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DROPLET MODEL NUCLEAR DENSITY DISTRIBUTIONS AND SINGLE PARTICLE POTENTIAL WELLS†

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Abstract

A description is given of the nuclear density distributions and single particle potential wells that arise in the course of Thomas-Fermi calculations of average nuclear properties. Simple expressions are given for the calculation of the essential characteristics of these distributions, and it is shown how the results obtained here may be used to approximate the densities and potential wells in terms of Fermi functions.

†Work performed under the auspices of the U. S. Atomic Energy Commission.

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1. Introduction

The primary purpose of this work is to present a method for determining the single particle potential wells appropriate for use in Shell Model calculations. The study is based on a calculation (in terms of the Thomas-Fermi statistical method) of average nuclear properties using a phenomenological velocity dependent force.

In ref. 1 we found that the Thomas-Fermi method of Seyler and Blanchard[2]) could be applied with profit to the calculation of nuclear binding energies and density distributions. It also predicts velocity dependent neutron and proton single particle potential wells, and the potentials obtained in this way for particles at the Fermi surface may be compared with the static wells normally employed for investigating energy levels in that region. However, in spite of its broad applicability, the Thomas-Fermi Model has two major drawbacks (which also apply to Hartree-Fock calculations), one in practice and one in principle.

The practical drawback is that since the coupled integral equations which arise in this method cannot be solved analytically the determination of the properties of each separate nucleus requires a somewhat complex computer calculation. Furthermore, the numerical results which are obtained for some of the quantities of interest (such as the density distributions or the potential wells) are given as numerical functions which, in practical applications, do not possess the flexibility of closed algebraic expressions.

The objection in principle is that the model gives, as a rule, little insight into the physical origin of the nuclear properties that it predicts. The connection between the nature of the two body force assumed and the final

results is obscure and all that can usually be said with certainty is that if one uses the force specified and the given calculational procedure then a certain result will be obtained.

In our work these objections have been overcome through the development of an approach we have called the Droplet Model. This simple algebraic theory, which is described in detail in ref. 1, gives the properties of finite nuclei in terms of a set of coefficients that are deduced from Thomas-Fermi calculations of infinite and semi-infinite nuclear matter. In place of complex, Thomas-Fermi Model computer calculations for the properties of finite nuclei one has merely to deal with algebraic expressions in terms of N and Z. Moreover, the physical origin of the results can be determined from the algebraic structure of the Droplet Model expressions.

In the next two sections of this paper the Thomas-Fermi method is applied to infinite and semi-infinite nuclear matter respectively. The properties of the neutron and proton potential wells which are deduced in these sections are then combined with previously determined Droplet Model expressions in a third section in order to provide a description of the potential wells to be expected for finite nuclei. The fourth section is concerned with comparing the predictions of this method with single particle potential wells deduced from fitting energy levels. The final section is a discussion of the results.

2. Volume Properties

As the first step in our formulation of a macroscopic theory of single particle potential wells we used the Thomas-Fermi Model described in the appendix to estimate the numerical values of the potentials felt by neutrons and protons in infinite nuclear matter.

In terms of the notation of eq. (4.28) of ref. 1 an expression can be derived for the potential felt by a neutron at the Fermi surface which is

$$\nu = - \alpha \Phi^3 (1 - \frac{6}{5} \Phi^2) - \beta \Psi^3 (1 - \frac{3}{5} \Phi^2 - \frac{3}{5} \Psi^2) \quad . \tag{1}$$

This expression, which is in dimensionless form, and a similar one for the proton potential may be converted to a form that can be applied directly. The resulting expression for the potential may then be written as an expansion in terms of small deviations of the neutron and proton densities from their equilibrium values.

We find that the potential well depths (N for neutrons and Z for protons) are given by

$$V\binom{N}{Z} = - 51.4 \ (\pm) \ 46.2 \ \delta - 28.3 \ \varepsilon + 1.9 \ \delta^2 \ \text{MeV} \quad , \tag{2}$$

where

$$\varepsilon = - \frac{1}{3} (\rho - \rho_0)/\rho_0 \quad , \tag{3}$$

$$\delta = (\rho_N - \rho_Z)/\rho \quad . \tag{4}$$

As used here ρ_N is the neutron density, ρ_Z the proton density, ρ the total density and ρ_0 the equilibrium density of standard nuclear matter. The first term on the right side of eq. (2) is the common potential depth felt by both neutrons and protons at the Fermi surface of symmetric ($\rho_N = \rho_Z = \frac{1}{2}\rho_0$) nuclear matter. The second term (+ for neutrons and - for protons) is the isospin dependence of the potential. The last two terms, which are of higher order and are not used in the following discussion, are the density dependence and quadratic isospin dependence of the potential.

3. Surface Properties

The surface properties to be expected for the single particle potential may be determined by solving the nuclear matter problem in the semi-infinite case. Using the same Thomas-Fermi method as in the last section we can find the surface density distributions of the neutrons and protons as a function of $\bar{\delta}$ (the bulk value of δ, which describes the system away from the surface region). The potential wells, which are self consistent with these density distributions and are appropriate for particles at the neutron or proton Fermi surfaces, can also be calculated. Figures 1 and 2 are examples of such semi-infinite density and potential well distributions.

