A NEW SEMIEMPIRICAL SHELL CORRECTION
TO THE DROPLET MODEL*
Gross Theory of Nuclear Magics§

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A new semiempirical atomic mass formula is presented. Special emphasis has been put on a theoretical basis for the microscopic (shell-correction) part, which is added to the macroscopic droplet-model expression. The latter includes the response to the surface diffuseness. The shell function, which is simple and analytic, is derived by bunching the average single-particle spectrum of nuclei with correct size according to the magic numbers. Shell effects from the inner shells are taken care of. In addition, ideas of changing magicities along neutron (proton) magic isotope (isotope) chains, and of damping of the off-Fermi-energy-shell contributions are introduced. These may be important for reliable extrapolations to very neutron-rich (or neutron-deficient) regions of the nuclear chart.

The final mass formula is a fairly simple analytic expression. In the preliminary fit with 50 free parameters, presented here, 1312 experimentally known atomic masses are reproduced with a rms error,

\[ \left( \sum_{\text{1312}} (M^{\text{exp}} - M^{\text{cal}})^2 / (1312 - 50) \right)^{1/2} \text{of 670 keV}. \]

Comparisons with experimental data are presented in figures for the isobaric mass parabolas, masses, radii, and quadrupole moments. Atomic mass predictions for some 8000 nuclei with $Z = 3$ to 114 and $N = 3$ to 184, with $S_n$ (or $S_p$) $> 0$ and with $S_n > -2$ MeV are presented in the main table of this issue. The simple FORTRAN-IV program (mass excess in MeV as a function of $Z$ and $A$) is available from the authors on request.

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§Gross, visible "without the aid of a microscope"; magics, science of magic effects
INTRODUCTION

A semiempirical model for the ground-state properties of nuclei is presented with the characteristic features:

1. The mass is separated into a macroscopic term and a microscopic (shell-correction) term.
2. The macroscopic part is described by the droplet-model\(^1\) expression, which takes care of the gross properties of the masses and radii.
3. The microscopic (shell) part is derived here theoretically from the Fermi gas model by a bunching procedure of its single-particle spectrum, which has been modified for the actual size of nuclei. In addition, it allows for proposed changes of the magicities (of the gaps in the single-particle spectra with magic level numbers), for a damping of the off-Fermi-energy-shell effects, and for the nuclear deformation.
4. The resulting shell function [Eqs. (22)-(24), (39)-(42)] is simple, analytic, and with two free parameters per shell which describe the magnitude and location of the gap at the Fermi energy for a magic number of particles of any kind.
5. The mass formula [Eqs. (22)-(24), (33)-(44)] reproduces 1312 experimentally known masses with a rms error of 670 keV (see Fig. 3). The isotopic mass-parabola properties, radii, and quadrupole moments are reproduced fairly well (see Figs. 2, 4, 5).
6. The parameter values for the gaps are reasonable.
7. The predictions are stable against small consistent changes\(^2\) of the parameters, so that different fit strategies lead to very similar results.

The motivation of our work is to predict nuclear ground-state properties (such as masses, radii, deformations) of nuclei far from the region of \(\beta\)-stability. This can be undertaken safely only if the model:

1. describes the smooth trends of these properties for known nuclei,
2. can take care of the fluctuation (shell effects) due to the detailed nuclear structure,
3. contains only free parameters which are physical quantities.

The now widely adopted strategy of Swiatecki was to separate the mass \(\tilde{M}\) into an average part \(\bar{M}\) assumed to be smooth, and a residual shell correction \(\hat{M}\).

\[
\tilde{M} = \bar{M} + \hat{M}. \tag{1}
\]

For \(\bar{M}\) the droplet model (DM) of Myers and Swiatecki\(^3\) is well established. (It is dangerous to extrapolate a mass formula, which does not contain the DM or at least the liquid-droplet model as its main smooth part.)\(^4\) The DM is known to be the second-order approximation to the microscopically self-consistent Thomas-Fermi approach. For \(\bar{M}\) there are two different strategies: either one extracts \(\bar{M}\) from huge (and difficult) Hartree-Fock (HF) calculations (or, neglecting the self-consistency, from the Nilsson-Strutinsky procedure) or one invents a simple expression with few free parameters.

We present a new shell function for \(\hat{M}\) which has the advantage that its analytic structure is derived theoretically and that it is consistent with the assumption of the smooth part \(\bar{M}\), that is, \(\bar{M}\) contains the influence of the absolute sizes of the nuclei on their shell effects. The shell function is gained by bunching the Fermi gas level density according to the known magic numbers.

METHOD

Gross Level Density

To construct the shell function we start from the smooth part \(\bar{\rho}\) of the single-particle level density\(^5\) of a nucleus of \(N\) neutrons and \(Z\) protons with respective radii \(R_{n,p}(N,Z)\).

