1/2} \ . \tag{10}$$

For a cavity that is not very deep or very large, surface-layer corrections to the above formulae may be readily derived (following, for example, the method of Reference (70)). In any case, insofar as the statistical assumption is valid, the level density $g(\varepsilon_n)$ and related quantities are smooth functions of ε_n or n. In the case of an irregular cavity, devoid of any symmetries, the eigenvalues would, in general, be nondegenerate and the inaccuracy of the statistical assumption would be relatively small, reflecting only the discrete spacing of the eigenvalues and random fluctuations around the average. The presence of degeneracies will cause deviations from the statistical (Liquid Drop or Droplet Model) behavior, the deviations being in proportion to the strength of the degeneracies in question. Thus the approximate 2 x 2 spin-isospin degeneracy of the nuclear problem has long been known to contribute to the special stability of light

"alpha-particle" nuclei and was early suggested (71, p. 7) as a factor in the even-odd staggering of nuclear masses (corresponding to the special stability of even-even nuclei). Much more drastic are the deviations associated with the $(2\ell+1)$ degeneracy of eigenvalues in a spherically symmetric potential (ℓ is the angular momentum quantum number), or the even stronger degeneracies associated with the isotropic harmonic oscillator potential or the inverse-distance potential. In all these cases, instead of an almost smooth spectrum of levels one has a "bunched" spectrum, with several levels per bunch and with gaps in between that would otherwise be populated by the debunched levels. The reason for the relative stability of systems with a particle number corresponding to a closed shell (a particle number corresponding to a filled bunch of levels) is clear: when one begins to fill a new bunch of levels, the eigenvalues are at first anomalously high compared to an average (one has to overcome an anomalously large gap) so the first particles are relatively poorly bound. On the other hand, when completing the filling of a bunch, one is putting particles into eigenvalues that are by now lower than debunched eigenvalues would

be (they would be half-way up the next gap). Thus, the eigenvalues ε_n, considered as a function of the particle number, n, go up and down like a zig-zag, crossing and recrossing the average (a vertical zig followed by a sloping zag). The total energy is a running integral over this zig-zag, and its deviation from the average will be a series of arches, with deepest cusped points corresponding to the especially well-bound closed shells. The tops of the arches--half-filled shells--will have anomalously poor bindings (high masses). Mathematically, the binding energy anomaly--the shell effect--can thus be written as((13), Equation (2))

$$V_{SHELLS} = \sum_{n=1}^{n_{max}} \varepsilon_n(\text{bunched}) - \sum_{n=1}^{n_{max}} \varepsilon_n(\text{unbunched}) \tag{11}$$

$$= \int_0^{n_{max}} \varepsilon(\text{bunched})dn - \int_0^{n_{max}} \varepsilon(\text{unbunched})dn \quad . \tag{12}$$

This formula underlines both the treatments of shell effects in Refs. (9-13) and (15-18, 72-76).

In the semi-empirical treatment of Reference (13) the unbunched spectrum of the separate proton and neutron eigenvalues was taken to be

that of the Thomas-Fermi method (proportional to $n^{2/3}$). This spectrum was then imagined cut up into bands corresponding to the known neutron or proton magic numbers for spherical nuclei: N, Z = M_i, with M_i = 2, 8, 14 (or 20), 28, 50, 126, 184 . The bands were squeezed by a (common) adjustable factor and slightly moved down together by a second adjustable factor to form the bunched spectrum. Insertion in Equation (12) then gave the proton and neutron shell corrections for the spherical shape. Since the bunching responsible for the known magic numbers is associated with the spherical shape, this bunching and the resulting shell effects should be damped out as the shape is distorted from the sphere. This was achieved in the semi-empirical method by multiplying the shell effect for the spherical shape by a shell damping function in the form of a gaussian, $\exp(-\sigma^2)$, where is the root mean square deviation of the nuclear surface from the sphere, in units of an adjustable range parameter a. When this three-parameter algebraic shell correction is added to a Liquid Drop or Droplet Model formula, a fair account can be given of the nuclear ground state masses, equilibrium deformations, and fission barrier

heights. (The comparison with the ground state masses is shown in Figure 2).

The Strutinsky method (15-18,75) may be considered as resulting from Equation (12) by changing the variable of integration from n to ε:

$$V_{SHELLS} = \int_{-\infty}^{\varepsilon_F} g(\varepsilon)\,\varepsilon\,d\varepsilon - \int_{-\infty}^{\varepsilon_F} \tilde{g}(\varepsilon)\,\varepsilon\,d\varepsilon \quad , \tag{13}$$

where $g(\varepsilon)$ is the actual level density, $d\varepsilon/dn$, of the bunched eigevalues, and $\tilde{g}(\varepsilon)$ is the level density of the unbunched eigenvalues. The Fermi energy ε_F is determined by particle-number normalization,

$$N \text{ or } Z = \int_{-\infty}^{\varepsilon_F} g(\varepsilon)\,d\varepsilon \quad . \tag{14}$$

In practice, the bunched level density $g(\varepsilon)$ (a series of delta functions) is obtained by calculating numerically all the eigenvalues in a suitable shell model potential with spin-orbit coupling. (A modified oscillator (73), a Woods-Saxon well (18) or a potential obtained by folding a Yukawa interaction into a sharp-surfaced generating density (75)). The level density $\tilde{g}(\varepsilon)$ is most often

obtained by smoothing $g(\varepsilon)$ by means of an essentially Gaussian smearing function of suitable range c, i.e.,

$$\tilde{g}(\varepsilon) = \int_{-\infty}^{+\infty} g(\varepsilon) \frac{e^{-(\varepsilon-\varepsilon')^2/c^2}}{c\sqrt{\pi}} [1 + \text{Modification}] d\varepsilon' \quad . \quad (15)$$

The "Modification" is a polynomial in the argument $(\varepsilon-\varepsilon')/c$, chosen to maximize the smoothing of the rapid oscillations in g, while doing the least damage to the long-range smooth dependence of g on energy.

