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ABSTRACT

Nuclear properties—nuclear masses in particular—
lend themselves to a two-part approach in which average
properties and shell effects are treated separately. Re-
cent improvements in treating the shell-effect part of nu-
clear masses have stimulated an investigation of correc-
tions to the smooth part of the formula—the liquid-drop-
model part. The Thomas-Fermi statistical method is em-
ployed to calculate these corrections, and the coefficient
of the $A^{1/3}$ term is discussed in detail. In addition the
nuclear density distributions are shown which arise in the
course of the Thomas-Fermi calculations.

INTRODUCTION

The time has come to take another look at possible improvements in the liquid-drop-model part of the mass formula. Since such improvements are difficult to extract directly from the experimental masses, a theory is needed which relates these corrections to established nuclear properties. I will present here, according to the following outline, one possible approach to this problem:
- · Two-part Treatment of Nuclear Properties
- · The Thomas-Fermi Method
- · Results of the Calculations
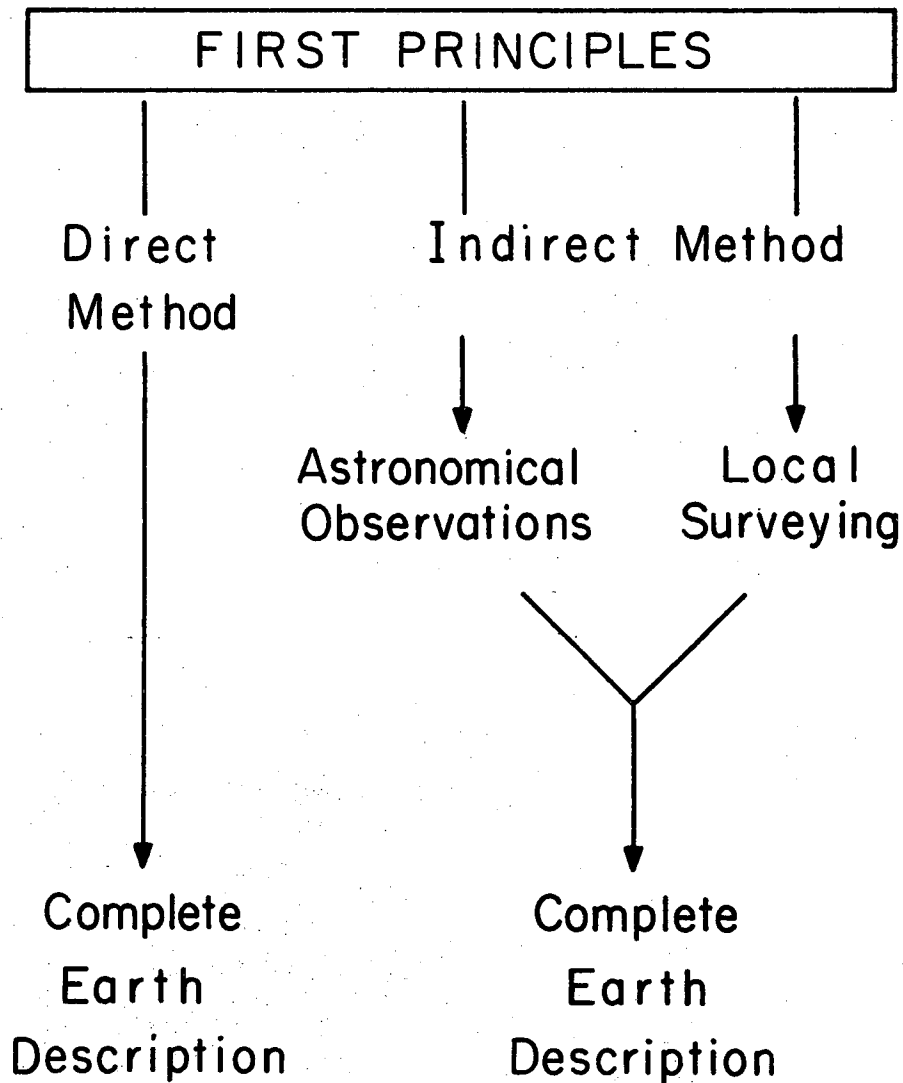
TWO-PART TREATMENT OF NUCLEAR PROPERTIES

From the earliest work on nuclear masses to the present, it has been recognized that a simple four-term liquid-drop-model formula–consisting of volume energy, surface energy, symmetry energy, and Coulomb energy– provides a good explanation of average mass trends (1). Attempts to improve the agreement as more mass data have become available have often involved higher-order contributions to the energy such as
- (a) the surface symmetry energy,
- (b) the surface curvature correction,
- (c) the compressibility correction,
- (d) the Coulomb exchange correction.
But, although one believes such terms are present, it has been difficult to find evidence for them directly in the trends of the experimental masses. The reason for this is that these corrections tend to be obscured by variations in the masses due to shell effects, and these variations – which appear as wiggles in plots of mass against particle number– must be removed before the details of the smooth trends can be extracted. The need to separate wiggles from smooth trends in other nuclear properties–not only masses–calls for a characteristic two-part formulation of nuclear theory.

An analogy can be used to demonstrate the value of a two-part approach. Suppose the problem is to map the surface of the earth instead of the nuclear mass surface. Then there are two ways of proceeding from first principles (which here include various observational data such as angles between surface features, elevations, etc.). One is the direct approach of extending local measurements

over wider and wider regions until all points on the globe
are linked together in a self-consistent way. The second
way, and the only one that is satisfactory at present, is to
add detailed local measurements to a smooth reference
geoid whose shape has been determined from astronomical
data.

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┌─────────────────────────────────────────┐
│          FIRST  PRINCIPLES              │
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Direct
Method

Indirect Method

Astronomical
Observations

Local
Surveying

Complete
Earth
Description

Complete
Earth
Description

Each part of the two-part approach calls on separate observational data and is characterized by its own special techniques, and this is just as true in the nuclear case.