For \(\bar{\rho}\) we use the Fermi gas expression but here drop the correction due to the nuclear surface which has been discussed elsewhere.\(^5\) Thus

\[
\bar{\rho}_{n,p}(t;N,Z) = \left( \frac{2m^*_{n,p}}{\hbar^2} \right)^{1/2} \frac{2}{3\pi} R^3_{n,p} \sqrt{t}, \tag{2}
\]

where \(m^*\) is the effective nucleon mass and \(t\) is the kinetic energy of a single nucleon.

For the radii \(R_{n,p}\) we get from the DM the expression

\[
R_{n,p} = r_0 A^{1/3} \left[ \frac{1 + \frac{I}{36}(1 + \delta)}{1 - \frac{I}{36} \Omega} \right]^{1/3}, \tag{3}
\]

where \(A \equiv N + Z, I \equiv (N - Z)/A,\) and \(r_0, \delta,\) and \(\Omega\) are the nuclear radius constant, the bulk-neutron excess, and the bulk-density excess, respectively, as given in the DM (see the contribution of W. D. Myers to this issue).

For the sake of abbreviation we define the scaling energies

\[
a_{n,p} \equiv C_{n,p} \left( \frac{R_{n,p}}{r_0} \right)^2 \tag{4}
\]

with

\[
C_{n,p} \equiv \left( \frac{9\pi}{4} \right)^{2/3} \frac{\hbar^2}{2m^*_{n,p}} r_0^{-2}. \tag{5}
\]

Applying the known scaling\(^6\) of Fermi gas spectra of finite nuclei, \(e = t/a_{n,p}\), we can translate (2) into the level density for the scaled spectrum:

\[
\bar{\rho}(e) \equiv \bar{\rho}(t) a_{n,p} = \frac{3}{2} \sqrt{e} \tag{6}
\]

which is independent of \(N\) and \(Z\).

We assume a superposition of shell functions for neutrons and protons,

\[
\bar{\rho}(N,Z) = \rho_{\bar{M}}(N,I) + \rho_{\bar{M}}(Z,I). \tag{7}
\]

We further assume that \(\rho_{\bar{M}}\) and \(\rho_{\hat{M}}\) are of the same

\(^1\)Degenerate levels are counted as separate levels
analytic structure. Thus we need only to prescribe the construction of the shell function for one kind of nucleon. One can simplify the notation and write $\mathcal{K}$ for the nucleon number of any one kind, that is, $\mathcal{K}$ means either $N$ or $Z$ and $a$ stands for $a_N$ or $a_Z$, respectively.

The Fermi energy $\varepsilon(\mathcal{K})$ is gained by integrating Eq. (6),

$$\varepsilon(\mathcal{K}) = \frac{3}{5} \mathcal{K}^{5/3}.$$  \hfill (8)

The total scaled kinetic energy of the $\mathcal{K}$-fermion system is

$$\frac{1}{a} M_{\mathcal{K}}(\mathcal{K}) = \frac{3}{5} \mathcal{K}^{5/3}. \hfill (9)$$

**Bunching**

We bunch the given average level density $\bar{\rho}(\varepsilon)$ to create "magic" gaps on top of those levels which belong to a magic number (see Fig. 1). The level density in each bunch is assumed to be proportional to that in the unbunched case,

$$\tilde{\rho}(\varepsilon; \mathcal{K}, i) \equiv \rho_i \bar{\rho}(\varepsilon) = \rho_i \frac{3}{2} \sqrt{\varepsilon}, \hfill (10)$$

with the bunching strength $\rho_i$. Since the number of nucleons belonging to the $i$th bunch is $\mathcal{K}_i - \mathcal{K}_{i-1}$, we have the relationship

$$\frac{1}{\rho_i} = (\mathcal{K}_i - \mathcal{K}_{i-1})^{-1} (\varepsilon_i^{5/2} - \varepsilon_i^{5/2}) \hfill (11)$$

between $\rho_i$ and the top and bottom energies $\varepsilon_i$ and $\varepsilon_i$ of the $i$th bunch.

The Fermi energy $\varepsilon(\mathcal{K})$ is to be derived from

$$\frac{1}{\rho_i} = (\mathcal{K}_i - \mathcal{K}_{i-1})^{-1} (\varepsilon_i^{5/2} - \varepsilon_i^{5/2}) \hfill (12)$$

for $\mathcal{K}_{i-1} < \mathcal{K}_i \leq \mathcal{K}_i$.