The method used to characterize the "location" L and "width" W of the surfaces in these figures is discussed in the appendix. The dependence of these quantities, which characterize the neutron and proton densities and single particle potential wells, on the bulk asymmetry $\bar{\delta}$ is shown in fig. 3. Here we see that the widths of the surfaces of the neutron and proton potential wells $W_V(N)$ and $W_V(Z)$ do not depend linearly on $\bar{\delta}$. The same is true of the widths of the surfaces of the density distributions themselves $W_\rho(N)$ and $W_\rho(Z)$. The

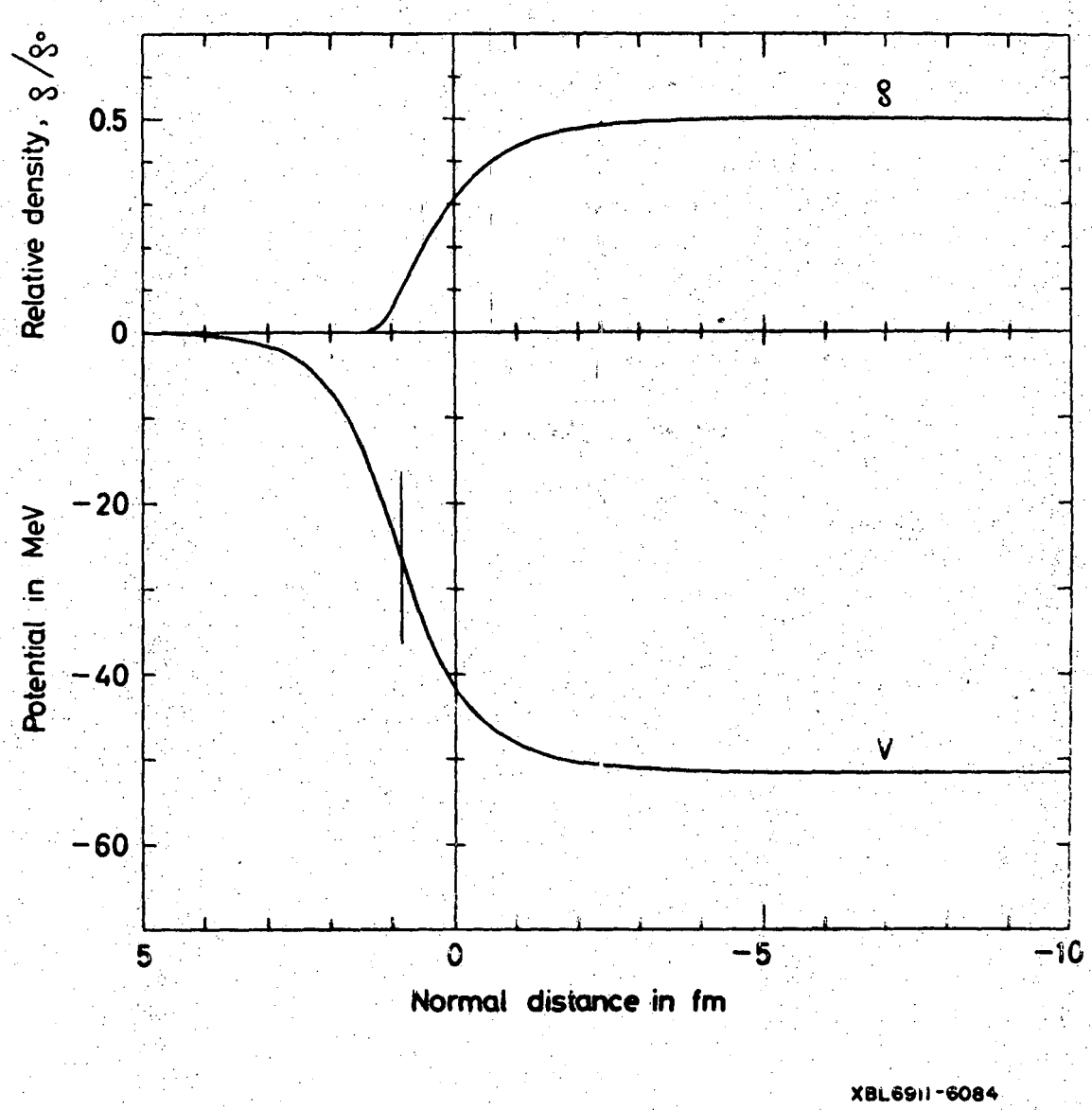

Fig. 1. The Thomas-Fermi density distribution ρ plotted relative to the "effective location of the surface" as defined in the appendix. In this case (the case of particle number symmetry where $\bar{\delta} = 0$) the neutron and proton density distributions are equal and are both represented by the curve labeled ρ. The potential felt by particles at the Fermi surface is also plotted. This curve, which is labeled V, has the effective location of its surface outside that of the density, at a point that is indicated by a vertical bar.

