In Memoriam

This paper is dedicated to the memory of our friend and colleague John L. Norton, who wrote the original versions of the computer programs that we use to calculate the single-particle energies and resulting shell and pairing corrections for a deformed folded-Yukawa single-particle potential.

NUCLEAR GROUND-STATE MASSES AND DEFORMATIONS

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Abstract: We tabulate the atomic mass excesses and nuclear ground-state deformations of 8979 nuclei ranging from ^{16}O to $A = 339$. The calculations are based on the finite-range droplet macroscopic model and the folded-Yukawa single-particle microscopic model. Relative to our 1981 mass table the current results are obtained with an improved macroscopic model, an improved pairing model with a new form for the effective-interaction pairing gap, and minimization of the ground-state energy with respect to additional shape degrees of freedom. The values of only nine constants are determined directly from a least-squares adjustment to the ground-state masses of 1654 nuclei ranging from ^{16}O to ^{263}106 and to 28 fission-barrier heights. The error of the mass model is 0.669 MeV for the entire region of nuclei considered, but is only 0.448 MeV for the region $N \geq 65$.

1 Introduction

We presented our first macroscopic-microscopic global nuclear mass calculation 14 years ago [1,2]. This calculation, which was based on a finite-range liquid-drop model for the macroscopic energy and a folded-Yukawa single-particle potential for the microscopic corrections, was somewhat limited in scope. With only 4023 nuclei included, it did not extend to the proton or neutron drip lines or to the region of superheavy nuclei. Also, the quantities tabulated were limited to ground-state masses, Q_2 and Q_4 moments, and microscopic corrections.

Our next publication of calculated nuclear masses occurred seven years ago [3,4]. In these calculations new pairing models had been incorporated and two different macroscopic models were investigated, namely the finite-range liquid-drop model (FRLDM) [3] and the finite-range droplet model (FRDM) [4]. These abbreviations are also used to designate the full macroscopic-microscopic nuclear structure models based on the respective macroscopic models. The former is the macroscopic model used in the 1981 [1,2] calculations and the latter is an improved version [5] of the droplet model [6–8]. Because there were several unresolved issues in the 1988 calculations [3,4] these tables should be regarded as interim progress reports.

We have now resolved these issues, which were related to the pairing calculations [9], to the effect of higher-multipole distortions on the ground-state mass [10], and to some details of the shell-correction and zero-point-energy calculations [11]. The resolution of these issues has resulted in the present mass table. We first briefly review some important results obtained in the original 1981 calculation and enumerate the additional features of our new calculations.

Subsequent comparisons of predictions of our original 1981 model [1,2] with nuclear masses measured after the calculations were published showed that the model would reliably predict masses of nuclei that were not included in the determination of model constants [3,11]. With a properly defined model error [3], the error in new regions of nuclei is about the same as in the region where the constants were adjusted. In the most recent investigations [11,12] of the 1981 mass calculation in new regions of nuclei, the error for 351 new nuclei was only 6% larger than the error in the region where the model constants were adjusted. Furthermore, the error did not increase with distance from β stability.

Also, many other nuclear-structure properties were successfully predicted by the model for nuclei far from stability [13–16]. A special result of the 1981 mass calculation was the interpretation of certain spectroscopic results in terms of an intrinsic octupole deformation of nuclei in their ground state [1,17–19].

Here we present results of our new calculations of nuclear ground-state masses and deformations. Relative to the 1981 calculations we use an improved macroscopic-microscopic model, include additional shape degrees of freedom, extend the calculations to new regions of nuclei, and calculate a large number of additional nuclear ground-state properties. These additional properties will be published in a forthcoming article devoted to nuclear astrophysics [20].

Specifically, we have improved the model in the following areas:

- Our preferred macroscopic model is now the finite-range droplet model, which contains several essential improvements [4,5] over the original droplet model [6–8].
- The pairing calculations have been improved. Our pairing model is now the Lipkin-Nogami model [21–23]. We also use an improved functional form of the effective-interaction pairing gap and an optimized pairing constant [9,24].
- An eighth-order Strutinsky shell correction is used.
- The ϵ zero-point energy is still added to the calculated potential energy to obtain the ground-state mass, but no γ zero-point energy is added, since the method of calculation is not sufficiently accurate [11].
- We minimize the ground-state energy with respect to ϵ_3 and ϵ_6 shape degrees of freedom, in addition to the ϵ_2 and ϵ_4 shape degrees of freedom considered previously.
- Each ground-state shell-plus-pairing correction is based on single-particle levels calculated for the constants appropriate to the nucleus studied. Earlier, a single set of single-particle levels was used for an extended region of nuclei in conjunction with an interpolation scheme to improve accuracy.
- The calculation has been extended from 4023 nuclei to 8979 nuclei, which now includes nuclei between the proton and neutron drip lines and superheavy nuclei up to $A = 339$.