| FIRST PRINCIPLES |

Direct Method   Indirect   Method

Liquid – drop   Shell
Formula   Effects

Complete   Complete
Mass   Mass
Formula   Formula
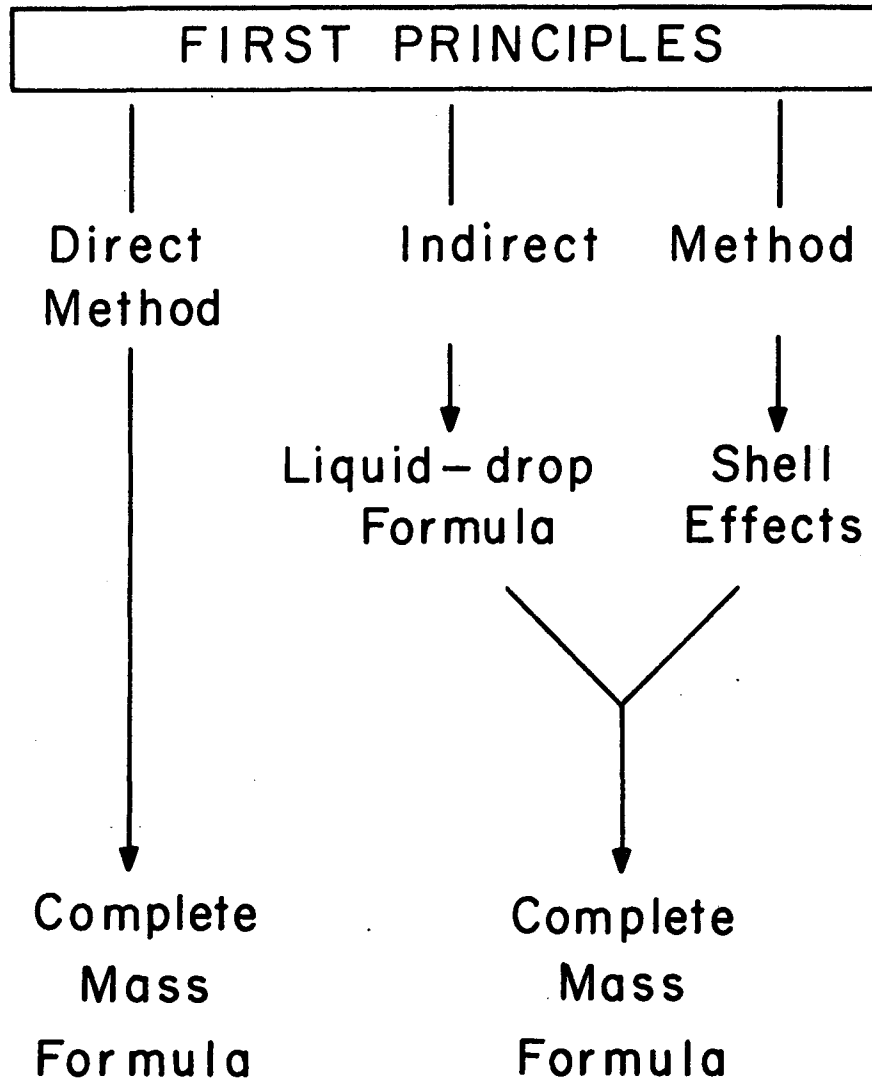
In both instances the direct method is too difficult at present, but the separate parts of the indirect method provide a tractable approach which yields satisfactory results.

There are many examples of application of this two-part approach to nuclear properties, the prediction of nuclear masses being one of the most familiar. In Fig. 1 we can see how well the masses are given by the liquid-drop model; Fig. 2 shows the remaining shell-effect variations and how they may be treated. The nuclear deformation energy may also be treated in this two-part way, and Fig. 3 illustrates how shell effects can be added to the liquid-drop model in order to predict the shape of nuclei. Finally, consider Fig. 4, which shows the smooth behavior of the liquid-drop-model fission barriers and the modifications to be expected from adding shell effects.

Recent emphasis in the application of the two-part approach to the calculation of nuclear masses has been on improving the corrections for single-particle effects (2-5). These wiggles can now be approximately accounted for, and when they are subtracted a very smooth empirical mass surface remains. The time is ripe to make refinements to the old four-term liquid-drop theory in analyzing this corrected smooth surface.

THE THOMAS-FERMI METHOD

The natural choice when undertaking a study of average nuclear properties is a statistical method of calculation like the Thomas-Fermi treatment of atoms. For example, see Refs. (6-8). In this approach the kinetic energy of the particles is assumed to be that of a Fermi gas without correction for density gradients. The validity of this assumption depends upon how slowly the density varies over a typical particle deBroglie wavelength. Detailed analysis of this question in Ref. (9) shows that gradient corrections are less than 10% when