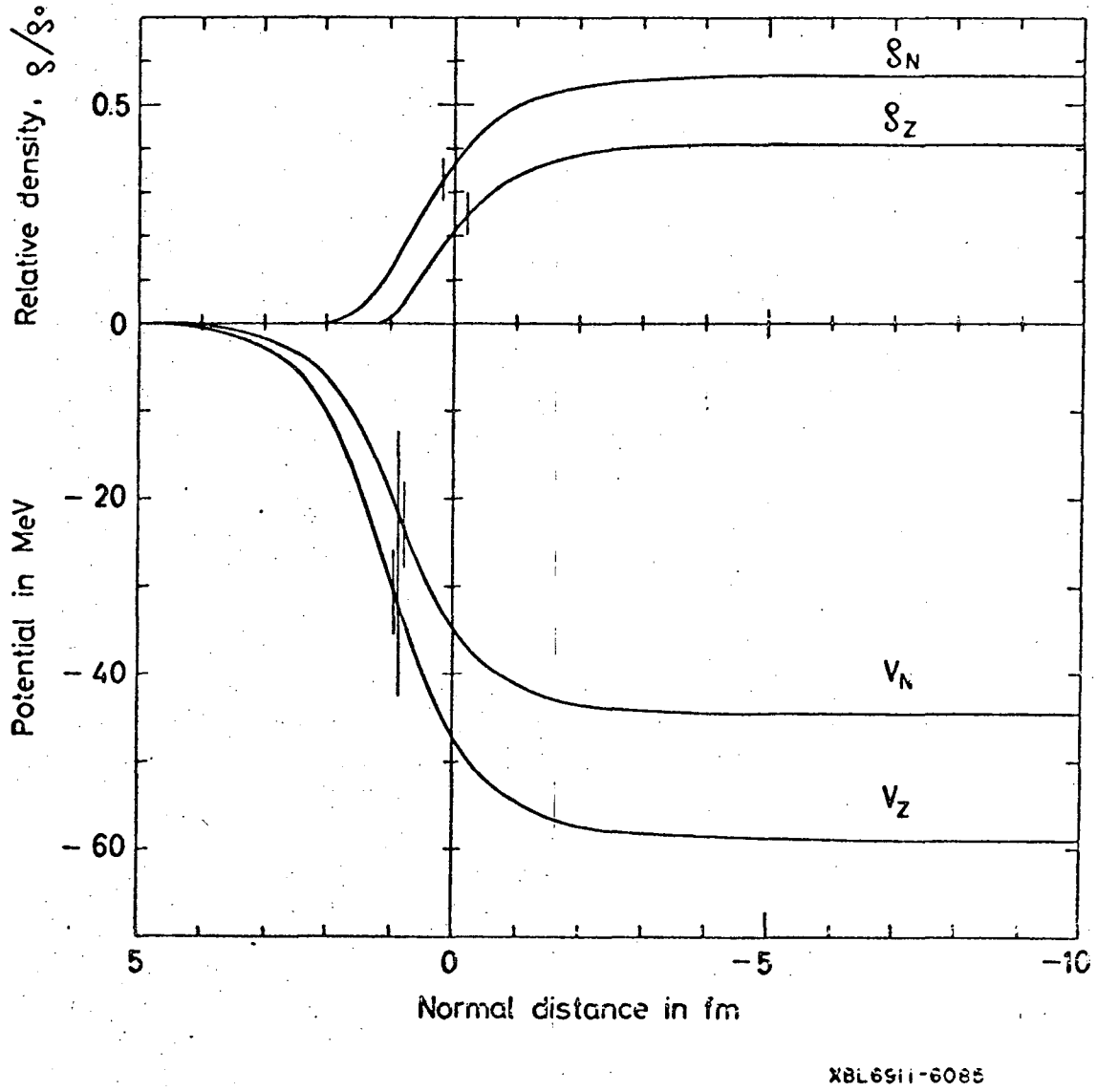

Fig. 2. The Thomas-Fermi density distributions and single particle potential wells for a case of non-vanishing asymmetry $\bar{\delta}$. As in fig. 1 the curves are plotted relative to the effective location of the surface of the total density. In addition, the locations of the neutron and proton surfaces are indicated by small vertical bars. The separate locations of the neutron and proton potential surfaces are given by the smaller bars on either side of the long vertical bar that indicates their average position.