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In the macroscopic-microscopic approach it is possible to calculate a large number of nuclear structure properties in addition to nuclear ground-state masses. These include the following:

Even-multipole ground-state deformations:

Quadrupole ϵ deformation	ϵ_2
Hexadecapole ϵ deformation	ϵ_4
Hexacontatetrapole ϵ deformation	ϵ_6
Related quadrupole β deformation	β_2
Related hexadecapole β deformation	β_4
Related hexacontatetrapole β deformation	β_6

Beta-decay properties:

Q value of the β decay	Q_β
β-decay half-life	T_β
β-delayed one-neutron emission probability	$P_{1\mathrm{n}}$
β-delayed two-neutron emission probability	$P_{2\mathrm{n}}$
β-delayed three-neutron emission probability	$P_{3\mathrm{n}}$

Lipkin-Nogami pairing quantities:

Neutron pairing gap	Δ_{n}
Proton pairing gap	Δ_{p}
Neutron number-fluctuation constant	$\lambda_{2\mathrm{n}}$
Proton number-fluctuation constant	$\lambda_{2\mathrm{p}}$

Odd-particle spins:

Projection of the odd-neutron angular momentum along the symmetry axis	Ω_{n}
Projection of the odd-proton angular momentum along the symmetry axis	Ω_{p}

Alpha-decay properties:

Q value of the α decay	Q_α
α-decay half-life	T_α

Octupole properties:

Octupole ϵ deformation	ϵ_3
Related octupole β deformation	β_3
Decrease in mass due to octupole deformation	ΔE_3

FRDM mass-related quantities:

Spherical macroscopic energy	$E_{\mathrm{mac}}^{\mathrm{sph}}$
Shell correction	E_{shell}
Pairing correction	E_{pair}
Microscopic correction	E_{mic}
Calculated mass excess	M_{th}
Experimental mass excess	M_{exp}
Experimental uncertainty	σ_{exp}
Discrepancy	ΔM
Calculated binding energy	E_{bind}

FRLDM mass-related quantities:

Finite-range liquid-drop model microscopic correction	$E_{\mathrm{mic}}^{\mathrm{FL}}$
Finite-range liquid-drop model mass excess	$M_{\mathrm{th}}^{\mathrm{FL}}$

Neutron and proton separation energies:

One-neutron separation energy	$S_{1\mathrm{n}}$
Two-neutron separation energy	$S_{2\mathrm{n}}$
One-proton separation energy	$S_{1\mathrm{p}}$
Two-proton separation energy	$S_{2\mathrm{p}}$

As mentioned above, we present here the calculated ground-state masses and deformations. Some of the remaining quantities will be presented in a forthcoming publication [20].

In the next section we specify the macroscopic-microscopic finite-range droplet model in some detail. We discuss in particular the constants of the model, paying special attention to how to count the number of constants of a model. We present a summary of *all* constants in the model, including both those constants that have been determined from a least-squares adjustment to ground-state masses and fission-barrier heights and those that have been determined from other considerations. After our model has been specified, we discuss how it has been applied to the current mass calculation.

2 Models

In the macroscopic-microscopic method the total potential energy, which is calculated as a function of shape, proton number Z, and neutron number N, is the sum of a macroscopic term and a microscopic term representing the shell-plus-pairing correction. Thus, the total nuclear potential energy can be written as

$$E_{\rm pot}(Z, N, {\rm shape}) = E_{\rm mac}(Z, N, {\rm shape}) + E_{\rm s+p}(Z, N, {\rm shape}) \tag{1}$$

We study here two alternative models for $E_{\rm mac}$, given by Eqs. (40) and (62) below. The shell-plus-pairing correction is given by Eqs. (75) and (76) below.

It is practical to define an additional energy, the microscopic correction $E_{\rm mic}$, which is different from the shell-plus-pairing correction $E_{\rm s+p}$. For a specific deformation $\epsilon_{\rm a}$, the latter is determined solely from the single-particle level spectrum at this deformation by use of Strutinsky's shell-correction method [25,26] and a pairing model. In contrast, the microscopic correction is given by

$$E_{\rm mic}(\epsilon_{\rm a}) = E_{\rm s+p}(\epsilon_{\rm a}) + E_{\rm mac}(\epsilon_{\rm a}) - E_{\rm mac}(\epsilon_{\rm sphere}) \tag{2}$$

This definition has the desirable consequence that the potential energy $E_{\rm pot}$ of a nucleus at a certain deformation, for example the ground-state deformation $\epsilon_{\rm gs}$, is simply

$$E_{\rm pot}(\epsilon_{\rm gs}) = E_{\rm mic}(\epsilon_{\rm gs}) + E_{\rm mac}(\epsilon_{\rm sphere}) \tag{3}$$

However, the reader should note that the term microscopic correction is sometimes used instead for shell-plus-pairing correction. When results are presented it is usually $E_{\rm mic}$ that is tabulated, because it represents all additional effects over and above the *spherical* macroscopic energy. In practical calculations it is $E_{\rm s+p}$ that is calculated. To obtain the total energy a *deformed* macroscopic energy term is then added to $E_{\rm s+p}$.

There exist several different models for both the macroscopic and microscopic terms. Most of the initial works following the advent of Strutinsky's shell correction method used the *liquid-drop model* [27,28] as the macroscopic model.

The preferred model in the current calculations has its origin in a 1981 nuclear mass model [1,2], which utilized the folded-Yukawa single-particle potential developed in 1972 [29,30]. The macroscopic model used in the 1981 calculation was a finite-range liquid-drop model, which contained a modified surface-energy term to account for the finite range of the nuclear force. The modified surface-energy term was given by the Yukawa-plus-exponential finite-range model [31]. The macroscopic part in this formulation does not describe such features as nuclear compressibility and corresponding variations in the proton and neutron radii.