The total scaled kinetic energy of the $(\mathcal{K}_i - \mathcal{K}_{i-1})$ nucleons of bunch $i$ is then

$$\frac{1}{a} \hat{M}_i(\mathcal{K}_i) = \rho_i \frac{3}{5} (\varepsilon_i^{5/2} - \sqrt{\varepsilon_i^{5/2}}). \hfill (13)$$

**Shell Function**

The shell function $M(\mathcal{K})$ for $\mathcal{K}$ particles $(\mathcal{K}_{i-1} < \mathcal{K} \leq \mathcal{K}_i)$ of one kind of nucleon can now be formulated by summing up Eq. (13) for the inner filled shells and the last shell, and subtracting the smooth part $M_{\mathcal{K}}(\mathcal{K})$ of the Fermi gas model:

$$M(\mathcal{K}) = M(\mathcal{K}_i) - M(\mathcal{K}_{i-1})$$

$$= \frac{1}{a} \hat{M}_i(\mathcal{K}_i) + \sum_{j=1}^{i-1} \frac{1}{a} \hat{M}_j(\mathcal{K}_j) - M_{\mathcal{K}}(\mathcal{K}) \hfill (14)$$

Using Eqs. (9) and (13), we get [with the subscript $i$ for either $i$ or $j$ until Eq. (29)]

$$\frac{1}{a} \hat{M}_i(\mathcal{K}_i) = \frac{3}{5} \left\{ \frac{2}{(\mathcal{K}_i - \mathcal{K}_{i-1})^{5/2}} - \frac{2}{(\mathcal{K}_i - \mathcal{K}_{i-1})^{5/2}} + \frac{2}{(\mathcal{K}_i - \mathcal{K}_{i-1})^{5/2}} \right\} - \frac{2}{(\mathcal{K}_i^{5/2} - \mathcal{K}_{i-1}^{5/2})} \hfill (15)$$

Fig. 1. Schematic diagram of the bunching procedure.
Thus, besides the contribution of the uppermost shell, the shell-correction energy contains consistently the (nonvanishing) contributions of the lower-lying shells. In comparing to the shell function of Myers and Swiatecki, we find they introduced an additional constraint that the “center of gravities” of the bunched and unbunched levels should be the same. Then the contributions of the filled inner shells automatically vanish, and so they have to mock up their contribution by introducing a global term assumed to be proportional to $A^{-1/3}$. In addition, they interpolate linearly between the unbunched case ($p_i = 1$) and the complete bunching case ($p_i = \infty$) with the weight factor as a global fit parameter.

Magic Gaps

The shell function $\bar{\mu}(\mathfrak{R})$ should, on physical grounds, depend not too much on the absolute values of the border levels $\varphi_i$ and $\varphi_i^*$ as on the magic gaps

$$G_i = \varphi_i^* - \varphi_i^*,$$  \hspace{1cm} (16)

separating the bunch $i + 1$ from bunch $i$. The magic gaps in a single-particle spectrum of a finite nucleus should be proportional to its average level spacing $\bar{\rho}^{-1}$. Therefore we rewrite the shell function introducing the dimensionless quantity $\gamma_i$, which we will call magicity,

$$\gamma_i = G_i \bar{\rho} \varphi(\mathfrak{R}_i).$$  \hspace{1cm} (17)

The magicity $\gamma_i$ measures the essential part of the gap width after taking out the assumed $\bar{\rho}^{-1}$ and dependencies.

Besides the magnitude of the gap $G_i$ we have to specify its location. This we do in relating it to the magic levels $\varphi_i \equiv \varphi(\mathfrak{R}_i)$ of the unbunched level density,

$$\varphi_i = \varphi_i^* - \varphi_i^*$$  \hspace{1cm} (18)

by introducing the relative gap location $x_i$.

We have converted the two bordering levels $\varphi_i$, $\varphi_i^*$ of a magic gap into the two parameters $\gamma_i$ and $x_i$, the magicity and the relative gap location. Inserting Eq. (17) in Eq. (18) we get

$$\varphi_i = \mathfrak{R}_i^{2/3} \left(1 - \frac{2}{3} \frac{x_i \gamma_i}{\mathfrak{R}_i} \right)$$  \hspace{1cm} (19)

and

$$\varphi_i^* = \mathfrak{R}_i^{2/3} \left(1 + \frac{2}{3} \frac{(1 - x_i \gamma_i^*)}{\mathfrak{R}_i} \right).$$

Linearized Shell Function

The somewhat clumsy but exact expression (15) with (19) for the shell function can be simplified by making use of a physical property of the realistic single-particle spectra of nuclei.