An additional feature of the Strutinsky method is the inclusion of a correction to the binding energy arising from the pairing of nucleons moving in time-reversed orbits. This pairing correction is important for a realistic description of nuclear energies and is relatively easily treated by means of the Bardeen-Cooper-Schrieffer method, once the eigenvalues ε_n have been calculated with the aid of a computer (73,18,75). The final correction to the smooth, local binding energy consists then of separate shell and pairing corrections for the neutrons and protons.

The Strutinsky method has essentially no adjustable parameters and, given the requisite computational effort, provides the shell

correction for any nuclear shape. When combined with a suitable Liquid Drop or Droplet formula, it has been spectacularly successful in accounting for known features of nuclear deformation energies and in making predictions of new phenomena.

For examples, the reader is referred to Secion 6 and to the vast literature reviewed in Reference (76). The foundation of the method and, in particular, its relation to self-consistent Hartree-Fock treatments of the nuclear problem, are discussed by Brack and others (18,77) and Bohr-Mottelson (78) Vol. II p. 367-371.

6. SPECIFIC TREATMENTS

In the foregoing sections we described the principal physical ingredients that go into typical macroscopic theories of nuclear binding and deformation energies. In the present section we shall review briefly the relevant literature and provide some details in a few cases. The various developments can be traced in the proceedings of a long series of conferences on atomic masses (79-85), a series on nuclei far from stability (86-90), and a series of conferences on the physics and chemistry of fission (91-94).

Reference (12) was one of the first extensive tabulations of predicted masses that combines the Liquid Drop model with semi-empirical algebraic shell corrections (11,13). It also stressed the dependence of nuclear binding energies, including shell effects, on the shape of the nucleus (rather than concentrating on the ground-state masses only). We shall give some details of this mass formula as an example of this type of treatment.

The (atomic) mass was written as a sum of a liquid drop part and a shell correction, as follows:

$$M(N,Z,\text{shape}) = M_{LD}(N,Z,\text{shape}) + M_{SHELLS}(N,Z,\text{shape}). \tag{16}$$

The liquid drop part is given by

$$M_{LD} = M_n N + M_H Z - a_1(1 - \kappa I^2)A + a_2(1 - \kappa I^2)A^{2/3}B_s$$
$$+ c_3 Z^2 A^{-1/3} B_c - c_4 Z^2 A^{-1} + \delta \ . \tag{17}$$

The first two terms are the masses of the neutron and of the hydrogen <u>atom</u> (this then allows for the masses of the Z atomic electrons), the next two are the volume and surface energies, with a common quadratic dependence on the relative neutron excess I. The shape dependence of the surface energy is contained in B_s, the ratio of the area of the shape in question to that of a sphere of equal volume. The next term is the electrostatic energy, whose shape dependence is contained in B_c (the ratio of the Coulomb energy of the shape in question to that of the sphere). The next term is a (shape-independent) correction to the electrostatic energy due to the diffuseness of the charge distribution. The last term is the even-odd correction, taken empirically as $\pm 11A^{1/2}$ MeV for odd-odd or even-even nuclei and zero

for odd-mass nuclei. The quantities a_1, a_2, κ, c_3 are four adjustable parameters (c_4 is related to c_3).

The shell correction, which results from cutting up the nuclear energy spectrum into bands defined by the magic numbers M_i, as described in Section 5, is given by

$$M_{SHELLS} = C\, s(N,Z) e^{-\theta^2} \quad , \tag{18}$$

where θ = (RMS deviation of shape from sphere)/a

$$S(N,Z) = \frac{F(N)+F(Z)}{(A/2)^{2/3}} - cA^{1/3} \tag{19}$$

$$F(N) = q_i(N - M_{i-1}) - \frac{3}{5}(N^{5/3} - M_{i-1}^{5/3}), \text{ for } M_{i-1} \leq N \leq M_i$$

with

$$M_i = 2,8,14(\text{or } 20),28,50,82,126,184 \quad . \tag{20}$$

The quantities C, a, c are three adjustable parameters.

For a given N and Z the ground-state mass and deformation were calculated from Equation (16) by minimizing the total energy with respect to ellipsoidal distortions. The mass table generated in this way (12) listed the Liquid Drop mass, the Shell correction, the deformation, various decay energies, and the predicted fission barrier for about 8000 different combinations of N and Z. (The inclusion of

fission barriers is necessary for a firm determination of the adjustable surface and Coulomb energy coefficients.)