The droplet model [6–8], an extension of the liquid-drop model [27,28] that includes higher-order terms in $A^{-1/3}$ and $(N - Z)/A$, does describe such features. However, in its original formulation the droplet model was very inaccurate for nuclei far from stability and also failed catastrophically [31] to reproduce fission barriers of medium-mass nuclei. These deficiencies led Myers to suggest that the surface-energy terms of the droplet model also be generalized to account for the finite range of the nuclear force. Thus, the Yukawa-plus-exponential model for the surface tension was incorporated into the droplet model. During this work it also became apparent that the description of nuclear compressibility was unsatisfactory, since the squeezing of the central density of light nuclei was overpredicted. The deficiency was serious because it starts to become important already at about $A = 120$ and becomes even more pronounced for lighter nuclei. To account for compressibility effects for light nuclei and for other higher-order effects an empirical exponential term was added [4,5].

The additions of the finite-range surface-energy effects and exponential term to the droplet model [5] resulted in dramatic improvements in its predictive properties, as summarized in the discussion of Table A in Ref. 4. Mass calculations based on both the FRLDM [3] and the FRDM [4] were presented in the 1988 review of mass models in Atomic Data and Nuclear Data Tables. These calculations also used an improved pairing model relative to that used in the 1981 work. In the 1988 results the error in the FRDM was 8% lower than that in the FRLDM.

However, there were two major unresolved issues in the 1988 calculations. First, there existed some deficiencies in the pairing model and the values of the constants that were used. Second, ϵ_3 and ϵ_6 shape degrees of freedom were still not included, so deviations between calculated and measured masses due to the omission of these shape degrees of freedom were still present. Extensive investigations of pairing models and their constants have now been completed and resulted in an improved formulation of the pairing model [9]. We have now also minimized the potential energy with respect to ϵ_3 and ϵ_6 shape degrees of freedom. An overview of the results has been given in a paper on Coulomb redistribution effects [10]. The FRDM, which includes Coulomb redistribution effects, is now our preferred nuclear mass model.

Although the FRDM is now our preferred model, we also present results for the FRLDM for comparative purposes and for use in studies that assume constant nuclear density. We therefore specify below both models. Because several of the model constants are determined by least-squares-minimization of the model error, we start by defining model error.

2.1 Model error and adjustment procedure

In many studies the model error has been defined as simply the root-mean-square (rms) deviation, which as usual is given by

$$\mathrm{rms} = \left[\frac{1}{n}\sum_{i=1}^{n}(M_{\mathrm{exp}}^{i} - M_{\mathrm{th}}^{i})^2\right]^{\frac{1}{2}} \tag{4}$$

Here M_{th}^{i} is the calculated mass for a particular value of the proton number Z and neutron number N, and M_{exp}^{i} is the corresponding measured quantity. There are n such measurements for different N and Z. The choice (4) is a reasonable definition when all the errors $\sigma_{\mathrm{exp}}^{i}$ associated with the measurements are small compared to the model error. However, for large $\sigma_{\mathrm{exp}}^{i}$ the above definition is unsatisfactory, since both the theoretical and experimental errors contribute to the rms deviation. The definition (4) will therefore always overestimate the intrinsic model error.

When the experimental errors are large, it is necessary to use an approach that "decouples" the theoretical and experimental errors from one another. This can be accomplished by observing that the calculated masses are distributed around the *true* masses with a standard deviation σ_{th}. There exist powerful statistical methods for determining the intrinsic model error σ_{th}. The model error obtained in this way contains no contributions from the experimental uncertainties $\sigma_{\mathrm{exp}}^{i}$. To introduce such an error concept a new set of equations for determining model parameters and error were derived [3] by use of statistical arguments and the maximum-likelihood (ML) method. Here we generalize from the original assumption [3] $e_{\mathrm{th}}^{i} \in \mathrm{N}(0,\sigma_{\mathrm{th}})$ that the theoretical error term e_{th}^{i} is normally distributed with zero mean deviation from the true mass to $e_{\mathrm{th}}^{i} \in \mathrm{N}(\mu_{\mathrm{th}},\sigma_{\mathrm{th}})$ to allow for an error with a mean μ_{th} that is different from zero and a standard deviation σ_{th} around this mean [12]. This leads to the generalized equations

$$\sum_{i=1}^{n}\frac{[M_{\mathrm{exp}}^{i} - (M_{\mathrm{th}}^{i} + \mu_{\mathrm{th}}{}^{*})]}{{\sigma_{\mathrm{exp}}^{i}}^{2} + {\sigma_{\mathrm{th}}}^{2*}}\frac{\partial M_{\mathrm{th}}^{i}}{\partial p_{\nu}} = 0, \quad \nu = 1, 2, \ldots, m \tag{5}$$

$$\sum_{i=1}^{n} \frac{\left[M_{\rm exp}^{i} - (M_{\rm th}^{i} + {\mu_{\rm th}}^{*})\right]^{2} - ({\sigma_{\rm exp}^{i}}^{2} + {\sigma_{\rm th}}^{2*})}{({\sigma_{\rm exp}^{i}}^{2} + {\sigma_{\rm th}}^{2*})^{2}} = 0 \tag{6}$$