The magic gaps $\Delta G_i$ are some few MeV and are thus one order of magnitude smaller than the absolute value of the kinetic energy $\omega_e$ of the border level

$$G_i \ll \omega_e.$$  \hspace{1cm} (20)

With the expression (17), and as far as $|x_i| \leq 1$, this becomes

$$\frac{2}{3} \left| \frac{x_i \gamma_i}{\mathfrak{R}_i} \right| \ll 1.$$ \hspace{1cm} (21)

The shell function (15) with (19) can thus be linearized with respect to (21) with the result

$$\frac{1}{d} \bar{\mu}(\mathfrak{R}) \approx \left[1 - \left(\xi_{i-1} + \eta_i\right)^{-1} \right] \times \left[ \frac{2}{3} \frac{x_i \gamma_i}{\mathfrak{R}_i} \right]$$  \hspace{1cm} (22)

with

$$x_i^*(\mathfrak{R}) = \frac{2}{3} \mathfrak{R}_i^{2/3} (\mathfrak{R}_i - \mathfrak{R}_{i-1})$$

$$- \frac{3}{5} \mathfrak{R}_{i-1} (\mathfrak{R}_i^{2/3} - \mathfrak{R}_{i-1}^{2/3}),$$  \hspace{1cm} (23)

$$x_i^*(\mathfrak{R}) = \frac{2}{3} \mathfrak{R}_i^{2/3} (\mathfrak{R}_i - \mathfrak{R}_i)$$

$$+ \frac{3}{5} \mathfrak{R}_i (\mathfrak{R}_i^{2/3} - \mathfrak{R}_i^{2/3})$$

$$- \frac{2}{5} \mathfrak{R}_i^{2/3} (\mathfrak{R}_i - \mathfrak{R}_{i-1}),$$

where the specific bunching strengths

$$\eta_i = \frac{x_i \gamma_i}{\mathfrak{R}_i - \mathfrak{R}_{i-1}}, \xi_{i-1} = \frac{(1 - x_i \gamma_i)}{\mathfrak{R}_i - \mathfrak{R}_{i-1}}$$  \hspace{1cm} (24)

relate to the bunching strength $p_i$ by $(1 - p_i^{-1}) = \eta_i + \xi_{i-1}$. They give the ratio between the number of levels which had filled the gaps before the bunching and the total number of levels $\mathfrak{R}_i - \mathfrak{R}_{i-1}$. The functions $\xi_{i-1}$, $\eta_i$ are always positive since the lower (upper) gap has the effect of rising (lowering) the bunch by compression.

In the weak bunching limit, we have $p_i^{-1} \rightarrow 1$ and thus

$$\xi_{i-1} + \eta_i \ll 1.$$  \hspace{1cm} (25)

In experimentally known nuclei, this is not too bad an approximation. One may neglect the denominator in Eq. (22) and thus end up with a completely linearized shell function. However, we will not use this approximation.

Changing Magicities

It has been suggested that some of the magic gaps
close or open for very neutron-rich or neutron-deficient nuclei. To take into account changing magicities, we consulted a Woods-Saxon calculation. The calculations with a potential, the size for which was again determined by the DM, suggest a correlation between the differences $\Delta l_i$ of the orbital angular momenta of the single-particle levels defining the gap. A reason for this may be the following. The neutron (proton) wavefunction with higher $l$ is pushed out into the neutron (proton) skin of the nucleus. Due to the lack of protons (neutrons) as interacting partners there, the binding is weaker.

Thus we assume that $\gamma_i$ contains a multiplicative factor

$$ h_i = 1 - \xi \Delta l_i (\Delta \mu)^2 \quad (26) $$

with positive coefficient $\xi$ and

$$ \Delta l_i = l_i - l_{i+1}. \quad (27) $$

In Eq. (26) $\Delta \mu$ stands for the number of neutrons (protons) in the neutron (proton) skin, which is given in the DM to be

$$ \Delta \mu = \begin{cases} \frac{(1 - \delta)(1 - \delta)}{1 - \delta} A & \text{for neutron skin} \\ \frac{(1 - \delta - 1)(1 + \delta)}{(1 + \delta) A} & \text{for proton skin.} \end{cases} \quad (28) $$

The Woods-Saxon calculation gives the magic numbers $\mathcal{N}_i$ and $\mathcal{L}_i$ as

$$ N_i(\Delta \mu) = 2(-1), 8(-1), 14(0), 20(-1), 28(+2), 40(-3), 50(+2), 82(+2), 126(-3), 184(-2), \quad (29) $$

$$ Z_i(\Delta \mu) = 2(-1), 8(-1), 14(0), 20(-1), 28(+2), 40(-3), 50(0), 82(-5), 114(+3). $$

Inserting the $\Delta l_i$ into Eq. (26) results in a closing of magic gaps with positive $\Delta l_i$ and an opening of gaps with negative $\Delta l_i$. Thus, for instance, $^{16}$He, $^{20}$O, $^{40}$Ca, and $^{176}$Sn are favored to be strongly doubly magic, in contrast to $^{76}$Ca.