In later versions of this type of treatment the shape dependence of the shell correction was modified, on physical grounds, to $(1-2\epsilon^2)\exp(-\epsilon^2)$ (14). Later this shell correction was combined with the Droplet Model, to create another table of nuclear masses and other properties (30). A feature of this table is that it includes predicted (effective sharp) radii of the neutron and proton distributions. These followed from minimizing the energy with respect to the Droplet Model degrees of freedom describing the neutron and proton density distributions. The Droplet Model formula has a structure similar to Equation (16) but is more complicated and has four additional shape-dependent functionals in addition to B_s and B_c. It also includes the exchange correction (linear in Z) for the anticorrelation of the protons and a semi-empirical "Wigner Term", proportional to $|I|$, believed to reflect the tighter binding of particles in identical (or closely similar) quantized orbitals (30).

Part of the Droplet Model mass table just mentioned (30) also appears in the extremely useful collection of calculated masses that has been assembled by Maripuu (95). This same collection also contains a Droplet Model calculation by von Groote, Hilf & Takahashi (28) that improves the agreement with the measured masses by introducing additional flexibility into the schematic shell correction function. In another contribution to this collection, Seeger & Howard (96) combine a LDM (modified along Droplet Model lines) with shell corrections calculated using the Strutinsky method.

At this point it is probably good to remind the reader that the adoption of Strutinsky shell corrections (15-18,72,77,97-99) constitutes a major advance but also a break with the previous semi-empirical shell corrections, which were algebraic in nature. The improved predictive power of the Strutinsky method and its essentially unlimited range of applicability are obtained at the cost of a major increase in calculational complexity. No aspect of this method is amenable to hand calculation, and large electronic computer calculations are required for every result.

An enormous literature based on applications of the Strutinsky method has grown up around the prediction of the various nuclear properties, including the properties of superheavy elements that are thought to form an island of stability beyond the end of the known periodic table. Besides the early work by Strutinsky (15-17), some of the landmark papers in this area are those of Nilsson et al. (73), Brack et al. (18), Boslterli et al. (75), and the review in this series by Nix (76). Figure 5 gives an illustration of results obtained with the Strutinsky method.

A significant recent compilation of nuclear properties that makes use of the Strutinsky method is that of Möller & Nix (37,38). The LDM part of their energy expression employs a surface energy determined by folding a particular combination of a Yukawa and an exponential interaction into the specified nuclear density distribution, as explained in Section 4. This treatment of the Proximity part, in addition to providing an approximation to the interaction energy of approaching nuclei, appears to have a very significant effect on lowering the fission barriers of medium and light nuclei. Several

other refinements are included in the treatment (corrections for the proton form factor, an exact treatment of the diffuseness correction to the electrostatic energy, the effect of a slight charge asymmetry in the nuclear force, corrections for zero-point motions in the ground state). But the correction that produced a really significant improvement in the fit to nuclear ground-state masses resulted from the simple inclusion of a shape-independent A° term (i.e. a constant) in the Liquid Drop part of the formula. This cut the RMS deviations in the ground-state masses from 1.93 MeV to 0.97 MeV and seemed to remove virtually all systematic smooth deviations between theory and experiment. This may be the first time that significant contact between experiment and the Leptodermous expansion has taken place at the A° level.

The treatment of the Proximity Part of the macroscopic energy with the aid of a folding technique (36) requires numerical integrations similar to those involved in the evaluation of the electrostatic energy. The more restricted but algebraic treatment that follows from the Proximity Force Theorem in Section 4 has been found useful for

discussing the interaction energy between nuclei. The expression for V_p, given in Section 4, when combined with the electrostatic interaction energy of two rigid spheres, overestimates the experimental interaction barriers between two nuclei (as measured for projectiles and targets throughout the periodic tables) by about 4 ± 2% (100). (A discrepancy in this sense is not unexpected, since actual nuclei are not rigid and, by deforming under the influence of the nuclear forces, may lower the interaction barrier).

In addition to the theories of nuclear binding and deformation energies, which are the subject of this review, we should mention two treatments that do not go beyond the discussion of equilibrium nuclear masses. The first is that of Zeldes and co-workers (101-105). They employ shell model considerations in constructing algebraic expressions containing a large number of parameters adjusted to account for various aspects of the nuclear level scheme. A table of mass predictions based on this approach has been prepared by Liran & Zeldes (106). It agrees extremely well with the known masses on which it is based and is most reliable for short-range extrapolations.

Another approach is that of nuclear mass relations, which was reviewed in this series by Garvey (45). For example, there is the isobaric-multiplet mass equation (107-109), which is obtained from the (more general) Wigner supermultiplet theory (110,111). This equation asserts that the (2T + 1) masses of an isobaric multiplet with isospin T should be related by the expression,

$$M(T_z) = a + bT_z + cT_z^2 \quad . \tag{21}$$

In this same category of mass relations, but of wider applicability, is the Garvey & Kelson (41-46) approach illustrated in Figure 6, which is based on adding and subtracting masses so that, within the framework of a shell model treatment, the various interactions between the particles would cancel. The masses of six nuclei should sum to zero when combined according to these patterns. If five masses are known, these relations can be used to predict the mass of the missing member. In this way tables of predicted masses can be built up by successive application of the basic relations. However, in their simplest forms, the predictions can go badly astray if naively applied to long-range extrapolations (112, 48). The advantages and limitations of this type

of mass relations have been investigated by Jänecke & others (47-53), who find a number of ways of enhancing their long-range predictive power. The method has also been applied by Monahan & Serduke (113-115).