$$\sum_{i=1}^{n} \frac{\left[M_{\rm exp}^{i} - (M_{\rm th}^{i} + {\mu_{\rm th}}^{*})\right]}{({\sigma_{\rm exp}^{i}}^{2} + {\sigma_{\rm th}}^{2*})} = 0 \tag{7}$$

where p_ν are the unknown parameters of the model. The notation ${\sigma_{\rm th}}^{2*}$ means that by solving Eqs. (6) and (7) we obtain the estimate ${\sigma_{\rm th}}^{2*}$ of the true ${\sigma_{\rm th}}^{2}$. Equation (5) is equivalent to minimizing S with respect to p_ν, where

$$S = \sum_{i=1}^{n} \frac{\left[M_{\rm exp}^{i} - (M_{\rm th}^{i} + {\mu_{\rm th}}^{*})\right]^{2}}{{\sigma_{\rm exp}^{i}}^{2} + {\sigma_{\rm th}}^{2*}} \tag{8}$$

Thus, we are led to two additional equations relative to the usual least-squares equations that arise when model parameters are estimated by adjustments to experimental data under the assumption of a perfect theory with $\sigma_{\rm th} = 0$ and $\mu_{\rm th} = 0$. For the FRLDM the least-squares equations (5) are linear, whereas for the FRDM they are non-linear.

When the model contains a term $a_0 A^0$ that is strictly constant, Eq. (7) is identical to the member in Eq. (5) that corresponds to the derivative with respect to this constant. Thus, one should in this case put ${\mu_{\rm th}}^* = 0$ and solve only the remaining $m+1$ equations. One may therefore in this case characterize the error of the model in the region where the parameters were adjusted solely by the quantity $\sigma_{\rm th}$. In other cases one should solve the full set of equations. If ${\mu_{\rm th}}^*$ is significantly different from zero the theory needs modification. Even if $\mu_{\rm th} = 0$ in the original data region, it is entirely possible (although undesirable) that one obtains a mean error ${\mu_{\rm th}}^*$ that is substantially different from zero when one analyzes model results for new data points to which the parameters were not adjusted. In this case the most complete characterization of the theoretical error requires both its mean $\mu_{\rm th}$ and its standard deviation $\sigma_{\rm th}$ around this mean.

To allow for a single error measure that is similar to an rms deviation between the data and model we later also calculate the square root of the second central moment of the error term, $\sigma_{{\rm th};\mu=0}$, in our studies of model behavior in new regions of nuclei. This quantity is obtained by setting ${\mu_{\rm th}}^* = 0$ when solving Eq. (6). In contrast to the rms measure, it has the advantage that it has no contributions from the experimental errors.

Equations (5)–(7) constitute a system of $m+2$ equations that are to be solved together. It is instructive to rewrite Eqs. (6) and (7) as

$${\sigma_{\rm th}}^{2*} = \frac{1}{\sum_{i=1}^{n} {w_i}^{k_\sigma}} \sum_{i=1}^{n} {w_i}^{k_\sigma} \left[(M_{\rm exp}^{i} - M_{\rm th}^{i} - {\mu_{\rm th}}^{*})^2 - {\sigma_{\rm exp}^{i}}^{2} \right] \tag{9}$$

$${\mu_{\rm th}}^{*} = \frac{1}{\sum_{i=1}^{n} {w_i}^{k_\mu}} \sum_{i=1}^{n} {w_i}^{k_\mu} \left[(M_{\rm exp}^{i} - M_{\rm th}^{i}) \right] \tag{10}$$

where

$${w_i}^{k} = \frac{1}{({\sigma_{\rm exp}^{i}}^{2} + {\sigma_{\rm th}}^{2*})^{k}} \tag{11}$$

$$k_\sigma = 2 \tag{12}$$

$$k_\mu = 1 \tag{13}$$

The unknowns ${\mu_{\rm th}}^*$ and ${\sigma_{\rm th}}^{2*}$ can easily be determined from Eqs. (9) and (10) by an iterative procedure whose convergence is extremely rapid, requiring only about four iterations. An *interpretation*, not a proof, of Eq. (9) is that the experimental error is "subtracted out" from the difference between the experimental and calculated masses.

A common misconception is that one has to "throw away" data points that have errors that are equal to or larger than the error of the model whose parameters are determined. When a proper statistical approach, such as the one above, is used, this is no longer necessary.