$$\frac{|\text{grad } \rho|}{\rho^{4/3}} \lesssim 12.$$

The criterion is satisfied over most of the charge distribution in an atom; which explains why the simple Thomas-Fermi approach works so well. The introduction of gradient corrections into the atomic calculations has been shown to have little influence on the results (9). For nuclei the criterion is met over the central region and through the surface out to the point where the density has dropped to about 1/6 of its central value. Consequently, the neglect
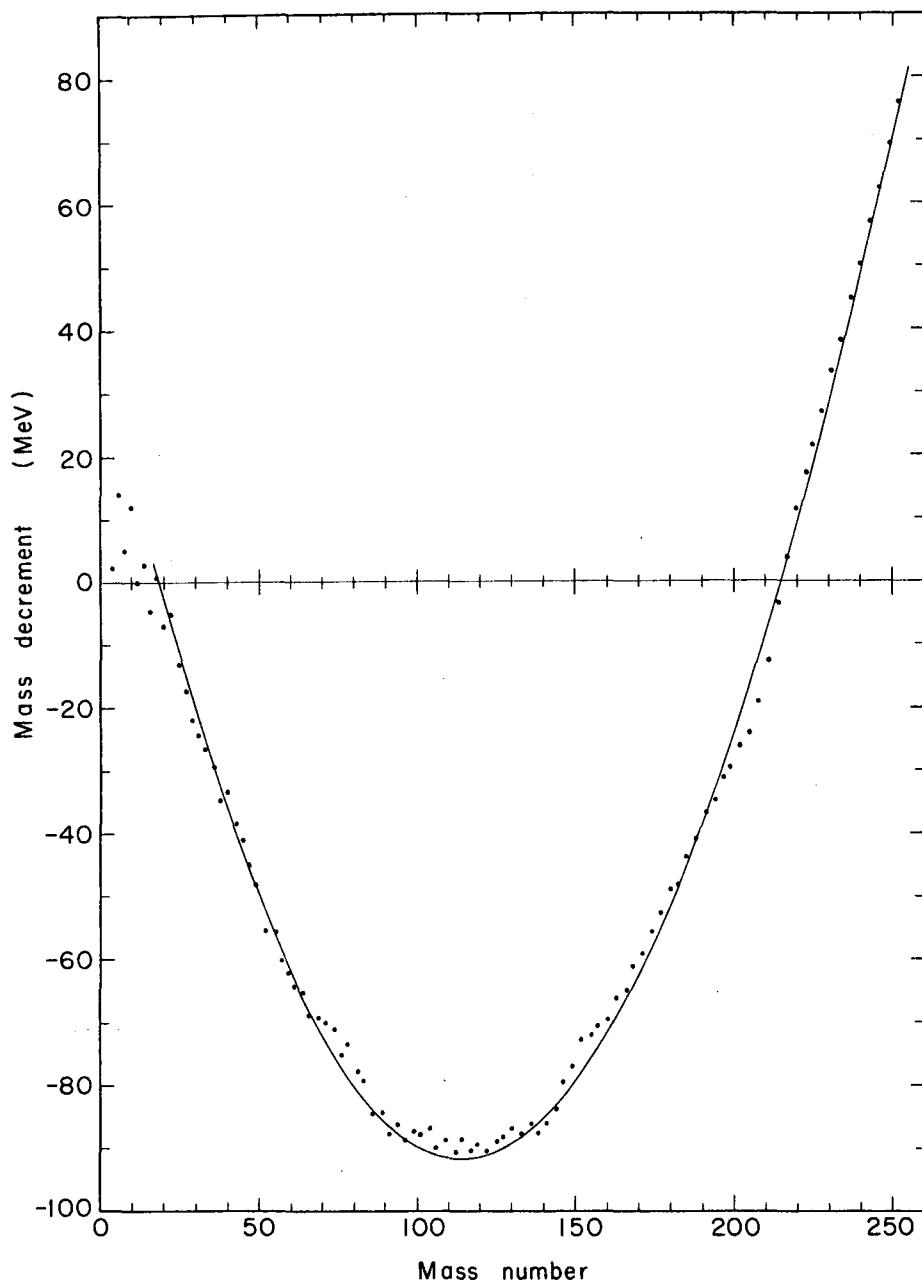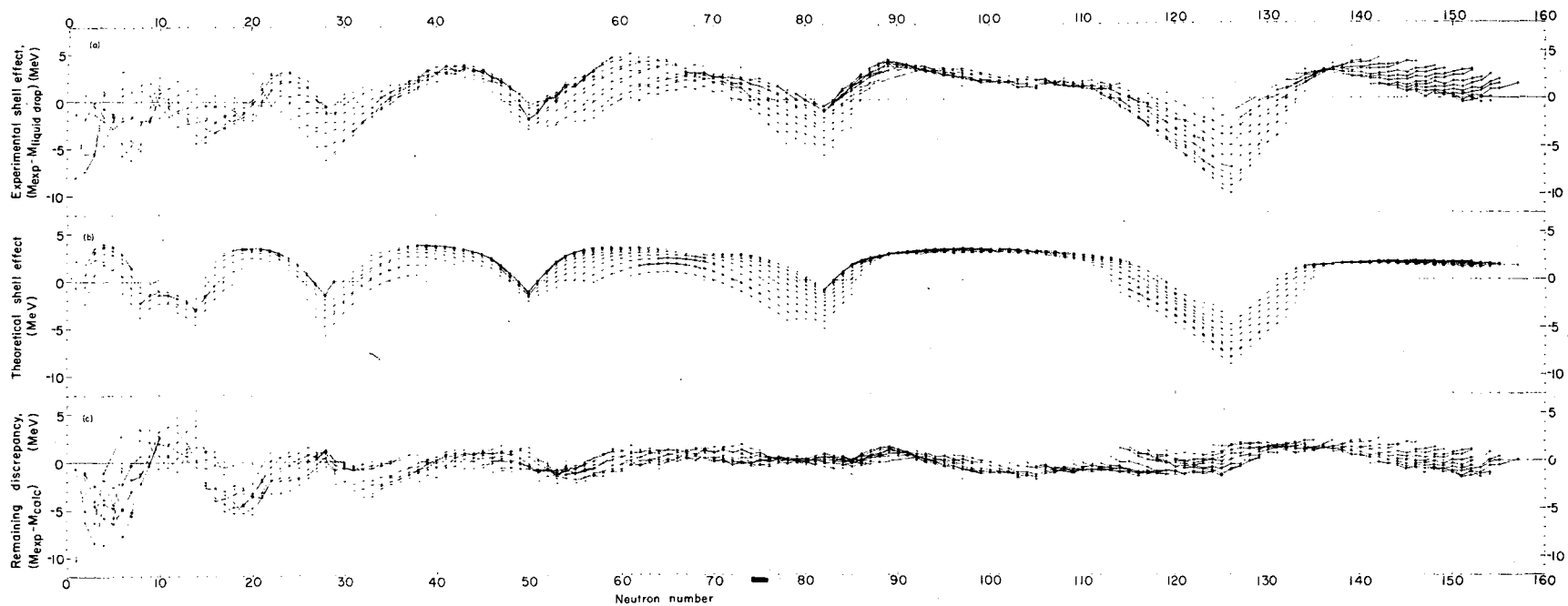
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Fig. 1. From Ref. (2); Mass decrements of 97 beta-
stable nuclei compared with the smooth curve
corresponding to a liquid-drop-model mass for-
mula. Note that the overall trend of the decre-
ments is reproduced throughout the periodic
table. The scatter of the points is due to shell
effects.