**Damping of Shells off the Fermi Energy**

The single-particle properties of nuclear levels near the magic gaps are experimentally and theoretically most pronounced at and near the Fermi surface. Far above and below the Fermi energy the many-particle correlations become important. These effects result in a damping of the shell structure of the levels far above the Fermi sea and in a washing out of the shell gaps deep inside the Fermi sea.

We have taken care of these effects in a crude way by allowing for a slight damping of the off-Fermi-energy contributions of the single-particle spectrum to the shell function. We assume that $\gamma_i$ contains a damping factor

$$ g_i = \exp \left\{ -\alpha \left( \mathcal{R}_{i/2} - \mathcal{R}_{i/2}^2 \right) / \left( \mathcal{R}_{i/2} - \mathcal{R}_{i/2}^2 \right)^2 \right\} $$

for the uppermost gap

$$ g_i = \exp \left\{ -\alpha \left( \mathcal{R}_{i/2} - \mathcal{R}_{i/2}^2 \right) / \left( \mathcal{R}_{i/2} - \mathcal{R}_{i/2}^2 \right)^2 \right\} $$

for the lower gaps

with one parameter $\alpha$ common to all nuclei. This reduces the influence of the lower shells on the shell function and introduces an $(\rho - \rho_e)$-dependent compression of the bunch $i$.

**Deformation**

The ground-state deformation of nuclei are calculated in the usual way by minimizing the mass of the nucleus

$$ M(N,Z,x_2) = \tilde{M}(N,Z,x_2) + s \tilde{M}(N,I,x_2) + \rho \tilde{M}(Z,I,x_2) $$

with respect to the ellipsoidal deformation $\epsilon$. For the deformation dependence of the smooth part $\tilde{M}$, the deformable DMP is used. The gross feature of the shape dependence of our shell function $\tilde{M}$ can in principle be extracted from a study of the changing of the shell gaps with deformation in a deformable Woods-Saxon or
Hartree-Fock calculation

\[ G_r(\mathfrak{Q}, I; \text{shape}) = G_r(\mathfrak{Q}, I; \mathfrak{L}) \mathfrak{L}(\text{shape}). \] (31)

This will be studied elsewhere. Here we use the simple procedure of Myers and Swiatecki\(^7\) who try to represent the effect of gap destruction due to deformation by multiplying the total shell correction with a shape-dependent function

\[ \tilde{M}(\mathfrak{Q}, I; \theta) = M(\mathfrak{Q}, I)(1 - 2\theta^2) \exp(-\theta^2), \] (32)

where \( \theta^2 = \int dr \left( \frac{R - R_0}{d_0} \right)^2 \).

Fig. 3. Theoretical shell correction (top), experimental shell correction (middle), and the residual errors (bottom), in MeV.
MASS FORMULA

Here we summarize the final mass formula presented in this contribution. The predictions of the Table are given as the mass excess \( \Delta M = M - A \) in MeV

\[
\Delta M(N,Z) = -B(N,Z) + (M_nN + M_pZ). \tag{33}
\]

where \( B \) is the binding energy in MeV, and

\[
M_n = 8.07144 \text{ MeV, } M_p = 7.28899 \text{ MeV} \tag{34}
\]

are the neutron and proton mass excesses, respectively.\(^ \text{10} \)

The mass formula itself consists of the following terms

\[
M(N,Z) = \tilde{M}(N,Z;\theta) + M_{\text{pair}}(N,Z) + M_{\text{nuc}}(N,Z) + M_{\text{harm}}(N,Z;\theta), \tag{35}
\]

where for \( \tilde{M} \) we use the DM expression\(^ \text{2.9} \) (Myers, this issue\(^ * \)), but with the following values of coefficients.

\[
\begin{align*}
 a_1 & = 16.19 \text{ MeV, volume energy} \\
 b_2 & = 20.85 \text{ MeV, surface energy} \\
 J & = 38.20 \text{ MeV, symmetry energy} \\
 r_0 & = 1.167 \text{ fm, nuclear-radius constant} \\
 b_0 & = 0.7 \text{ fm, diffuseness width} \\
 a_3 & = 0 \text{ MeV, curvature correction} \\
 Q & = 17.7 \text{ MeV, effective-surface stiffness} \\
 K & = 300 \text{ MeV, compressibility} \\
 L & = 100 \text{ MeV, density symmetry} \\
 M & = 0 \text{ MeV, symmetry anharmonicity}
\end{align*}
\]

The Coulomb coefficients are

\[
\begin{align*}
 c_1 & = \frac{3}{5} \frac{e^2}{r_0} = 0.7403 \text{ MeV, Coulomb energy} \\
 c_2 & = \frac{e^2}{336} \left( \frac{1}{a} + 18 \right) \tag{36}
\end{align*}
\]

\[
\begin{align*}
 c_4 & = \frac{8}{5} \frac{e^2}{2\pi^2} \frac{b_0^2}{b_1} \\
 c_5 & = \frac{1}{64} \frac{a^2}{Q} \\
 c_6 & = 4.838 \times 10^{-4} \text{ MeV, surface redistribution of second kind}
\end{align*}
\]

For the pairing term, we make the simple assumption

\[
M_{\text{pair}} = \left\{ \begin{array}{ll} +\Delta & \text{for odd-odd} \\ 0 & \text{for odd-}A \\ -\Delta & \text{for even-even} \end{array} \right. \tag{37}
\]

with \( \Delta = 10/\sqrt{A} \text{ MeV} \).