We will see below that the discrepancy between our mass calculations and measured masses systematically increases as the size of the nuclear system decreases. It is therefore of interest to consider that the mass-model error is a function of mass number A. A simple function to investigate is

$$\sigma_{\rm th} = \frac{c}{A^{\alpha}} \tag{14}$$

where c and α are two parameters to be determined. Whereas under the assumption of a constant model error one determines this single error constant from Eq. (9), we find that the ML method for the error assumption in Eq. (14), with two unknowns, and assuming $\mu_{\rm th} = 0$, yields the equations

$$\sum_{i=1}^{n} \frac{(M_{\rm exp}^i - M_{\rm th}^i)^2 - \left[{\sigma_{\rm exp}^i}^2 + \left(\dfrac{c^*}{{A_i}^{\alpha^*}}\right)^2\right]}{\left[{\sigma_{\rm exp}^i}^2 + \left(\dfrac{c^*}{{A_i}^{\alpha^*}}\right)^2\right]^2 {A_i}^{\alpha^*}} = 0 \tag{15}$$

$$\sum_{i=1}^{n} \frac{(M_{\rm exp}^i - M_{\rm th}^i)^2 - \left[{\sigma_{\rm exp}^i}^2 + \left(\dfrac{c^*}{{A_i}^{\alpha^*}}\right)^2\right]}{\left[{\sigma_{\rm exp}^i}^2 + \left(\dfrac{c^*}{{A_i}^{\alpha^*}}\right)^2\right]^2 {A_i}^{\alpha^*+1}} = 0 \tag{16}$$

These equations are considerably more complicated to solve than Eq. (9). We solve them by minimizing the sum of the squares of the left members of Eqs. (15) and (16).

2.2 Shape parameterizations

The original parameterization of the folded-Yukawa single-particle model was the three-quadratic-surface parameterization [29,32]. It was designed to allow great flexibility in describing shapes late in the fission process. However, it is less suitable for describing ground-state shapes.

To allow a better description of ground-state shapes and to allow close comparison with results of Nilsson modified-oscillator calculations, we incorporated the Nilsson perturbed-spheroid parameterization, or ϵ parameterization, into the folded-Yukawa single-particle computer code in 1973 [30,33,34].

In our work here we use the ϵ parameterization for all calculations related to ground-state properties. In our adjustment of macroscopic constants we also include 28 outer saddle-point heights of fission barriers. The shapes of these saddle points were obtained in a three-parameter calculation in the three-quadratic-surface parameterization in 1973 [33].

2.2.1 Perturbed-spheroid parameterization

The ϵ parameterization was originally used by Nilsson [35] in the modified-oscillator single-particle potential. It was introduced to limit the dimensions of the matrices from which the single-particle energies and wave functions are obtained by diagonalization. This requirement leads to somewhat complex expressions for the nuclear shape. Here we employ its extension to higher-multipole distortions. For completeness we define it with axially asymmetric shapes [36–38] included, although this symmetry-breaking shape degree of freedom has not yet been implemented in the folded-Yukawa single-particle model. Note that a factor $\frac{1}{2}\sqrt{\frac{4\pi}{9}}$ is missing in front of the $V_4(\gamma)$ function in Eq. (3) of Ref. 38.

As the first step in defining the ϵ parameterization a "stretched" representation is introduced. The stretched coordinates ξ, η, and ζ are defined by

$$\begin{aligned}
\xi &= \left\{\frac{m\omega_0}{\hbar}\left[1-\frac{2}{3}\epsilon_2\cos\left(\gamma+\frac{2}{3}\pi\right)\right]\right\}^{1/2} x \\
\eta &= \left\{\frac{m\omega_0}{\hbar}\left[1-\frac{2}{3}\epsilon_2\cos\left(\gamma-\frac{2}{3}\pi\right)\right]\right\}^{1/2} y \\
\zeta &= \left\{\frac{m\omega_0}{\hbar}\left[1-\frac{2}{3}\epsilon_2\cos\gamma\right]\right\}^{1/2} z
\end{aligned} \tag{17}$$

where $\hbar\omega_0$ is the oscillator energy, ϵ_2 the ellipsoidal deformation parameter, and γ the non-axiality angle. It is then convenient to define a "stretched" radius vector ρ_{t} by

$$\rho_{\mathrm{t}} = (\xi^2+\eta^2+\zeta^2)^{1/2} \tag{18}$$

a stretched polar angle θ_t by

$$u = \cos\theta_t = \frac{\zeta}{\rho_{\mathrm{t}}} = \left[\frac{1-\frac{2}{3}\epsilon_2\cos\gamma}{1-\frac{1}{3}\epsilon_2\cos\gamma(3\cos^2\theta-1)+\left(\frac{1}{3}\right)^{1/2}\epsilon_2\sin\gamma\sin^2\theta\cos2\phi}\right]^{1/2}\cos\theta \tag{19}$$

and a stretched azimuthal angle ϕ_{t} by

$$v = \cos2\phi_{\mathrm{t}} = \frac{2\eta}{(\xi^2+\eta^2)^{1/2}} = \frac{\left[1+\frac{1}{3}\epsilon_2\cos\gamma\right]\cos2\phi+\left(\frac{1}{3}\right)^{1/2}\epsilon_2\sin\gamma}{1+\frac{1}{3}\epsilon_2\cos\gamma+\left(\frac{1}{3}\right)^{1/2}\epsilon_2\sin\gamma\cos2\phi} \tag{20}$$