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Fig. 2. From Ref. (3): Experimental and calculated shell effects in the nuclear masses, and their difference, as functions of neutron number. Isotopes of an element are connected by a line.
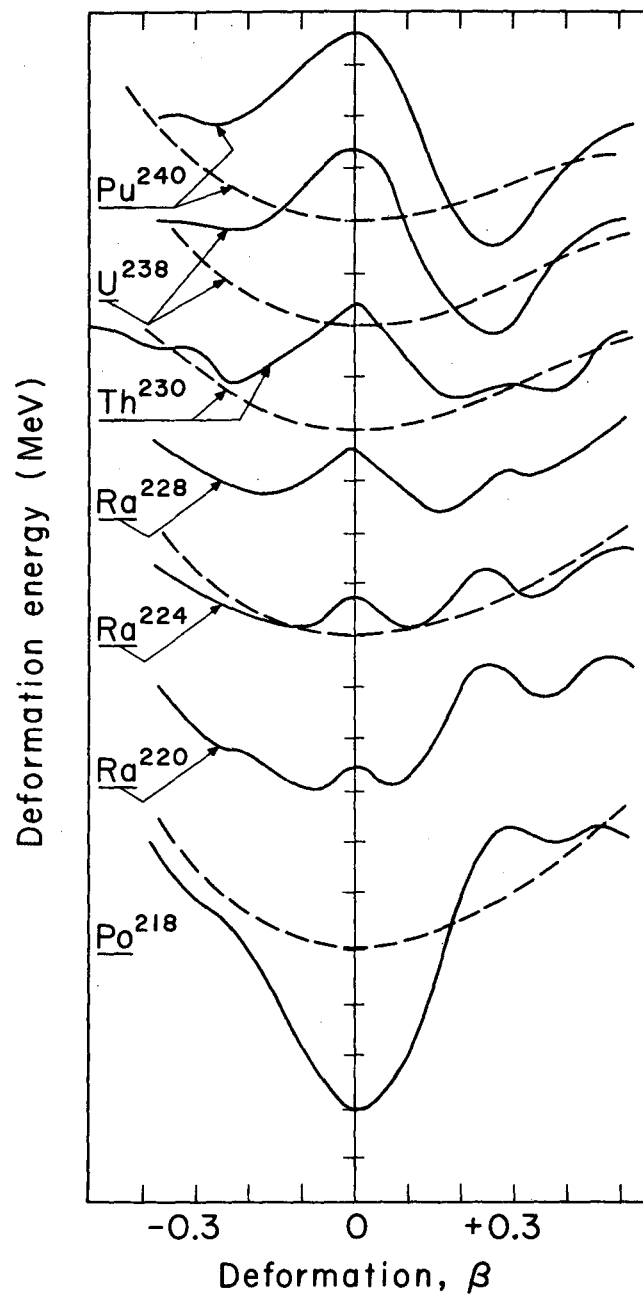
Fig. 3. In Ref. (4) this figure is used to illustrate the rela-
tive deformation energy of various nuclei in MeV.
This energy–the solid line–line is obtained by adding
the results of a shell-model calculation to the liquid-
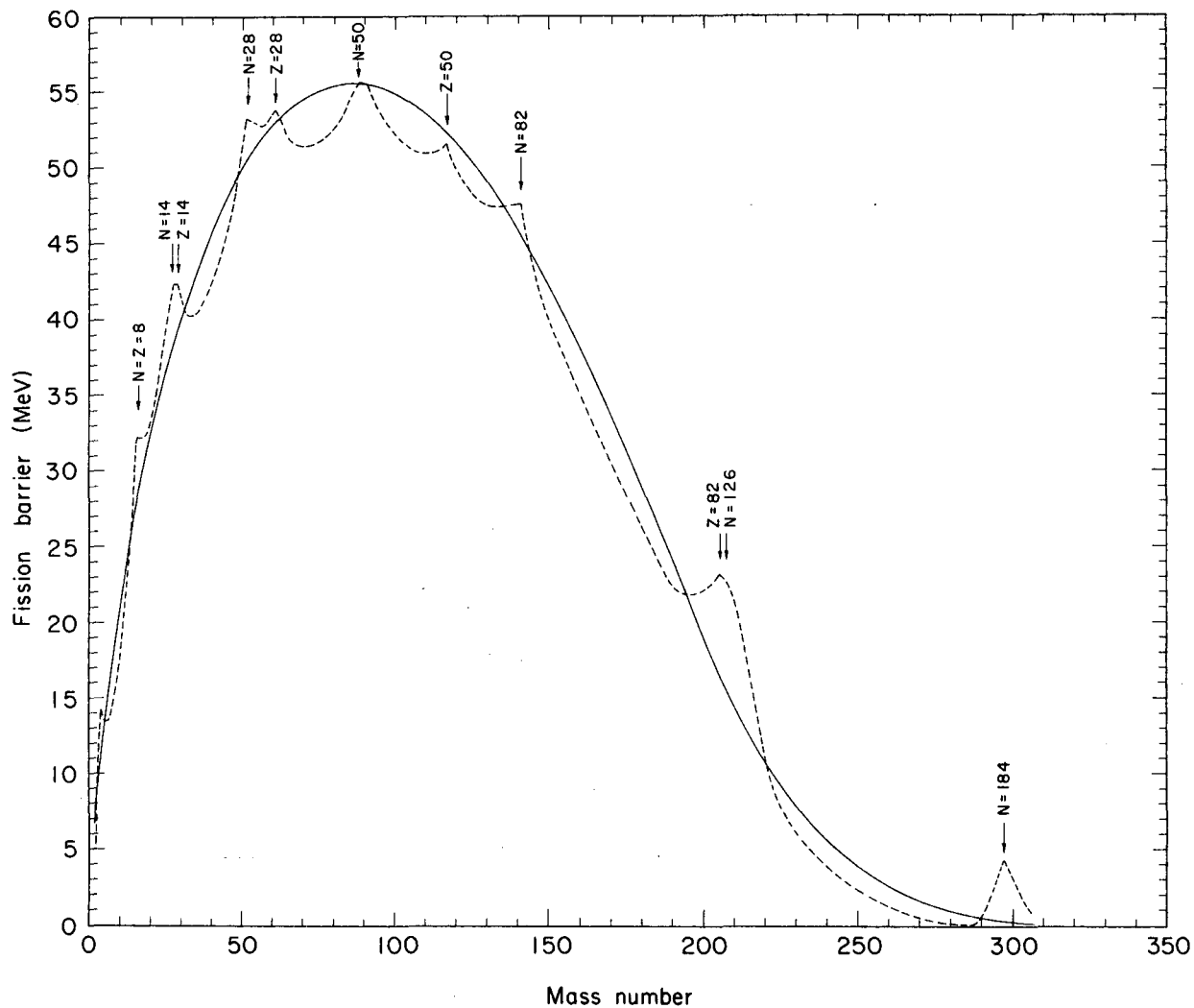drop-model result shown by the dashed lines.

Fig. 4. Fission barrier energy (MeV) for nuclei along Green's approximation to the valley of stability. In this figure [from Ref. (2)] the smooth curve is the liquid-drop-model result, and the dashed curve shows what modification is to be expected from the introduction of shell effects.

of gradient corrections is expected to have little influence
on the outcome of the calculation except for the outer
fringe of the density distribution.

In addition to the Thomas-Fermi expression for the
kinetic energy, the law of interaction between the particles
must be specified. In this work a phenomenological inter-
action was chosen which leads to saturation and which is
simple enough to allow calculations with no further approxi-
mations. This interaction—which was first applied in this
context by Seyler and Blanchard (7)—consists of a Yukawa
force whose strength decreases with increasing relative
momentum of the particles, and is of different magnitude
between "like" and "unlike" particles. The "like" strength
applies to proton-proton or neutron-neutron interactions,
while the "unlike" strength applies to the neutron-proton
interaction. This interaction may be written

$$V = - C_{like \atop (or\ unlike)} \quad [1-(p_{12}/p_c)^2] \ \frac{e^{-(r_{12}/r_y)}}{(r_{12}/r_y)} ,$$

where r_{12} is the relative distance, and p_{12} the relative
momentum of the particles. The parameter p_c governs
the velocity dependence of the potential. It is the value of
the relative momentum at which the attractive force—whose
strength is decreasing with increasing relative momentum—
would vanish, and beyond which the force would become
repulsive. The four parameters of the interaction—the two
strengths C_1 and C_u, the Yukawa range r_y, and the criti-
cal momentum p_c—will be determined later from the prop-
erties of nuclei.

With the kinetic and interaction energies specified
one may ask, as in the atomic problem, what spatial dis-
tribution of nucleons minimizes the total energy. This
leads to a standard variational problem which in the atomic
case results in the nonlinear Thomas-Fermi differential
equation. For nuclei this minimization leads to an integral
equation which might be called the Seyler-Blanchard equa-
tion. The systematic working out of the consequences of
this equation leads to a compact theory of all smooth nu-
clear properties analogous to the Thomas-Fermi theory of
atomic properties.