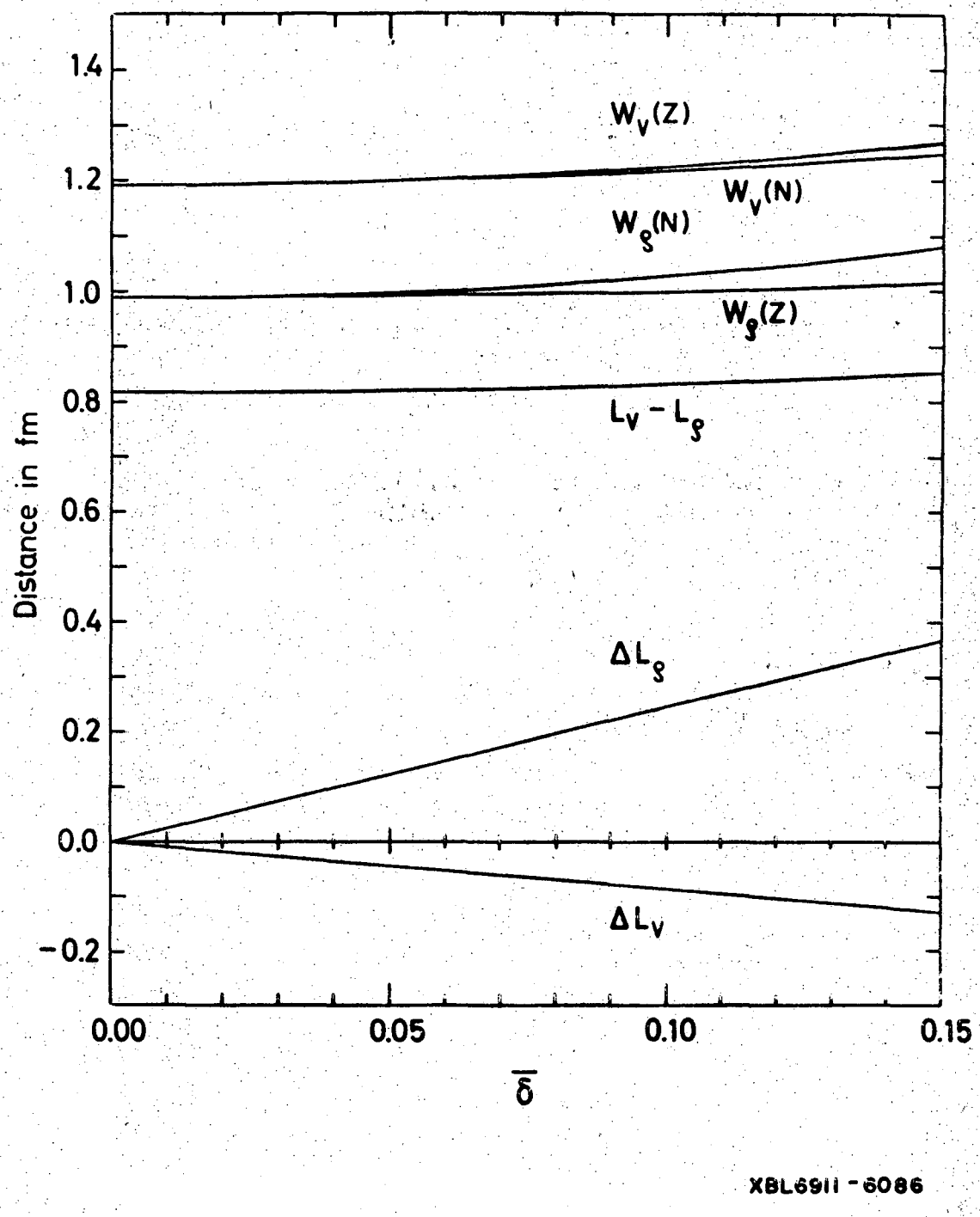

Fig. 3. The widths W and locations L of the neutron and proton density distributions and potential wells for semi-infinite Thomas-Fermi systems of the kind shown in figs. 1 and 2 are plotted against the value of the bulk asymmetry $\bar{\delta}$.

distance between the average locations of the surfaces of the potential and density $L_V - L_\rho$ is also seen to be linearly independent of $\bar{\delta}$. However, the distance between the locations of the neutron and proton surfaces ΔL_ρ does depend linearly on $\bar{\delta}$. This dependence is found to be exactly that predicted by the Droplet Model in the equation preceding eq. (2.20) of ref. 1, which is

$$t = \frac{3}{2} r_0 \, (J/Q) \, \bar{\delta} \quad , \tag{5}$$

where t is the neutron skin thickness ($t = \Delta L_\rho$) and r_0, J and Q are Droplet Model coefficients whose values are given in (17) below. Substitution of the numerical values of these coefficients into (5) yields

$$t = 2.45 \, \bar{\delta} \text{ fm} \quad , \tag{6}$$

for semi-infinite systems (and for finite systems without Coulomb energy). For real nuclei Coulomb effects must be taken into account and then according to sec. 2 of ref. 1 eq. (5) becomes

$$t = \frac{3}{2} (I - \bar{\delta}) \, r_0 A^{1/3} \quad , \tag{7}$$

where $\bar{\delta}$ is the average value of δ over the bulk central region of the nucleus (its value can be obtained from the Droplet Model expression which is eq. (16) below) and the definition of I, which is

$$I = (N-Z)/A \quad . \tag{8}$$

The distance by which the neutron potential well lies outside the proton well ΔL_V also depends linearly on $\bar{\delta}$. This dependence may be deduced from fig. 3 to be

$$\Delta L_V = -\ 0.43\ \bar{\delta}\ . \tag{9}$$

We can also see from the figure that for small values of $\bar{\delta}$

$$W_\rho(N) = W_\rho(Z) = 0.99 \text{ fm} + \text{terms of order } \bar{\delta}^2\ , \tag{10}$$

$$W_V(N) = W_V(Z) = 1.19 \text{ fm} + \text{terms of order } \bar{\delta}^2\ , \tag{11}$$

and

$$L_V - L_\rho = 0.82 \text{ fm} + \text{terms of order } \bar{\delta}^2\ . \tag{12}$$

This last quantity depends linearly on the curvature of the surface as one goes from semi-infinite to finite systems because the potential felt at a given distance outside a convex surface is smaller than it would be if the surface were flat. This causes the effective location of the potential well surface to move inward. For the Thomas-Fermi Model being investigated here this dependence was found to be

$$L_V - L_\rho = [0.82 - 0.28\ (2/R_\rho)] \text{ fm}\ , \tag{13}$$

where $2/R_\rho$ is the curvature of the surface of the density distribution.