In the folded-Yukawa model the single-particle potential is very different from that in the Nilsson modified-oscillator model. However, the definition of the ϵ parameterization will be most clear if we follow the steps in the Nilsson model. The implementation in the folded-Yukawa model will then be simple. The Nilsson modified-oscillator potential is defined by

$$\begin{aligned}
V = \frac{1}{2}\hbar\omega_0{\rho_{\mathrm{t}}}^2 \Bigg\{ & 1+2\epsilon_1P_1(\cos\theta_{\mathrm{t}}) \\
& -\frac{2}{3}\epsilon_2\cos\gamma P_2(\cos\theta_{\mathrm{t}})+\frac{1}{3}\epsilon_2\sin\gamma\left(\frac{8}{5}\pi\right)^{1/2}\left[Y_2^2(\theta_{\mathrm{t}},\phi_{\mathrm{t}})+Y_2^{-2}(\theta_{\mathrm{t}},\phi_{\mathrm{t}})\right] \\
& +2\epsilon_3P_3(\cos\theta_{\mathrm{t}})+2\epsilon_4V_4(\cos\theta_{\mathrm{t}},\cos2\phi_{\mathrm{t}})+2\epsilon_5P_5(\cos\theta_{\mathrm{t}})+2\epsilon_6P_6(\cos\theta_{\mathrm{t}})\Bigg\} \\
& -\kappa\hbar\mathring{\omega}_0\left[2\vec{l}_{\mathrm{t}}\cdot\vec{s}+\mu(\vec{l}_{\mathrm{t}}^{\,2}-<\vec{l}_{\mathrm{t}}^{\,2}>)\right]
\end{aligned} \tag{21}$$

where $\vec{l}_{\mathrm{t}}$ is the angular-momentum operator in the stretched coordinate system, $\vec{s}$ is the spin operator [35], and

$$V_4(u,v) = a_{40}P_4+\sqrt{\frac{4\pi}{9}}\left[a_{42}(Y_4^2+Y_4^{-2})+a_{44}(Y_4^4+Y_4^{-4})\right] \tag{22}$$

Here the hexadecapole potential $V_4(u,v)$ is made dependent on γ in such a way that axial symmetry is maintained when $\gamma = 0$, $60°$, $-120°$, and $-60°$, for mass-symmetric shapes and for

$\epsilon_6 = 0$. This is accomplished by choosing the coefficients a_{4i} so that they have the transformation properties of a hexadecapole tensor. However, this is achieved only for mass-symmetric shapes and for $\epsilon_6 = 0$. The ϵ parameterization has not been generalized to a more general case. Thus [38]

$$
\begin{aligned}
a_{40} &= \frac{1}{6}(5\cos^2\gamma + 1) \\
a_{42} &= -\frac{1}{12}\sqrt{30}\sin 2\gamma \\
a_{44} &= \frac{1}{12}\sqrt{70}\sin^2\gamma
\end{aligned}
\tag{23}
$$

It is customary to now assume that the shape of the nuclear surface is equal to the shape of an equipotential surface given by Eq. (21). By neglecting the $\vec{l}_{\rm t} \cdot \vec{s}$ and $\vec{l}_{\rm t}^{\,2}$ terms and solving for $\rho_{\rm t}$ and then using Eqs. (17)–(20) to derive an expression for r in the non-stretched laboratory system we obtain

$$
\begin{aligned}
r(\theta,\phi) = \; & \frac{R_0}{\omega_0/\mathring{\omega}_0}\left\{\left[1-\frac{2}{3}\epsilon_2\cos\left(\gamma+\frac{2}{3}\pi\right)\right]\left[1-\frac{2}{3}\epsilon_2\cos\left(\gamma-\frac{2}{3}\pi\right)\right]\left[1-\frac{2}{3}\epsilon_2\cos\gamma\right]\right\}^{-1/2} \\
& \times\left[1-\frac{1}{3}\epsilon_2\cos\gamma-\frac{2}{9}\epsilon_2^{\,2}\cos^2\gamma+\epsilon_2\left(\cos\gamma+\frac{1}{3}\epsilon_2\cos 2\gamma\right)u^2\right. \\
& \left. -\left(\frac{1}{3}\right)^{1/2}\epsilon_2\sin\gamma\left(1-\frac{2}{3}\epsilon_2\cos\gamma\right)(1-u^2)v\right]^{1/2} \\
& \times\left[1-\frac{2}{3}\epsilon_2\cos\gamma\frac{1}{2}(3u^2-1)+\left(\frac{1}{3}\right)^{1/2}\epsilon_2\sin\gamma(1-u^2)v\right. \\
& \left. +2\epsilon_1P_1(u)+2\epsilon_3P_3(u)+2\epsilon_4V_4(u,v)+2\epsilon_5P_5(u)+2\epsilon_6P_6(u)\right]^{-1/2}
\end{aligned}
\tag{24}
$$

In the Nilsson model the starting point is to define the potential. After the potential has been generated the shape of the nuclear surface is deduced by the above argument. In the folded-Yukawa model the starting point is different. There, the equation for the nuclear surface, given by Eq. (24) in the case of the ϵ parameterization, is specified in the initial step. Once the shape of the surface is known, the single-particle potential may be generated as described in later sections.