With respect to the analogy between the nuclear
theory presented here and the Thomas-Fermi atomic the-
ory, it should be pointed out that there is one important

difference. This has to do with exchange corrections. In
the standard atomic case exchange effects are simply ne-
glected because their influence is known to be small. In
nuclei such effects are not small but their proper treatment
is difficult. The approach used here is a compromise in
which such effects are not neglected, but are treated in a
qualitative way through the velocity dependence of the inter-
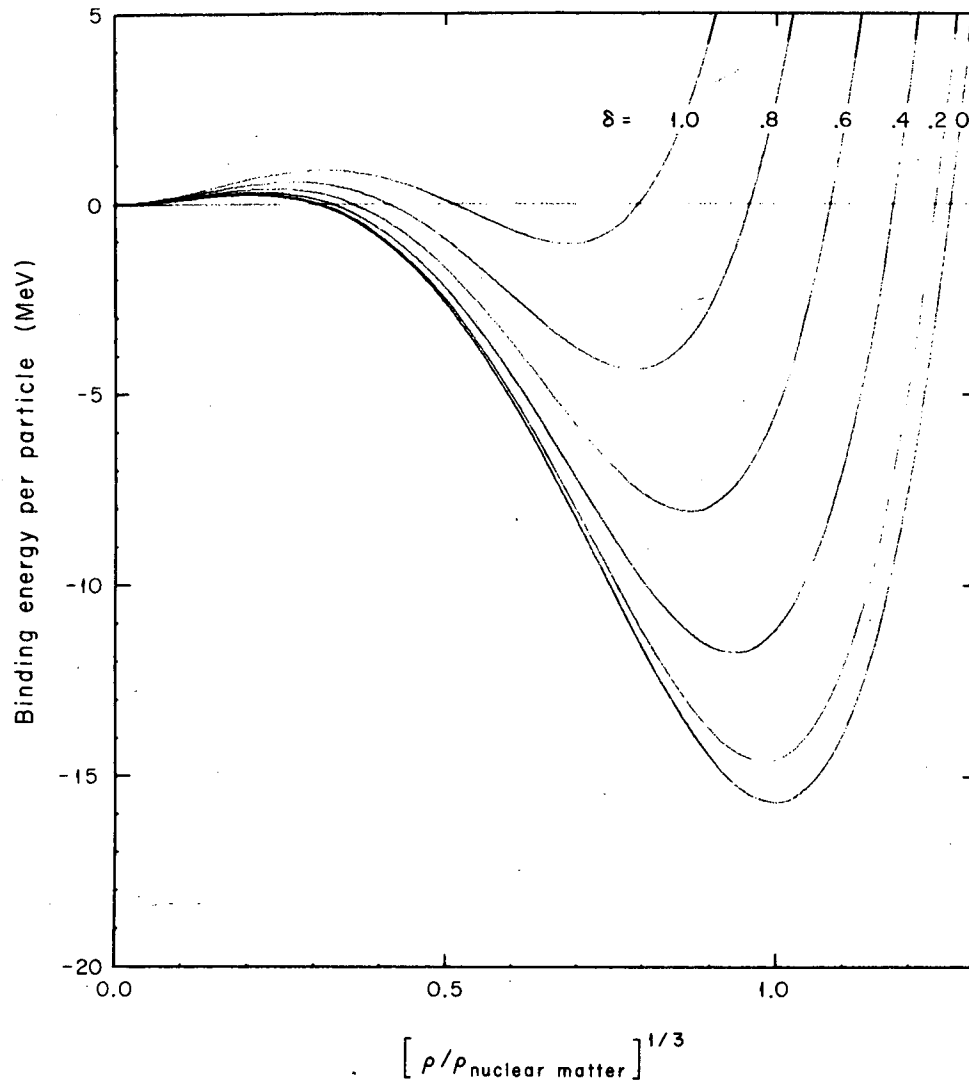action.

RESULTS OF THE CALCULATIONS

The implications of this approach will be shown by
considering the following natural sequence of calculations:
1. Infinite nuclear matter
2. Semi-infinite nuclear matter
3. Finite nuclei, without Coulomb energy
4. Finite nuclei, with Coulomb energy
The infinite nuclear matter problem takes the form of a
simple algebraic relation when this method is used, and Fig.
5 shows how the energy per particle of nuclear matter de-
pends on density and composition. The requirement that
the experimental values of the volume energy, symmetry
energy, and density of nuclear matter be reproduced pro-
vides three relations among the four free parameters of the
theory. At this stage, and without specifying the fourth
parameter, we are able to make our first predictions, which
are that the calculated compressibility of nuclear matter is
large (about 295 MeV) and that the energy per particle of
neutron matter is small (about -1 MeV).

The problem may also be solved in the semi-infinite
case, and the resulting density distribution, and part of the
potential associated with it, are shown in Fig. 6. This
case—nuclear matter bounded by a flat surface—may be
thought of as a solution for the surface region of a very large
nucleus. Also shown in the figure is a curve representing
the difference between the energy of the surface particles at
any point through the surface and the energy they would have
if they were in the nuclear interior. We may call this the
surface energy function, since integration over it gives the
surface energy coefficient.

At this point the last free parameter may be chosen to
fix the numerical value of either the surface energy or sur-
face thickness. Since the emphasis here is on the mass for-
mula, I have chosen to fix the surface energy, with the re-
sult that the surface thickness—characterized by the distance
in which the density falls from 90% to 10% of its central

$$\delta = \quad 1.0 \qquad .8 \qquad .6 \qquad .4 \quad .2 \quad 0$$

Binding energy per particle (MeV)