4. Droplet Model

In order to make use of these relationships for predicting the properties of finite nuclei we must first calculate the radius of an equivalent sharp sphere which represents the density distribution. This radius, which is the analog for spherically symmetric finite systems of the quantity we have

called the location of the surface in the semi-infinite case, is given by the Droplet Model expression

$$R_\rho = r_0 A^{1/3} (1 + \bar{\varepsilon}) \quad . \tag{14}$$

The quantities $\bar{\varepsilon}$ (which appears above) and $\bar{\delta}$ (which finds application in the following discussion) are the average values over the central region of the nucleus of the quantities ε and δ defined in eqs. (3) and (4). The values of these quantities appropriate for a nucleus with N neutrons and Z protons, where A = N + Z and I = (N-Z)/A, are given by the Droplet Model expressions

$$\bar{\varepsilon} = (-2a_2 A^{-1/3} + L\bar{\delta}^2 + c_1 Z^2 A^{-4/3})/K \quad , \tag{15}$$

$$\bar{\delta} = [I + (3c_1/8Q) Z^2 A^{-5/3}]/[1 + (9J/4Q) A^{-1/3}] \quad . \tag{16}$$

These expressions (which are discussed in detail in sec. 2 of ref. 1) make use of coefficients which describe various properties of infinite and semi-infinite nuclear matter. These coefficients have been calculated with the aid of the Thomas-Fermi Model used in the last two sections and are found to have the values

a_2 = 22 MeV, surface energy coefficient

J = 35 MeV, symmetry energy coefficient

K = 300 MeV, compressibility coefficient

L = 99 MeV, density-symmetry coefficient

Q = 25 MeV, effective surface stiffness

c_1 = 0.745 MeV, Coulomb energy coefficient

where $c_1 = 3e^2/5r_0$ and

$r_0 = 1.16$ fm, the nuclear radius constant.

These coefficients differ slightly from those in ref. 1 for reasons that are given in connection with Table 3 in the appendix.

Once the radius of the density R_ρ is known from eq. (14) then the separate radii of the neutron and proton distributions can be calculated from the expression

$$R_\rho\binom{N}{Z} = R_\rho \; (\pm) \; \frac{1}{2} t \quad , \tag{18}$$

where t is obtained from eq. (7). The mean radius of the neutron and proton potential wells is given by

$$R_V = R_\rho + (L_V - L_\rho) \quad , \tag{19}$$

where $(L_V - L_\rho)$ is obtained from eq. (13), and the separate radii of the neutron and proton potential wells are given by

$$R_V\binom{N}{Z} = R_V \; (\pm) \; \frac{1}{2} \Delta L_V \quad , \tag{20}$$

ΔL_V being given by eq. (9).

The spatial distributions of the densities or potentials may be approximated by a Fermi function of the form

$$f(r) = \{1 + \exp[(r - R_{1/2})/a]\}^{-1} \quad . \tag{21}$$

In this connection, it can be shown that the relationship between the surface diffuseness parameter a and the width W of the surface region is given by the expression

$$a = (\sqrt{3}/\pi)W \quad . \tag{22}$$

It should also be noted that for large systems the half value radius parameter in the Fermi function $R_{1/2}$ is approximately the same as the equivalent sharp radius R. For finite systems, however, there is a geometric correction which can be shown to lead to the relationship

$$R_{1/2} = R\,(1 - (W/R)^2 + \cdots) \quad . \tag{23}$$

In Table 1 the most useful of the relationships derived here are summarized. The numerical values of the various parameters which enter have been inserted so as to make the expressions convenient to use.

5. Comparison

In order to facilitate comparison with experiment the Droplet Model predictions (calculated according to the expressions in Table 1) for various nuclear properties of interest are plotted in fig. 4. That the predicted proton radii correspond closely to the experimental results is not surprising since the parameters of the theory were chosen partly to insure this agreement. No parameters were adjusted to give the agreement which is seen to exist between the predicted potential well radii and depths and the values of these quantities determined by fitting single particle energy levels. The neutron potential well depth of ref. 5 differs from the predicted values because that author chose not to include the isospin dependence of the well. The radius of the neutron

Table 1. Droplet Model formulae.[a]

N = neutron number, Z = proton number,

$A = N + Z$, $I = (N-Z)/A$,

$\bar{\delta} = (I + 0.0112\, Z^2 A^{-5/3})/(1 + 3.15\, A^{-1/3})$

$\bar{\varepsilon} = -0.147\, A^{-1/3} + 0.330\, \bar{\delta}^2 + 0.00248\, Z^2\, A^{-4/3}$

Density

$R_\rho = 1.16\, A^{1/3}\, (1 + \bar{\varepsilon})$

$t = 0.773\, A^{1/3}\, (I - \bar{\delta})$

$R_\rho\binom{N}{Z} = R_\rho\, (\pm)\, \frac{1}{2}\, t$

For a Fermi function

$R_{\rho,1/2} = R_\rho\, [1 - (0.99/R_\rho)^2]$

$a_\rho = 0.55$

Potential

$R_V = R_\rho + 0.82 - 0.56/R_\rho$

$R_V\binom{N}{Z} = R_V(\mp)\, 0.22\, \bar{\delta}$

For a Fermi function

$R_{V,1/2} = R_V\, [1 - (1.19/R_V)^2]$

$a_V = 0.66$

$V\binom{N}{Z} = -51.4\, (\pm)\, 46.2\, \bar{\delta}$ MeV

[a]All distances are in fm.