Finally, as we mentioned in Section 2, a bold attempt is being made to go beyond the indirect approach and actually address the full many body problem of nuclear structure with the aid of the Hartree-Fock approximation. In spite of the difficult numerical calculations required, this area has seen a great deal of growth in the last decade; current developments have recently been reviewed in this series by Quentin & Flocard (40). A survey of nuclear radii throughout the periodic table using Hartree-Fock methods has been undertaken by Beiner, Lombard & Mas (116), who have also prepared a table of nuclear masses (117). A number of related studies is currently underway by Tondeur (118-122) and by Pearson and co-workers (123-126).

While still somewhat phenomenological in nature, because of the effective force (chosen for calculational convenience) and the Hartree-Fock approximation, this approach gives the Local, Proximity, and Global contributions to the energy within a single unified

self-consistent approach. This may be essential for the proper treatment of the problem when large excursions away from known nuclei (in shape, particle number, or N/Z) are being considered.

7. CONCLUDING REMARKS

After approximately half a century of nuclear physics there is available today a large amount of experimental information on the masses and deformation energies of nuclei relatively close to the line of beta stability. The interpretation of these measurements, which started off in the thirties with semi-empirical fits to ground-state masses, has improved over the years and has become integrated into detailed theories of nuclear structure and deformabilities. The resulting understanding of both the gross features, as approximated by a Liquid Drop or Droplet Model formula, and of the fine shell-effect details, calculated using the Strutinsky method, is generally adequate to account for the binding energies with an accuracy that may be considerably better than 1 MeV (better than 0.1%) for short-range extrapolations, but becomes uncertain for more distant extrapolations. The relatively recent breakthrough in describing quantitatively the shell effects was associated with the indirect approach, in which shell corrections are added to a smooth background, provided by the Liquid Drop Model. In the future, especially when very distant extrapolations

come into consideration (as in astrophysics) the direct approach of attacking the full many-body problem (in a suitable approximation) may become relatively more important. However, even then, the indirect macroscopic approach, suitably enriched to take into account the new situations (e.g. very neutron-rich neutron-star matter, or the bubble or foam topologies of collapsing supernovae) should continue to be a valuable tool for understanding these complex processes.

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Figure 1. The mass decrements (closely related to nuclear binding energies) are plotted for 97 beta-stable nuclei. The curve is a liquid-drop fit based on the "local" part of the nuclear potential-energy expresion. The deviations are due mostly to shell effects.

Figure 2. The shell correction to nuclear binding energies (i.e., the experimental mass minus a droplet model fit) is displayed as a function of neutron number [line (a)]. Line (b) is a theoretically calculated shell correction, using a schematic model of bunched levels in the upper part and the Strutinsky shell-correction method in the lower part. Line (c) is the remaining deviation (30).

Figure 3. The experimental nuclear binding energy per particle, corrected for the neutron excess, shell effects and the electrostatic energy, is plotted versus $A^{-1/3}$. The conformation of the experimental points to a linear trend down to mass numbers as low as 10 (see the labels along the data points) confirms the validity of the Leptodermous

Expansion and suggests a relatively small value for correction terms beyond the surface energy.

Figure 4. The orders of various terms in the expansion of the energy of a nucleus in powers of $A^{-1/3}$ and I^2. The Liquid Drop Model includes terms of order A, $A^{2/3}$ and I^2A. The Droplet Model is defined by the requirement that it should include, in addition, all terms of order $A^{1/3}$, $I^2A^{2/3}$ and I^4A.

Figure 5. The dashed lines represent the calculated Liquid Drop Model deformation energies of a number of superheavy nuclei. The solid lines show how the deformation energy is changed when Strutinsky shell effects are added (75).

Figure 6. Schematic representation of the so-called transverse and longitudinal mass relations. The boxes represent nuclei from the nuclidic chart with N horizontal and Z vertical. The presence of a plus or a minus sign in a box indicates that the mass value of the respective nucleus is to be added or substracted. If the Garvey-Kelson mass relations were exact, the sum of the six masses would be zero.