$$\left[\rho / \rho_{nuclear\ matter} \right]^{1/3}$$

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Fig. 5. The energy per particle for infinite nuclear matter
in MeV is shown as a function of both density and
composition, where $\delta = (N-Z)/A$. The parameters
entering the calculation are those given in Table I.
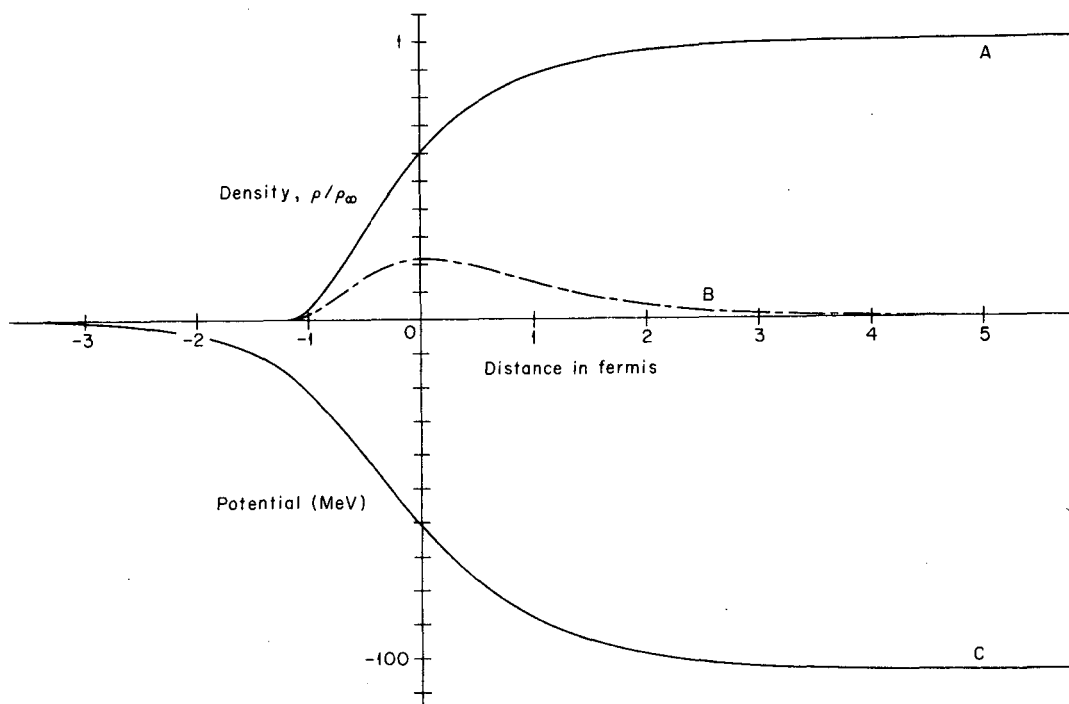
Fig. 6. Curve A is the predicted density distribution at the
boundary of symmetric, semi-infinite nuclear matter.
Curve B shows—in relative units—how the source of the
surface energy is distributed across the nuclear sur-
face. Curve C is the constant part of the velocity-
dependent potential that corresponds to the density dis-
tribution shown here. It is the average between neutrons
and protons of the potential which would be felt at each
point by a zero-velocity particle.

value-turns out to be 2.0 fermis. Table I lists the quanti-
ties used to determine the adjustable parameters, and the
values that result.

TABLE I

Input quantities from Ref. (2)

Value		Property
-15.677	MeV	Energy per particle of symmetric nuclear matter
28.062	Mev	Symmetry energy coefficient
1.2049	fm	Nuclear radius constant
18.56	MeV	Surface energy coefficient

Resulting values of the adjustable
parameters

Value		Parameter
367.7	MeV	C_1, Strength of neutron-neutron, proton-proton force
289.7	MeV	C_u, Strength of neutron-proton force
82.03	MeV	$(p_c^2/2M)$, Critical energy of the momentum dependence
0.6256	fm	r_y, Range of the interaction

With all the parameters fixed the next calculation to
consider is that of finite nuclei without Coulomb energy.
The important features of this new calculation are the den-
sity distributions, and the total binding energy as a function
of the mass number A. Figure 7 gives three examples of
the density distributions (which are the same for neutrons
and protons). Since these density distributions represent
average properties they do not have the wiggly appearance
of a single-particle calculation; hence, they may be thought
of as representing the average distribution for a number of
neighboring nuclei. They show an increase in the central
density of medium and heavy nuclei which is caused by the
squeezing of the central region by the nuclear surface.
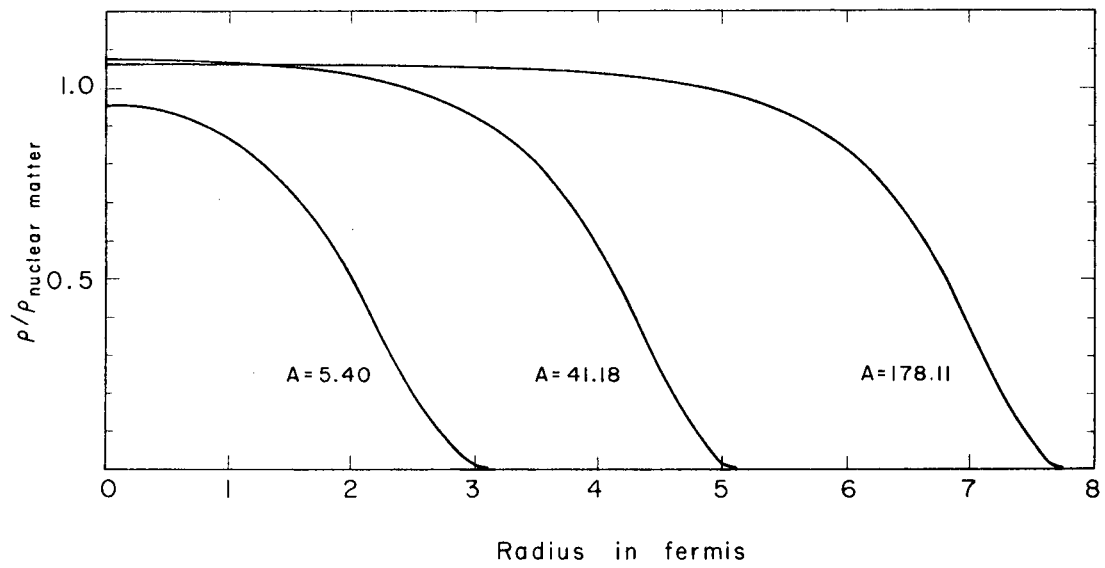
Fig. 7. Density distribution of three symmetric, finite nuclei shown for the case in which the Coulomb energy is not included in the calculation.

Other features of the density distribution also deserve dis-
cussion, but since we are here concerned primarily with
the mass formula let us turn to the other aspect of these
calculations, that is, the total energy. Before showing the
numerical results let us note some general features of the
A dependence of the nuclear energy. For saturating sys-
tems, such as nuclei, composed of particles interacting
via a short-range force we are led to expect a description
of the total energy in terms of an expansion in the dimen-
sionless ratio

$$\frac{(\text{ range of the force })}{(\text{radius of the system})} ,$$

which is proportional to $A^{-1/3}$. Because of this the various
contributions to the nuclear part of the binding energy of a
heavy nucleus form the following natural hierarchy of ef-
fects:

Order	Typical energy (MeV)	Effect
A	3000	Volume energy
$A^{1/3}$	600	Surface energy
$A^{2/3}$	50	Curvature and compressibility corrections
A^{0}	5	Finiteness and single-particle effects