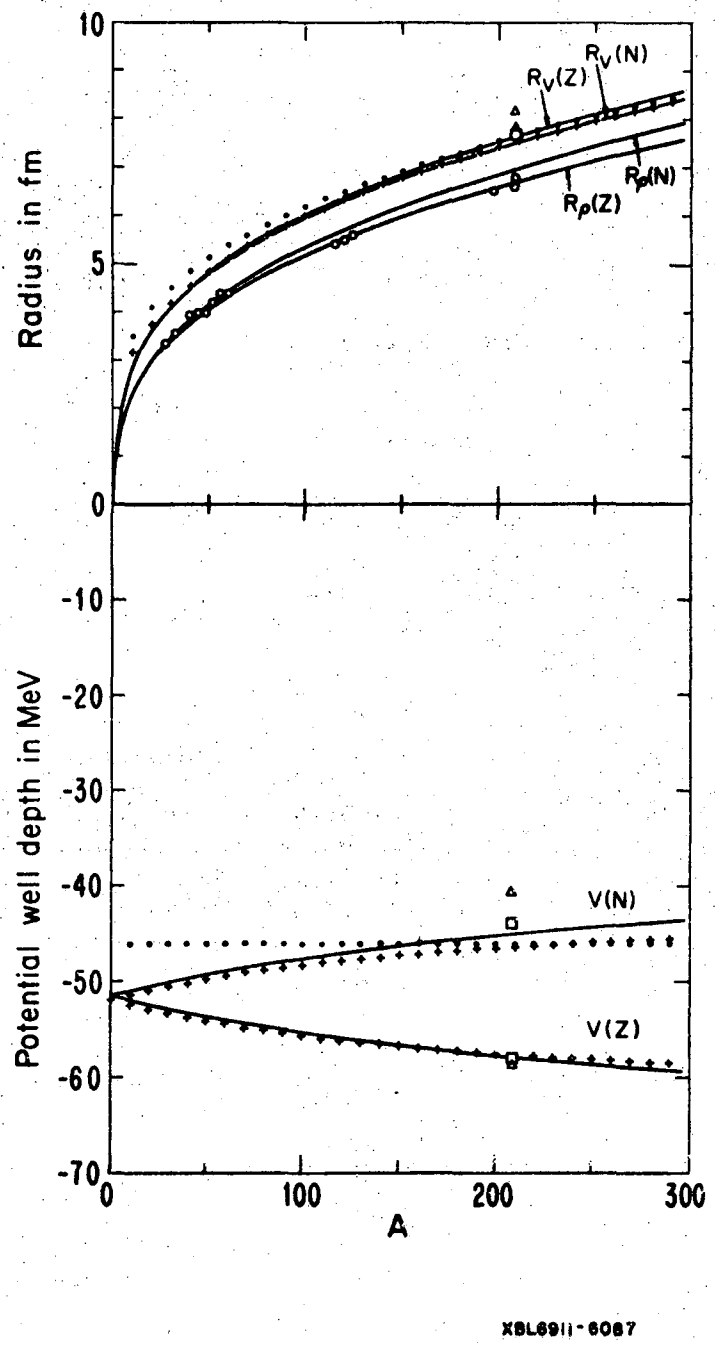

Fig. 4. The predictions of the algebraic theory, (as summarized in Table 1) are plotted as solid lines against the mass number A for nuclei along Green's approximation to beta stability,[3] which is I = 0.4 A/(200 + A). The various symbols represent experimental determinations of these same quantities as itemized in Table 2.

Table 2. Experimental radii and potential well depths.[a]

Symbol	Reference	Values
○	Ref. 4	$R_{\rho,1/2}(Z)$ and a_ρ determined separately for each nucleus
·····	Ref. 5	$R_{V,1/2}(N) = 1.16\ A^{1/3} + 0.6$ $a_V = 0.62$ $V(N) = -46.0$ MeV
+++++	Ref. 6	$R_{V,1/2}$ (N and Z) $= 1.24\ A^{1/3}$ $a_V = 0.63$ $V\binom{N}{Z} = -52\ (\pm)\ 27.5\ I$ MeV
for ^{208}Pb only		
□	Ref. 7	$R_{V,1/2}$ (N and Z) $= 7.52$ $a_V = 0.67$ $V(N) = -44.0$ MeV, $V(Z) = -58.0$ MeV
△	Ref. 8	$R_{V,1/2}(N) = 7.98$ fm, $R_{V,1/2}(Z) = 7.55$ $a_V = 0.70$ $V(N) = -40.6$ MeV, $V(Z) = -58.7$ MeV

[a]All the half value radii $R_{1/2}$ given here were converted to equivalent sharp radii R by means of the expression $R = R_{1/2}\ [1 + (\pi^2/3)(a/R_{1/2})^2]$ before being plotted in fig. 4. All distances are in fm.

potential well given in ref. 8 is larger than the predicted value and the potential is less deep than is predicted. Since there is a well known size-depth ambiguity in the determination of single particle wells these results may be consistent.