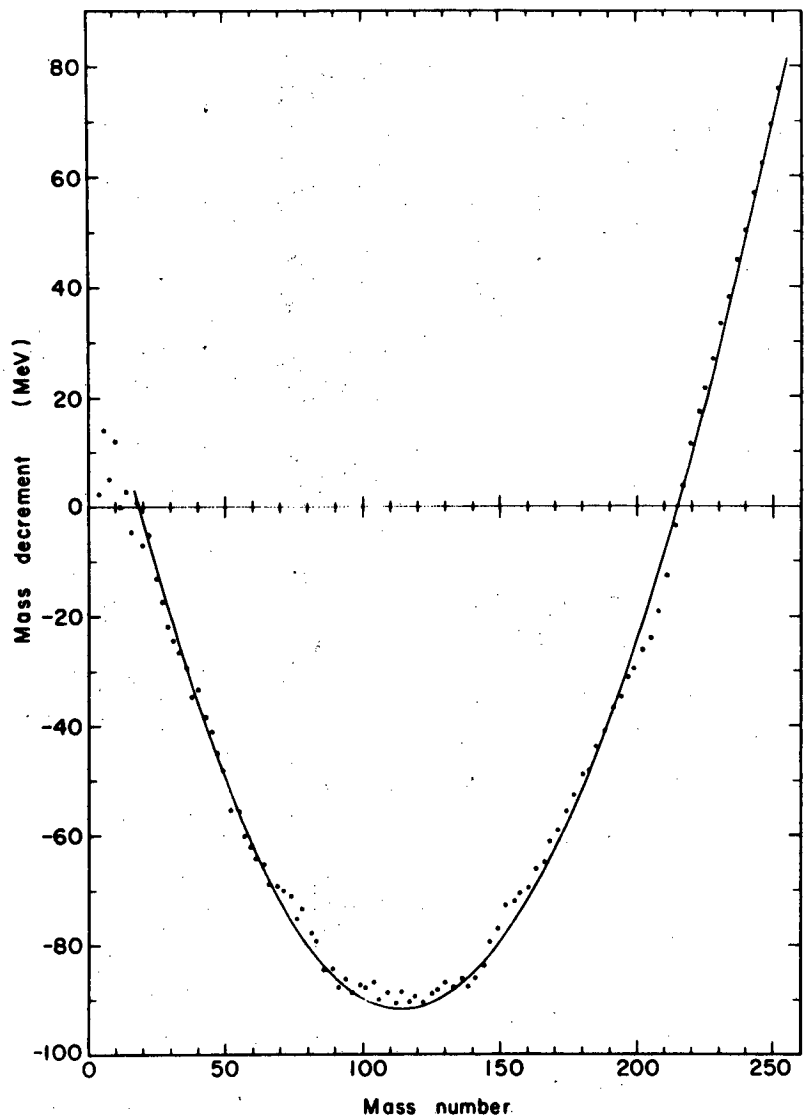

80
60
40
20
0
-20
-40
-60
-80
-100
Mass decrement (MeV)
0
50
100
150
200
250
Mass number

Fig. 1

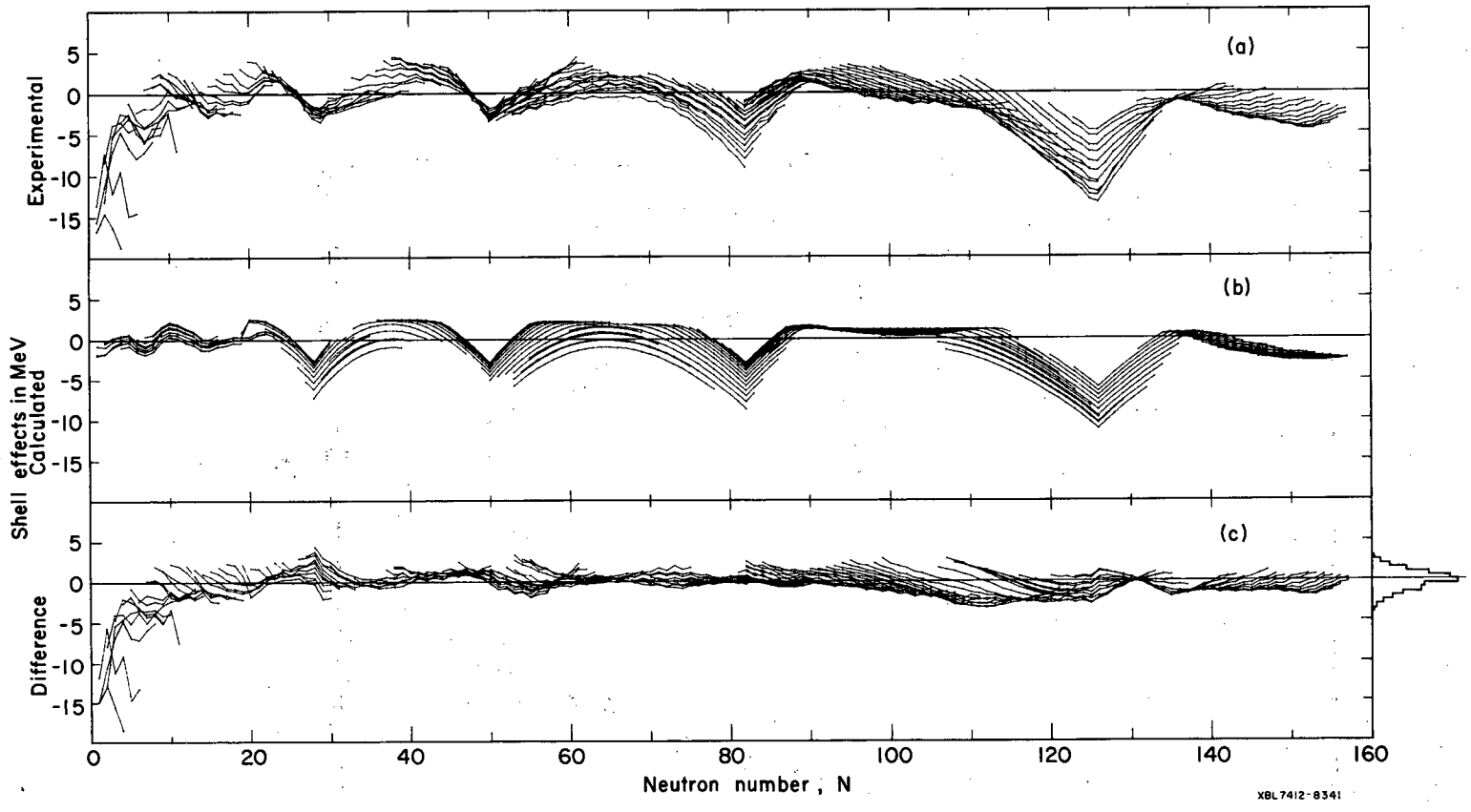

(a)
(b)
(c)
Experimental
Calculated
Difference
Shell effects in MeV
5
0
-5
-10
-15
0
20
40
60
80
100
120
140
160
Neutron number , N
XBL7412-8341