Figure 8 illustrates this point by showing how the energy
per particle of finite nuclei depends on $A^{-1/3}$. The curve
in the figure may be expressed as a Taylor series in $A^{-1/3}$,
and subsequent multiplication by A yields the following for-
mula for the nuclear part of the energy of symmetric finite
nuclei:

$$E = -15.677\, A + 18.56\, A^{2/3} + 6.98\, A^{1/3} - 12.3\, A^{0} + \cdots .$$

As noted before, the interaction parameters were chosen
to give the correct values for the volume and surface ener-
gies (the first two coefficients). The first new coefficient
to be predicted is that of the $A^{1/3}$ term. Two physical ef-
fects were found to make up this coefficient: the compress-
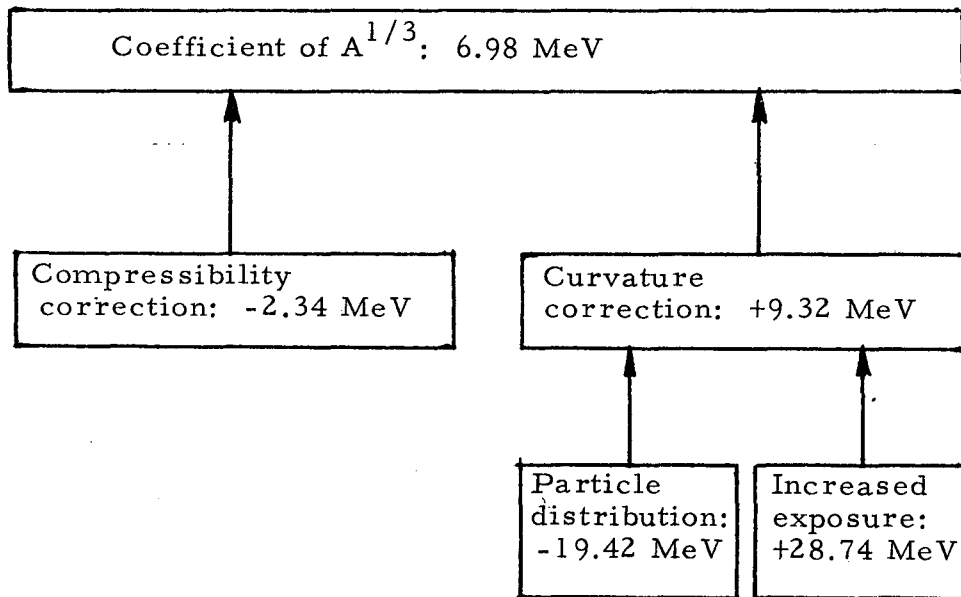ibility correction, and the surface curvature correction.
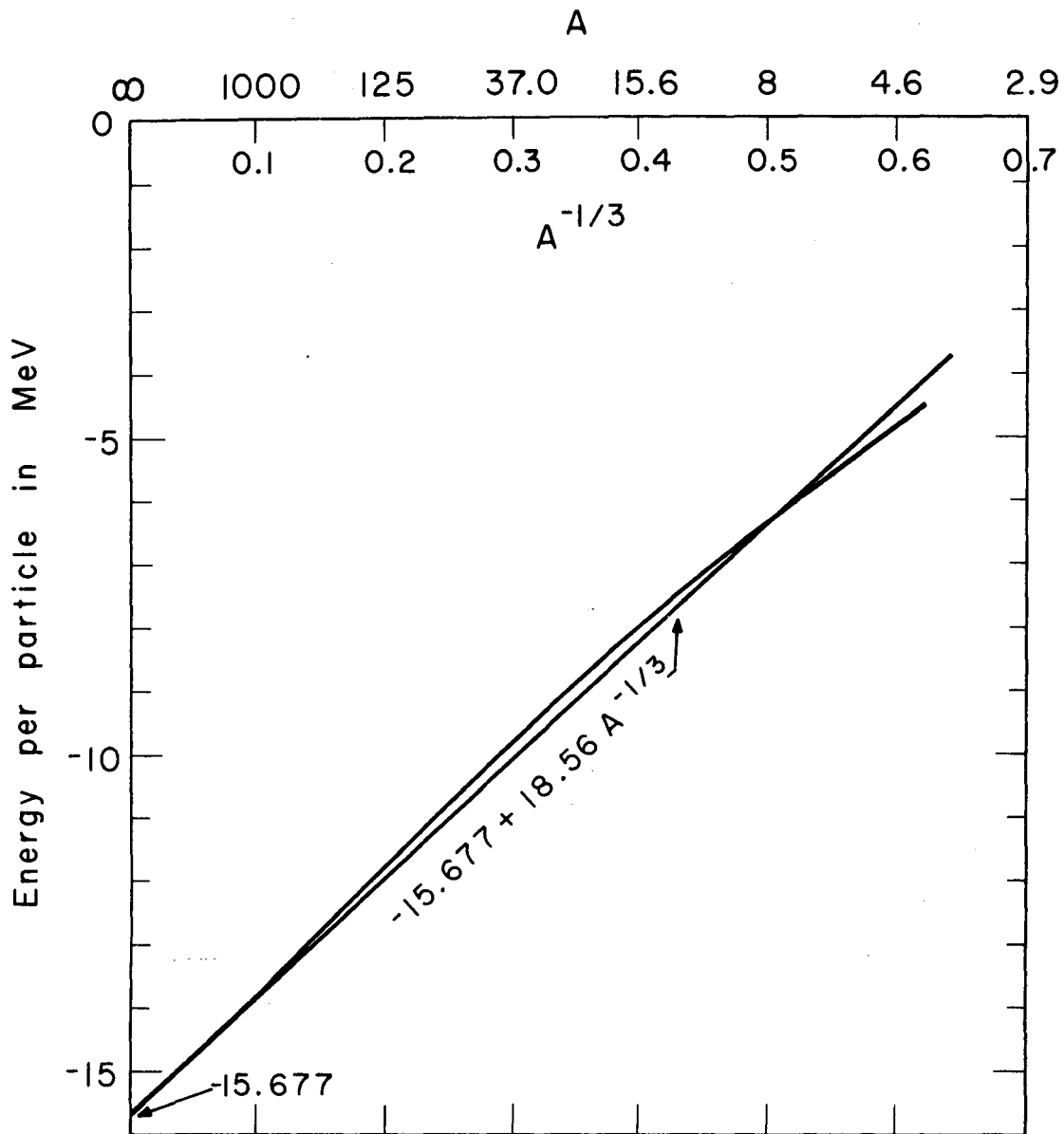
Fig. 8. The energy per particle of symmetric finite nuclei
without Coulomb effects plotted against $A^{-1/3}$. The
straight line shows the result of keeping only the two
lowest-order terms in the expansion of this function
in powers of $A^{-1/3}$, that is, only the volume and sur-
face-energy terms.

The first of these, the compressibility correction, accounts for the reduction of the surface energy at the expense of compressing the nuclear interior. This correction can easily be calculated from the expression

$$\text{Compressibility correction} = - \frac{2c_2^2}{K} = - 2.34 \text{ MeV},$$

where the surface energy coefficient c_2 is 18.56 MeV and the compressibility K is 295 MeV.