6. Discussion

The Droplet Model used here, which is developed in detail in ref. 1, is a general approach to the description of certain average nuclear properties. It is related to the specific methods such as Hartree-Fock and Thomas-Fermi in much the same way as thermodynamics is related to statistical mechanics. In the Droplet Model, just as in thermodynamics, the behavior of the system is given in terms of simple relationships which involve coefficients describing its macroscopic properties. For example, in thermodynamics a number of coefficients such as the specific heat, thermal expansion coefficient, and compressibility must be specified. In analogy the Droplet Model makes use of a number of coefficients such as the volume binding energy and symmetry energy, the surface energy, and the nuclear radius constant. Neither theory contains any provision for determining the values of these coefficients but once they are known the general behavior of the system follows. In applying thermodynamics one may obtain values of the necessary coefficients either from experiment or from detailed statistical mechanics calculations. In principle the Droplet Model coefficients can also be determined either from experiment or from detailed calculations, but in practice it seems that a combined approach is required.

In the liquid Drop Model, which is a restricted form of the Droplet Model, the four coefficients that enter the theory are easily obtained from experiment by fitting the Liquid Drop Model mass formula to experimental nuclear

masses. The five additional parameters which enter the theory at the Droplet Model level could, in principle, also be determined in this way. In practice this may prove difficult for two reasons. The first is that there is a great deal of scatter in the values of the experimental masses because of shell effects, which makes it difficult to determine fine details in the smooth part of the mass formula. The second problem is that the effects of some of the coefficients may be correlated so that their individual values are difficult to determine. In refs. 1 and 9 and in the present work a combined approach has been used. First, the values of the four basic coefficients (volume energy, symmetry energy, surface energy, and radius constant) were decided upon. In ref. 1 these were taken from a Liquid Drop Model mass formula which had been fitted to experimental masses. In ref. 9 and here they were chosen partly as before, partly so as to reflect new understanding of nuclear properties gained in ref. 1, and partly so as to give a better fit to nuclear charge radii. With these four coefficients fixed it was then necessary to find a way of estimating the values of the others. The Thomas-Fermi Model, which is described briefly in the appendix, was chosen for this purpose. The two body interaction used in this model has four parameters and these were adjusted so as to reproduce the four Droplet Model coefficients we had already fixed. The Thomas-Fermi Model was then used to calculate the values of the other coefficients. Of course, the values determined in this way depend to some extent on the model used.

The Thomas-Fermi Model that we found so useful for determining Droplet Model coefficients is also useful for investigating other aspects of macroscopic nuclear properties, some of which may be outside the scope of the Droplet Model approach. For example, this paper presents the results of applying the

Thomas-Fermi Model to nuclear single particle potential wells. Figure 4 shows how successful this approach has been. In spite of the fact that the Thomas-Fermi Model used here has only four parameters, and the fact that these are fixed by other considerations, the agreement between the potential wells predicted here and those determined in other ways is quite good.

In addition to the agreement obtained the method of calculation is also of interest. Even though the results presented here are those of the Thomas-Fermi Model we have not found it necessary to actually perform Thomas-Fermi calculations for finite nuclei. This is because we have employed a macroscopic approach to the problem. The Droplet Model was used to calculate some of the nuclear properties such as the bulk asymmetry and the neutron and proton radii. These results are then combined with information about the Thomas-Fermi potential wells (deduced from the infinite and semi-infinite cases) to give an algebraic theory. This algebraic theory, which is summarized in Table 1, is an excellent approximation to the exact Thomas-Fermi calculations but it is much more convenient to work with and it provides more insight into how the various nuclear properties are related.

The Droplet Model approach has found application in an improved semi-empirical nuclear mass formula[1]), and in the prediction of isotope shifts and the neutron skin thickness[9]). In this paper it has been successfully applied to predicting single particle potential wells, and there is work in progress to apply it to the calculation of fission barriers[10]). It seems as if it may be possible to encompass most macroscopic nuclear properties within a single algebraic theory which has at its heart the Droplet Model and which makes use of statistical methods such as the Thomas-Fermi Model for extending the theory to new applicatons.

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Appendix

The Thomas-Fermi Model

The Thomas-Fermi Model used here is that of Seyler and Blanchard[2]) as elaborated in ref. 1. In this statistical approach to nuclear properties it is assumed that the kinetic energies of particles at each point in the system are the same as they would be for a Fermi gas at the same density. Seyler and Blanchard go on to use, in addition to this basic assumption, a phenomenological, momentum dependent, two body interaction with four adjustable parameters. This interaction 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 the neutron-neutron and proton-proton interactions, while the "unlike" strength applies to the neutron-proton interaction. This interaction can be written

$$V(r,p) = - C_{\substack{\text{like} \\ \text{(or unlike)}}} \frac{e^{-(r/a)}}{r/a} [1 - (p/b)^2] \quad . \tag{24}$$

where V = the potential energy of two particles,

C = the strength of the interaction (different for "like" and "unlike" pairs),

r = the distance between the particles,

a = the range of the Yukawa force,

p = the magnitude of the relative momentum of the particles,

b = the critical value of the relative momentum at which the attractive force (whose strength decreases with increasing relative momentum) vanishes and beyond which the force becomes repulsive.