Fig. 2
upper

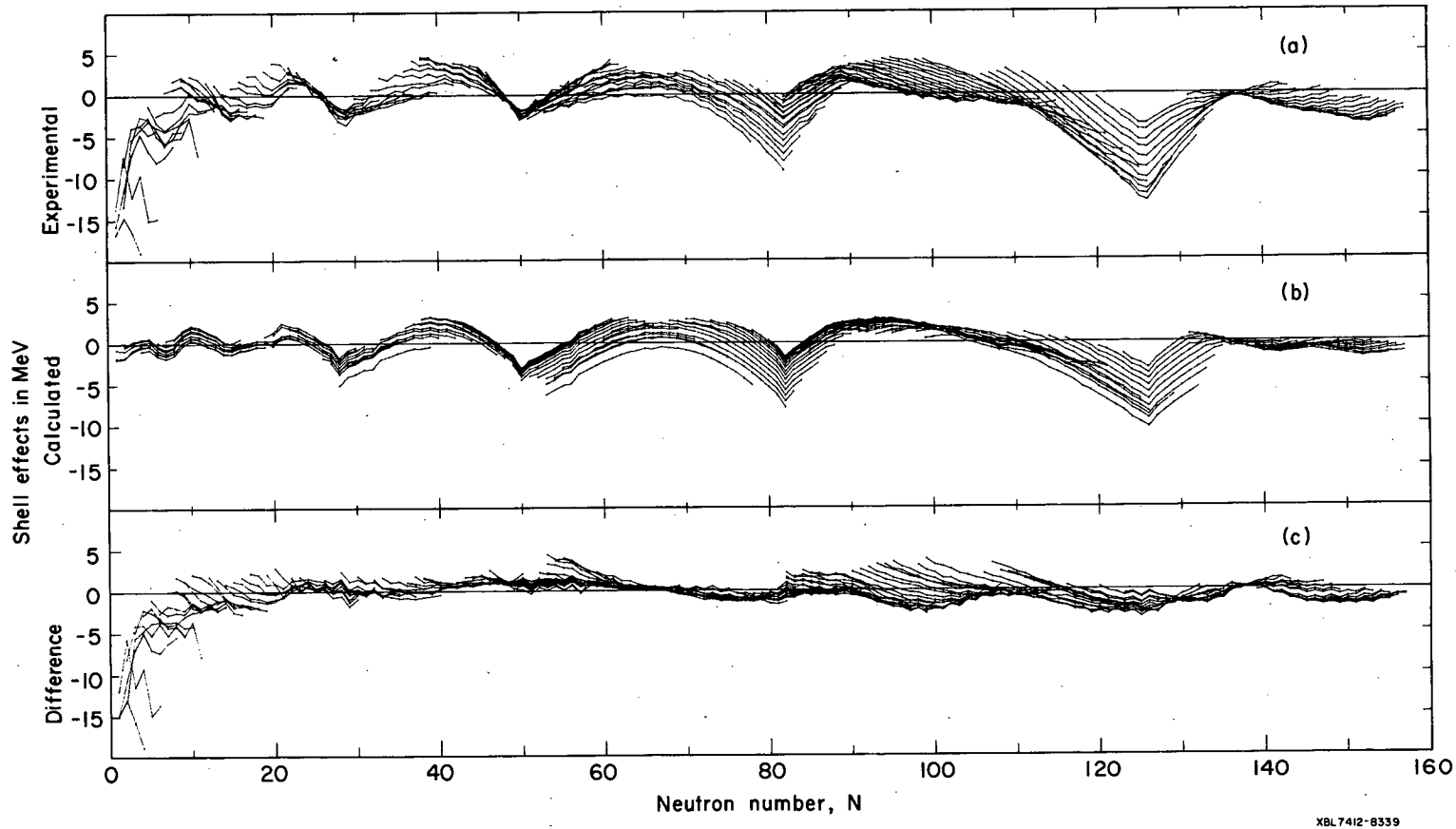

(a)
(b)
(c)
Experimental
Calculated
Difference
Shell effects in MeV
5
0
-5
-10
-15
0
20
40
60
80
100
120
140
160
Neutron number, N
XBL7412-8339