The remaining 9.32 MeV curvature correction has two distinct sources. The first represents the effect of the increased exposure—fewer neighbors—for particles close to a curved surface. The second represents the effect of the reduced number of particles with a given degree of exposure. The first effect, that of increased exposure, causes an increase in the surface energy which contributes 28.74 MeV to the correction. To illustrate the source of the other contribution, consider the vertical line in Fig. 6, which specifies the mean location of the surface. When the surface is curved there are more particles outside this point and fewer inside. The effect this has on the surface energy can be obtained by calculating the first moment of the surface energy function with respect to this point. The result of this calculation is a predicted contribution of -19.42 MeV to the curvature correction. Summarizing this discussion, we have

Coefficient of $A^{1/3}$: 6.98 MeV

Compressibility correction: -2.34 MeV

Curvature correction: +9.32 MeV

Particle distribution: -19.42 MeV

Increased exposure: +28.74 MeV

Continuing on to the next term in the series, it is interesting to note that the coefficient of the A^0 term is twice as large as that of the $A^{1/3}$ term and of opposite sign. This may explain why no strong evidence for an $A^{1/3}$ term has been observed in the experimental masses.

The next stage of the calculation, which is the inclusion of the Coulomb energy, brings us at last to the complete problem. As in the previous discussion the most interesting features are the density distributions and the binding energy. From the second of these I hope to extract the new correction terms which arise, such as

   (a)   the surface symmetry energy,
   (b)   the density redistribution effects, that are due to the Coulomb repulsion,
   (c)   the effect of surface diffuseness on the Coulomb energy.

This part of the work is not yet complete, but several preliminary calculations of the density distributions have been made, such as those shown in Fig. 9. This illustration shows both the neutron and proton density distributions for three nuclei near the valley of beta stability.

Since the Thomas-Fermi method provides one with a complete theory of the average properties of nuclei, much more than density distributions can be obtained. The immediate goal of the present investigation is to derive the magnitude and the N and Z dependence of the additional terms needed to improve the mass formula. Since each new term has a physical basis and a known method for its calculation, its dependence on the nuclear shape can also be determined. Thus, the resulting description of the smooth part of the nuclear binding energy will be general enough to include even highly deformed configurations. [For a related discussion see Ref. (8)]. When shell effects are added to this new formula—in the manner of Ref. (4)—this generality will permit improved predictions not only of nuclear ground-state masses, but also of ground-state deformations, and fission barrier energies.

SUMMARY

The purpose of this work is to make a contribution to the two-part approach to the nuclear mass formula. The emphasis here has been on improving the liquid-drop-model part of the formula. This improvement has been based on a statistical calculation of nuclear properties by use of the
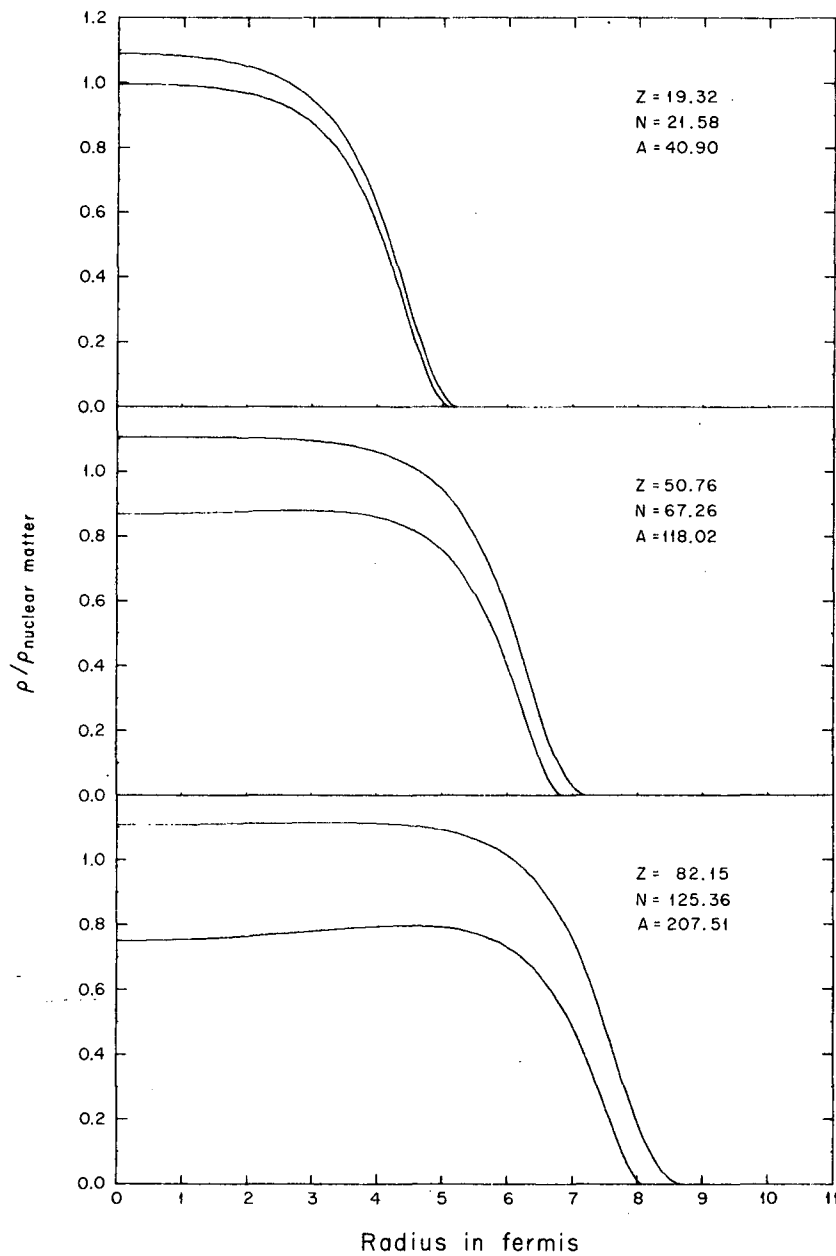
Fig. 9. Neutron and proton density distributions for three nuclei from along the valley of beta stability. Note the increasing neutron skin thickness, and the different ways the neutron and proton distributions approach zero.

Thomas-Fermi method, which is applicable when

$$\frac{|\text{grad } \rho|}{\rho^{4/3}} \lesssim 12.$$

Properties that can be calculated by the application of this method can be expressed as expansions in powers of the parameter

$$\frac{(\text{ range of the force })}{(\text{radius of the system})},$$

which is proportional to $A^{-1/3}$. With this expansion in mind the calculations have been used to extend the liquid-drop-model part of the mass formula to include a term in $A^{1/3}$, and work is in progress to determine the associated corrections to the Coulomb energy. When these additional terms have been calculated we will have an improved liquid-drop-model mass formula available. I hope it will have as long a life as the traditional liquid-drop-model formula it replaces.

FOOTNOTES AND REFERENCES

* Work done under auspices of the U. S. Atomic Energy Commission.

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