The Wigner term is

\[
M_W = W |1| \tag{38}
\]

with \( W = 30 \text{ MeV} \) and \( I = (N - Z)/4 \).

Our shell correction \( \tilde{M} \), Eq. (32), reads

\[
\tilde{M}(N,Z;\theta) = \tilde{M}(N,I) + \delta \tilde{M}(Z,I) 
\times (1 - 2\theta^2) \exp(-\theta^2). \tag{39}
\]

The expressions for \( \tilde{M} \) and \( \delta \tilde{M} \) can be presented in one piece if one performs the following: to gain \( \tilde{M} \), set \( \mathcal{R} = N \), let the subscript \( p = n \) and the coefficient \( r = +1 \); to gain \( \delta \tilde{M} \), replace \( \mathcal{R} \) by \( Z \) and let \( r = p = -1 \).

Then

\[
\tilde{M}(\mathcal{R},I) = c_r A^{-7/2} \left( \frac{1 - 3\tilde{\theta}}{1 + \tilde{\theta}} \right)^{1/2} \left( 1 + \frac{p}{r} \right)^{3/2} \tag{40}
\]

\[
\times \left[ \bar{S}(\mathcal{R},I) + \sum_{j=0}^{l-1} \bar{S}(\mathcal{R},j+1) + c_r \right]
\]

for \( \mathcal{R} - j < \mathcal{R} \leq \mathcal{R} \),

where \( \bar{c} \) are constants which mock up the shell correction due to the shells \( j < j_0 \). In the present fit, \( j_0 = 2 \), that is, nuclei with \( \mathcal{R} \leq 2 \) were not included.

The quantities \( \bar{S}(N,Z), \delta(N,Z) \) are given in Myers (this issue). The contribution of any bunch \( k \) is given by

\[
\bar{S}_k = \frac{1}{a_\ast} \frac{M_k}{[1 - (\bar{S}_{k-1} + \bar{c}_k)^{-1}(\delta_{k-1}^k - \delta_{k-1}^s)]}
\]

\[
\text{with}
\]

\[
\delta_{k-1}^s = \frac{2}{5} \mathcal{R}^{2/3} (\mathcal{R} - \mathcal{R}_{k-1}) - \frac{3}{5} \mathcal{R}_{k-1} (\mathcal{R}^{2/3} - \mathcal{R}_{k-1}^{2/3}),
\]

\[
\delta_{k-1}^s = \frac{2}{5} \mathcal{R}^{2/3} (\mathcal{R}_{k-1} - \mathcal{R}) + \frac{3}{5} \mathcal{R}_{k-1} (\mathcal{R}_{k-1}^{2/3} - \mathcal{R}_{k}^{2/3})
\]

\[
- \frac{2}{5} \mathcal{R}_{k-1}^{2/3} (\mathcal{R}_{k-1} - \mathcal{R}_{k-1})
\]

\[
\delta_{k}^s = (\mathcal{R}_{k} - \mathcal{R}_{k-1}) \delta_{k-1}^s - \delta_{k-1}^s / \mathcal{R}_{k}^{-1}
\]

\[
\bar{S}_k = (\mathcal{R}_{k} - \mathcal{R}_{k-1}) \delta_{k-1}^s - \delta_{k-1}^s / \mathcal{R}_{k}^{-1}
\]

\[
\text{and}
\]

\[
\eta_k = \frac{x_k^0 y_k^0}{(\mathcal{R}_{k} - \mathcal{R}_{k-1}) f_k} \equiv \hat{\eta}_k f_k
\]

\[
\delta_{k-1}^s = \frac{(1 - x_{k-1}^0) y_{k-1}^0}{(\mathcal{R}_{k} - \mathcal{R}_{k-1}) f_{k-1} - \delta_{k-1}^s / \mathcal{R}_{k}^{-1}}
\]

\[
\text{Since we include the effects due to the surface diffuseness,}\text{ the surface and the Coulomb-diffuseness energies read}
\]

\[
E_s = (a_2 + \frac{5}{4} \frac{Z^2}{A} \frac{b_0^4}{b_1^2}) \left( 1 + \eta^0 \right) \left( 1 - \frac{1}{2} \frac{b_0}{c_0} \right)
\]

\[
\text{and}
\]

\[
E_{\text{coul}} = \frac{5}{2} \frac{Z^2}{A} \left( \frac{b_0}{c_0} \right)^{1/2} \tag{41}
\]

\[
\text{The quantity } b_0 \text{ is the diffuseness width of semi-infinite nuclear matter and } \eta_k \equiv (b_0 - b_{k/3})/b_0 \text{ measures the deviation of the width } b_{k/3} \text{ of the actual proton distribution from } b_0.
\]