Fig. 2
lower

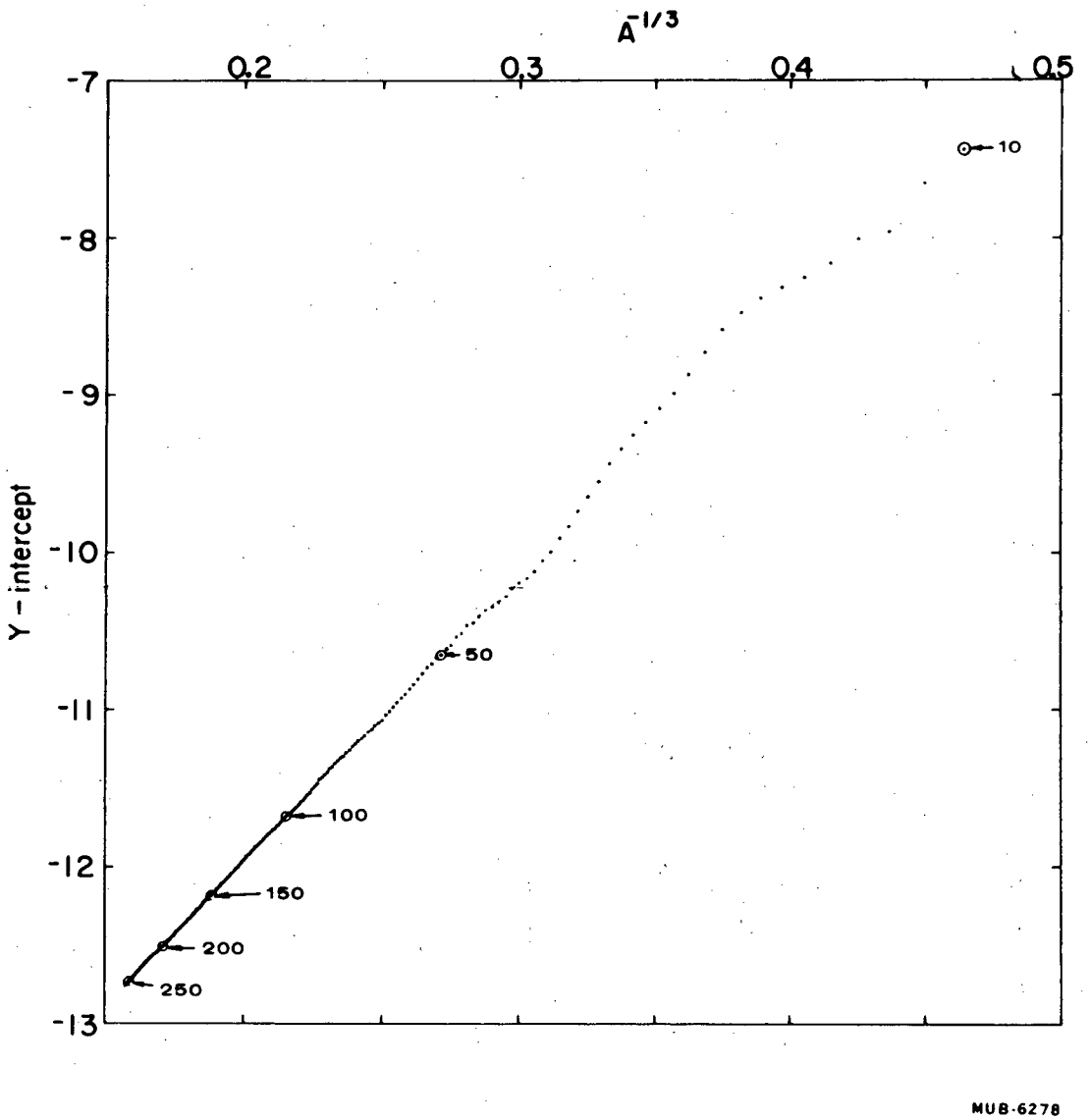
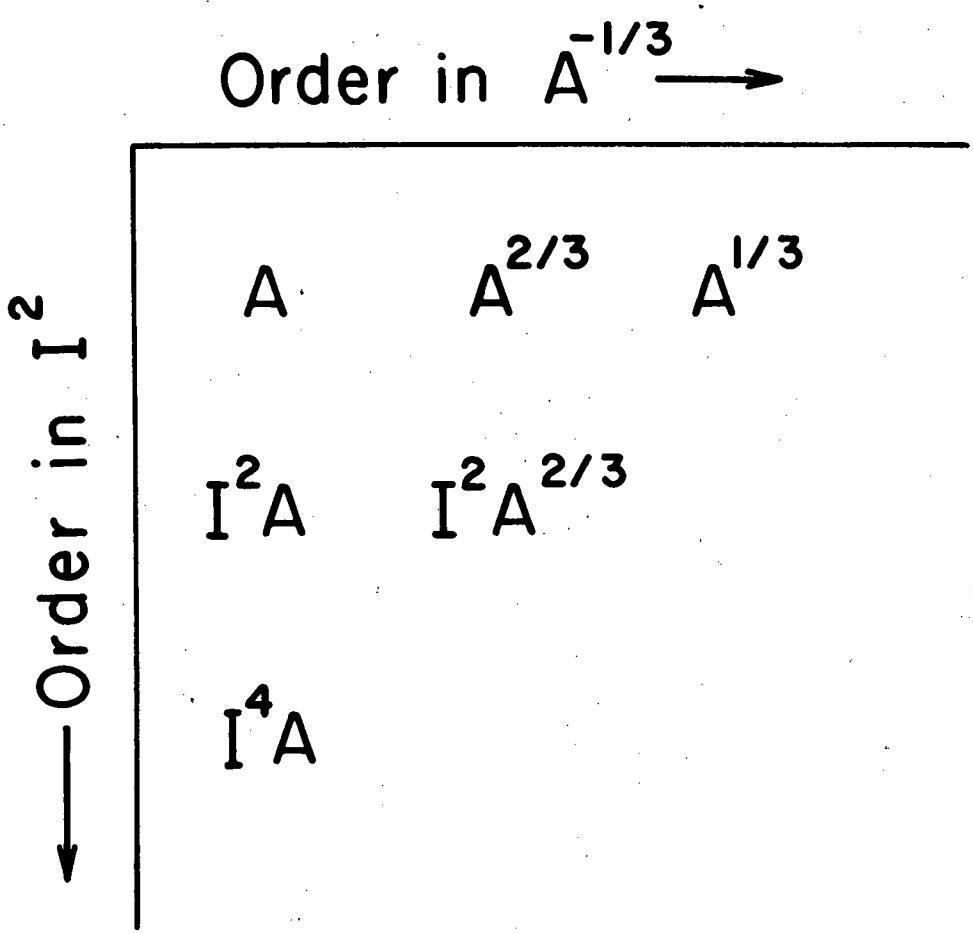