The quantity $\omega_0/\mathring{\omega}_0$ is determined by requiring that the volume remain constant with deformation, which gives

$$
\begin{aligned}
\left(\frac{\omega_0}{\mathring{\omega}_0}\right)^3 = \; & \frac{1}{4\pi}\left\{\left[1-\frac{2}{3}\epsilon_2\cos\left(\gamma+\frac{2}{3}\pi\right)\right]\left[1-\frac{2}{3}\epsilon_2\cos\left(\gamma-\frac{2}{3}\pi\right)\right]\left[1-\frac{2}{3}\epsilon_2\cos\gamma\right]\right\}^{-1/2} \\
& \times\int_0^{\pi}d\theta_{\rm t}\int_0^{2\pi}d\phi_{\rm t}\sin\theta_{\rm t}\left[1-\frac{2}{3}\epsilon_2\cos\gamma P_2(u)+\epsilon_2\sin\gamma\left(\frac{8\pi}{45}\right)^{1/2}(Y_2^2+Y_2^{-2})\right. \\
& \left. +2\epsilon_1P_1(u)+2\epsilon_3P_3(u)+2\epsilon_4V_4(u,v)+2\epsilon_5P_5(u)+2\epsilon_6P_6(u)\right]^{-3/2}
\end{aligned}
\tag{25}
$$

The above equation is derived by determining the volume inside the nuclear surface given by Eq. (24), with the integral $\int d^3r$ inside the surface evaluated in terms of the "non-stretched" coordinates θ and ϕ. After a variable substitution one arrives at the expression in Eq. (25).

The Legendre polynomials P_l occurring in the definitions of the ϵ parameterization are defined by

$$P_l(u) = \frac{1}{2^l l!}\frac{d^l}{du^l}(u^2-1)^l \quad , \qquad l = 0,\ 1,\ 2, \ldots, \infty \tag{26}$$

The first six Legendre polynomials are

$$\begin{aligned}
P_0(u) &= 1 \\
P_1(u) &= u \\
P_2(u) &= \frac{1}{2}(3u^2-1) \\
P_3(u) &= \frac{1}{2}(5u^3-3u) \\
P_4(u) &= \frac{1}{8}(35u^4-30u^2+3) \\
P_5(u) &= \frac{1}{8}(63u^5-70u^3+15u) \\
P_6(u) &= \frac{1}{16}(231u^6-315u^4+105u^2-5)
\end{aligned} \tag{27}$$

The associated Legendre functions P_l^m are defined by

$$P_l^m(u) = \frac{(1-u^2)^{m/2}}{2^l l!}\frac{d^{l+m}}{du^{l+m}}(u^2-1)^l \quad , \qquad l = 0,\ 1,\ 2, \ldots, \infty; \quad m = 0,\ 1,\ 2, \ldots, l \tag{28}$$

The spherical harmonics are then determined from the relations

$$Y_l^m(\theta,\phi) = (-)^m \left[\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}\right]^{1/2} P_l^m(\cos\theta)e^{im\phi} \quad , \qquad m \geq 0 \tag{29}$$

$$Y_l^{m*}(\theta,\phi) = (-)^m Y_l^{-m}(\theta,\phi) \tag{30}$$

which yield for the functions used here

$$\begin{aligned}
Y_2^2(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{2i\phi} \\
Y_2^{-2}(\theta,\phi) &= \sqrt{\frac{15}{32\pi}}\sin^2\theta e^{-2i\phi} \\
Y_4^4(\theta,\phi) &= \sqrt{\frac{315}{512\pi}}\sin^4\theta e^{4i\phi} \\
Y_4^{-4}(\theta,\phi) &= \sqrt{\frac{315}{512\pi}}\sin^4\theta e^{-4i\phi} \\
Y_4^2(\theta,\phi) &= \sqrt{\frac{45}{128\pi}}\sin^2\theta(7\cos^2\theta-1)e^{2i\phi} \\
Y_4^{-2}(\theta,\phi) &= \sqrt{\frac{45}{128\pi}}\sin^2\theta(7\cos^2\theta-1)e^{-2i\phi}
\end{aligned} \tag{31}$$

The sums

$$\begin{aligned}
SY_{22} &= Y_2^2(\theta,\phi) + Y_2^{-2}(\theta,\phi) \\
SY_{44} &= Y_4^4(\theta,\phi) + Y_4^{-4}(\theta,\phi) \\
SY_{42} &= Y_4^2(\theta,\phi) + Y_4^{-2}(\theta,\phi)
\end{aligned} \tag{32}$$

are required in the expression for the single-particle potential and in the corresponding equation for the nuclear surface. When the arguments of the spherical harmonics are the stretched angles θ_{t} and ϕ_{t} we obtain

$$\begin{aligned} SY_{22} &= \sqrt{\frac{15}{8\pi}}\sin^2\theta_{\mathrm{t}}\cos 2\phi_{\mathrm{t}} = \sqrt{\frac{15}{8\pi}}(1-u^2)v \\ SY_{44} &= \sqrt{\frac{315}{128\pi}}\sin^4\theta_{\mathrm{t}}\cos 4\phi_{\mathrm{t}} = \sqrt{\frac{315}{128\pi}}(1-u^2)^2(2v^2-1) \\ SY_{42} &= \sqrt{\frac{45}{32\pi}}\sin^2\theta_{\mathrm{t}}(7\cos^2\theta_{\mathrm{t}}-1)\cos 2\phi_{\mathrm{t}} = \sqrt{\frac{45}{32\pi}}(1-u^2)(7u^2-1)v \end{aligned} \tag{33}$$