The four quantities a, b, C_ℓ, and C_u are the adjustable parameters of the Thomas-Fermi treatment. The four pieces of data used to determine them and their resulting values are listed in Table 3.

Once the kinetic and potential energies of the system have been specified a standard variational procedure may be applied to find the spatial distribution of particles for which the total energy is stationary. This approach leads to a pair of coupled integral equations for the neutron and proton density distributions, which may be solved by computer iteration.

The density distributions found in this way may be used in conjunction with the two body interaction to calculate the self-consistent single particle potential wells, the total binding energy, and other nuclear properties. In addition, when the integral equations are solved in the infinite and semi-infinite cases the methods of ref. 1 can be applied to deduce the coefficients required in the Droplet Model.

SURFACE MOMENTS

For distributions (of density, potential, or other properties) that are encountered in the surface region of a saturating system an "equivalent sharp surface" or "the effective location of the surface" can be defined. These distributions are characterized by the face that they have a constant value in the bulk region and they go smoothly to zero in the vicinity of the surface. The "location" L of the surface of such a distribution f(x), where x is the measured along a normal to the surface, may be defined by the relation

$$\int_{-\infty}^{L} [f_0 - f(x)]\, dx = \int_{L}^{+\infty} f(x)\, dx \quad . \tag{25}$$

Table 3. Input quantities and interaction parameters.[a]

Value	Input quantities Property
15.677 MeV[b]	a_1, the volume energy coefficient
35 MeV[c]	J, the symmetry energy coefficient
1.16 fermi[d]	r_0, the nuclear radius constant
2.4 fermi[e]	t_{10-90}, the nuclear surface diffuseness 10-90% distance

Resulting values of the adjustable parameters

Value	Description
159 MeV	C_ℓ, the "like interaction strength
285 MeV	C_u, the "unlike" interaction strength
89.4 MeV	$(b^2/2M)$, the energy of a particle with the critical momentum b
0.694 fermi	a, the range of the interaction

[a]Some of the values given here differ from those given in ref. 1. (See the following footnotes to this table for details.)

[b]This value is the same as that used in ref. 1, its origin is in the mass formula fit of William D. Myers and Wladyslaw J. Swiatecki, Nucl. Phys. 81 (1966) 1.

[c]In ref. 1 it was discovered that previous values of this quantity which were determined from Liquid Drop Model fits to nuclear masses were too small and that the value given here is probably closer to the correct one.

[d]This value of the radius constant is better suited to predicting the spatial properties of nuclei than the one used in ref. 1.

(continued)

Table 3. Continued.

[e]Since a parameter set best suited for discussing spatial properties of nuclei was needed for this work and that of Ref. 9 the decision was made to use parameters which reproduce the experimentally observed surface diffuseness of 2.4 fermi rather than the surface energy as in ref. 1. This choice results in a surface energy coefficient of 22 MeV.

In this expression it is assumed that the function fills the half space $-\infty$ to L and has the value f_0 over most of this region, and that the half space L to $+\infty$ is mostly empty except for the transition region localized about L. For the density distribution, L is simply the location of the sharp surface which would contain the same number of particles at the given bulk density.

This concept of the "location" of a surface is a generalization of the "effective sharp radius" of a finite system. One usually thinks only of the density distribution in this connection, where the location L becomes the radius R_ρ and eq. (25) becomes

$$\frac{4}{3}\pi R_\rho^3 \rho_0 = 4\pi \int_0^\infty \rho(r)\, r^2 dr \quad . \tag{26}$$

One may also define an equivalent sharp radius for the potential well using the relation

$$\frac{4}{3}\pi R_V^3 V_0 = 4\pi \int_0^\infty V(r)\, r^2 dr \quad . \tag{27}$$

For the one-dimensional case of semi-infinite systems the location L of the surface may be defined in another way, which is equivalent to eq. (25) but which may be generalized to include higher order moments of the surface distribution. If, for example, we differentiate the distribution $f(x)$ and define $g(x)$ by the expression

$$g(x) = -\frac{df(x)}{dx} \quad , \tag{28}$$

where x is the outward normal distance from some point in the surface then the moments of $g(x)$ are the quantities of interest. We can define the "location" L of the surface to be

$$L = \int_{-\infty}^{\infty} g(x)\ x dx \Big/ \int_{-\infty}^{\infty} g(x)\ dx \tag{29}$$

An integration by parts is sufficient to show that this point in the surface corresponds to the point where an equivalent sharp surface would be located.

In a similar way the "width" W of the surface region can be defined as

$$W = \left[\int_{-\infty}^{\infty} g(x)\ (x-L)^2\ dx \Big/ \int_{-\infty}^{\infty} g(x)\ dx \right]^{1/2} . \tag{30}$$

Higher moments of $f(x)$ such as the skewness and the kurtosis, may also be of interest in some special cases.

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