$A^{-1/3}$
0.2
0.3
0.4
0.5
-7
-8
-9
-10
-11
-12
-13
Y - intercept
10
50
100
150
200
250
MUB-6278

Fig. 3



XBL687-3358

Fig. 4

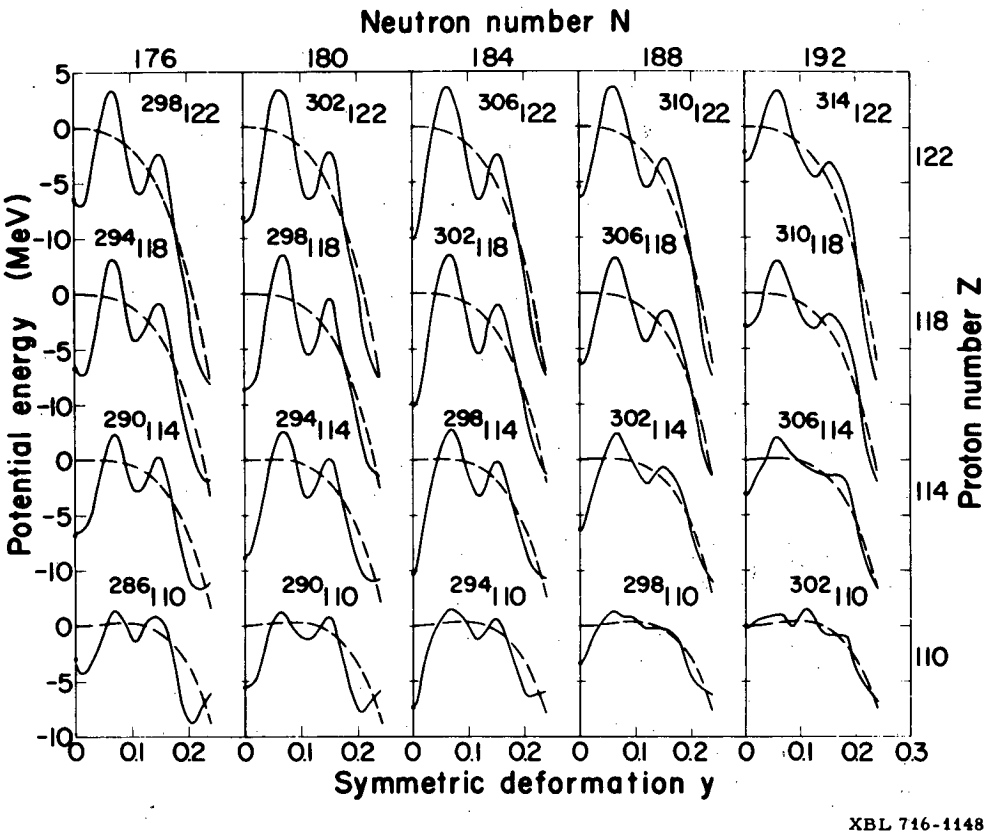
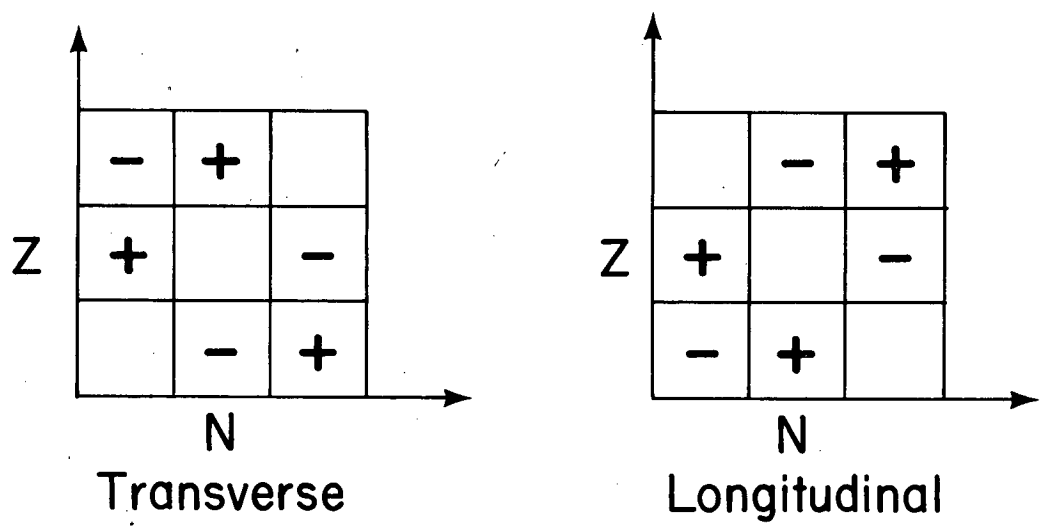

Neutron number N
176
180
184
188
192
Potential energy (MeV)
Proton number Z
122
118
114
110
Symmetric deformation y
XBL 716-1148

Fig. 5



XBL 822-130

Fig. 6

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