In the DM, \( \eta_k \) is calculated to be

\[
\eta_k = \frac{5}{2} \frac{Z^2}{A} \left( \frac{b_0}{c_0} \right)^{1/2} \left( 2 - 3.63 \frac{b_{k/3}}{c_0} \right)
\]

\[
\times \left( 0.33 \frac{Z^2}{A} \frac{b_{k/3}}{c_0} \right)^{1/2} \left( 2 - 7.26 \frac{b_{k/3}}{c_0} \right)
\]

\[
\text{The diffuseness widths } b_{k/3} \text{ are related to the diffuseness parameter } a_\ast \text{ of a Fermi distribution by } b_{k/3} = \eta_k a_\ast \sqrt{3}.
\]
where

$$f_k \equiv g_k h_k = g_k [1 - \xi \Delta \mu_k (\Delta \mu_k)^2]$$  \hspace{1cm} (41)

with $g_k$ being defined by Eq. (30), and, finally,

$$\Delta \mu_k = \alpha (1 - \delta) A (1 - \nu \delta),$$  \hspace{1cm} (42)

if this expression is positive, otherwise $\Delta \mu_k = 0$.

The assumptions for the damping of the shell strengths as well as for the changing of the magicities are included on physical arguments. In the present preliminary fit they have been assumed to be negligible (that is, $\alpha = \xi = 0$ which leads to $n_k = n_\nu^*$, $\xi_k = \xi_\nu^*$ and $c_k = c_\nu^*/(g_{k-1})$).

The values of the parameters of the shell term, specific bunching strengths $n_\nu^*$ and $\xi_\nu^*$ are

<table>
<thead>
<tr>
<th>$k$</th>
<th>$N_k(\Delta \lambda_k)$</th>
<th>$n_\nu^*$</th>
<th>$\xi_\nu^*$</th>
<th>$Z_\nu(\Delta \lambda_k)$</th>
<th>$n_\nu^*$</th>
<th>$\xi_\nu^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2(-1)</td>
<td>-</td>
<td>-0.0038</td>
<td>2(-1)</td>
<td>-</td>
<td>-0.0060</td>
</tr>
<tr>
<td>2</td>
<td>8(-1)</td>
<td>0.0210</td>
<td>0.0545</td>
<td>8(-1)</td>
<td>0.0002</td>
<td>0.0647</td>
</tr>
<tr>
<td>3</td>
<td>14(0)</td>
<td>0.0745</td>
<td>-0.0090</td>
<td>14(0)</td>
<td>0.0610</td>
<td>0.0388</td>
</tr>
<tr>
<td>4</td>
<td>20(-1)</td>
<td>-0.0327</td>
<td>0.0491</td>
<td>20(-1)</td>
<td>-0.0350</td>
<td>0.0303</td>
</tr>
<tr>
<td>5</td>
<td>28(+2)</td>
<td>0.1206</td>
<td>0.0353</td>
<td>28(+2)</td>
<td>0.0763</td>
<td>0.0618</td>
</tr>
<tr>
<td>6</td>
<td>40(-3)</td>
<td>-0.0268</td>
<td>0.0440</td>
<td>40(-3)</td>
<td>0.0237</td>
<td>-0.0033</td>
</tr>
<tr>
<td>7</td>
<td>50(+2)</td>
<td>0.1751</td>
<td>0.0497</td>
<td>50(0)</td>
<td>0.1094</td>
<td>0.0403</td>
</tr>
<tr>
<td>8</td>
<td>82(+2)</td>
<td>0.0572</td>
<td>0.0423</td>
<td>82(-5)</td>
<td>0.0375</td>
<td>0.0897</td>
</tr>
<tr>
<td>9</td>
<td>126(-3)</td>
<td>0.0680</td>
<td>0.0514</td>
<td>114(+3)</td>
<td>0.0438</td>
<td></td>
</tr>
<tr>
<td>10</td>
<td>184(-2)</td>
<td>0.0603</td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

and

$$C_\nu = 71.0 \text{ MeV, neutron Fermi-energy coefficient}$$
$$C_\nu = 72.0 \text{ MeV, proton Fermi-energy coefficient}$$
$$c_\nu^* = -0.109 \text{ neutron innermost-shell correction}$$
$$c_\nu^* = -0.108 \text{ proton innermost-shell correction}$$
$$\alpha_0 = 0.5 \text{ deformation}$$
$$r_0 = 0 \text{ damping}$$
$$\xi = 0 \text{ magicity change}$$

**COMPARISON WITH EXPERIMENT**

**Masses**

We have obtained the parameter values tabulated in the previous section by a least-squares-fit\(^*\) (without considering the experimental errors) to 1312 experimentally well-known atomic masses ($N, Z > 2$) which are reported by Wapstra and Bos in this issue.

**Smooth Part $\tilde{M}$**

The general trend of the smooth part $\tilde{M}$ in the valley of $\beta$-stability can be tested by plotting the isobaric mass-parabola quantities. We fit the DM part $M_{dM}$ for each isobar chain to a quadratic form in $(N - Z)$

$$\tilde{M}_A = V_A + \frac{1}{2} C_A (N - Z - Y_A)^2,$$ \hspace{1cm} (45)

following the analysis of Myers (this issue). The experimental quantities compared with $\tilde{M}_A$ are deduced from $M_{dM}$ by subtracting our theoretical shell term, the pairing and Wigner terms. Results are shown in Fig. 2. The average trends are nicely reproduced and the peculiarities of Myers' Fig. 1 for very-small-$A$ and very-large-$A$ nuclei are reduced. The residual systematic deviations disappear if we increase the value of the parameter $M$ in Eq. (36).

**Shell Part $\tilde{M}$**

We define the experimental shell correction as

$$\tilde{M}^{exp} = M^{exp} - (M_d^{cal} - \tilde{M}^{cal})$$ \hspace{1cm} (46)

which is compared with $\tilde{M}^{cal}$ in Fig. 3.

**Total Mass $M$**

The residual errors $M^{exp} - M^{cal} = \tilde{M}^{exp} - \tilde{M}^{cal}$ are plotted in Fig. 3. The results give a rms error...
The overall agreement is reasonable. The most pronounced deviations occur, of course, for the lightest elements. For $N, Z \geq 10$, the same parameter set gives a rms of 0.62 MeV for the then 1254 experimental masses. There still remain slight systematic deviations (for example, in the rare-earth and actinide regions) which we attribute to the deformation dependence of the shell correction.

The fit presented here is a preliminary one. The effects of damping (parameter $a$) and changing magicities (parameters $\eta$) as well as the microscopic shape dependence will be studied elsewhere.

The Table includes the predicted mass-excess values for the unknown nuclei with $Z = 3$ to 114, $N = 3$ to 184, and $S_n$ (or $S_{2n}$) $> 0$ and $S_p > -2$ MeV.

**Radii**

The average behavior of the equivalent neutron and proton radii $R_n$, $R_p$ and their weighted mean which represents the total-density radius $R$, is shown in Fig. 4 along Green's approximation\(^{14}\) of the valley of $\beta$-stability ($I = 0.4A/(A + 200)$). The difference between the neutron and proton radii (the neutron skin) ranges from about $-0.5\%$ to $6\%$ of $R$. For comparison we also plotted the calculated charge-radii for nuclei near magic numbers together with the different experimental values\(^{11}\) extracted from electron scattering. (The central radius of a three-parameter Fermi distribution is converted to the equivalent radius in the method used by Myers.) Within the uncertainties of the analysis of the experimental data the agreement is very good. There are strong indications that the general trend of the isotope shifts is reproduced.

Fig. 4. Results on radii. To show the mean trends of the equivalent sharp radii of spherical neutron-, proton-, and total-density distributions, these quantities are divided by $A^{1/3}$ and plotted against $A$ along Green's approximation\(^{14}\) of the valley of $\beta$-stability

- - - Neutron and proton radii
--- Total radius
$x$ Experimental values for charge distribution
● Droplet-model predictions for charge distribution
○ Droplet-model predictions for neutron distribution
**Quadrupole Moments**

The intrinsic quadrupole moments have been calculated with our mass formula. The results are shown in Fig. 5 together with the recent experimental data and their deviations. (The experimental values are taken from Ref. 12, selecting always the most recent data.) The gross features for the rare-earth and the transuranium regions are well reproduced. However, the too sudden beginning and end of the regions of deformation may be traced to the preliminary status of the deformation dependence of the shell function as discussed earlier.

**Decay Energies**

The theoretical decay energies for α-decay for the lead region have been checked with the experimental data, but the disagreement found for the conventional DM, as discussed elsewhere, could not be improved.

The window energies for β-delayed neutrons and protons, $Q_\beta^\lambda - S_\lambda$ and $Q_\alpha - S_\alpha$, respectively, were found to be improved in some cases. There is still work to be done, especially regarding the shape dependence of the shell function.

**References**


Fig. 5. Experimental and theoretical intrinsic quadrupole movements. The difference is displayed at the bottom.