2.2.2 Three-quadratic-surface parameterization

In the three-quadratic-surface parameterization the shape of the nuclear surface is defined in terms of three smoothly joined portions of quadratic surfaces of revolution. They are completely specified by [32]

$$\rho^2 = \begin{cases} {a_1}^2 - \dfrac{{a_1}^2}{{c_1}^2}(z-l_1)^2 \;, & l_1 - c_1 \le z \le z_1 \\ {a_2}^2 - \dfrac{{a_2}^2}{{c_2}^2}(z-l_2)^2 \;, & z_2 \le z \le l_2 + c_2 \\ {a_3}^2 - \dfrac{{a_3}^2}{{c_3}^2}(z-l_3)^2 \;, & z_1 \le z \le z_2 \end{cases} \tag{34}$$

Here the left-hand surface is denoted by the subscript 1, the right-hand one by 2, and the middle one by 3. Each surface is specified by the position l_i of its center, its transverse semiaxis a_i, and its semi-symmetry axis c_i. At the left and right intersections of the middle surface with the end surfaces the value of z is z_1 and z_2, respectively.

There are nine numbers required to specify the expressions in Eq. (34) but three numbers are eliminated by the conditions of constancy of the volume and continuous first derivatives at z_1 and z_2. The introduction of an auxiliary unit of distance u through

$$u = \left[\frac{1}{2}\left({a_1}^2 + {a_2}^2\right)\right]^{\frac{1}{2}} \tag{35}$$

permits a natural definition of two sets of shape coordinates. We define three mass-symmetric coordinates σ_i and three mass-asymmetric coordinates α_i by

$$\begin{aligned} \sigma_1 &= \frac{(l_2 - l_1)}{u} \\ \sigma_2 &= \frac{{a_3}^2}{{c_3}^2} \\ \sigma_3 &= \frac{1}{2}\left(\frac{{a_1}^2}{{c_1}^2} + \frac{{a_2}^2}{{c_2}^2}\right) \\ \alpha_1 &= \frac{1}{2}\frac{(l_1 + l_2)}{u} \\ \alpha_2 &= \frac{({a_1}^2 - {a_2}^2)}{u^2} \\ \alpha_3 &= \frac{{a_1}^2}{{c_1}^2} - \frac{{a_2}^2}{{c_2}^2} \end{aligned} \tag{36}$$

The coordinate α_1 is not varied freely but is instead determined by the requirement that the center of mass be at the origin.

2.2.3 Conversion to β parameters

A common parameterization, which we do *not* use here, is the β parameterization. However, since we want to present some of our results in terms of β shape parameters, we introduce the parameterization and a scheme to express shapes generated in other parameterizations in terms of β deformation parameters. In the β parameterization the radius vector r is defined by

$$r(\theta,\phi) = R_0(1 + \sum_{l=1}^{\infty}\sum_{m=-l}^{l} \beta_{lm} Y_l^m) \tag{37}$$

where R_0 is deformation dependent so as to conserve the volume inside the nuclear surface. When only axially symmetric shapes are considered the notation β_l is normally used for β_{l0}. Since the spherical harmonics Y_l^m are orthogonal, one may determine the β parameters corresponding to a specific shape in the ϵ parameterization by use of

$$\beta_{lm} = \sqrt{4\pi}\frac{\int r(\theta,\phi)Y_l^m(\theta,\phi)d\Omega}{\int r(\theta,\phi)Y_0^0(\theta,\phi)d\Omega} \tag{38}$$

where r is now the radius vector in the ϵ parameterization, given by Eq. (24). This conversion equation is in fact valid for a radius vector $r(\theta,\phi)$ defined by any parameterization.

When the β parameters corresponding to a specific shape in the ϵ parameterization are determined one should observe that higher-order β parameters may be non-zero even if higher-order ϵ parameters are identically zero. For this reason, and because β_5 is not tabulated, the nuclear ground-state shape is not completely specified by the β parameters in the Table, whereas the shape is completely defined by the ϵ parameters.

2.3 Finite-range droplet model

The *finite-range droplet model*, developed in 1984 [5], combines the finite-range effects of the FRLDM [31,39,40] with the higher-order terms in the droplet model. In addition, the finite-range droplet model contains the new exponential term

$$-CAe^{-\gamma A^{1/3}}\bar{\epsilon} \tag{39}$$

where C and γ specify the strength and range, respectively, of this contribution to the energy and the quantity $\bar{\epsilon}$ is a dilatation variable given by Eq. (49) below. The exponential term leads to an improved description of compressibility effects and is crucial to the substantially improved results obtained in the finite-range droplet model relative to the original droplet model. The necessity for this empirical exponential term, which is discussed extensively in Refs. 5 and 41, is clearly demonstrated in Refs. 5 and 41 and by the results obtained in Sec. 4.2 below.

Most of our results here are based on the finite-range droplet model for the macroscopic term. Relative to the formulation given in Ref. 5, which unfortunately has numerous misprints, we use a new model for the average neutron and proton pairing gaps. The complete expression for the contribution to the atomic mass excess from the FRDM macroscopic energy is obtained after minimization with respect to variations in $\bar{\epsilon}$ and $\bar{\delta}$, where $\bar{\delta}$ is the average bulk relative neutron excess given by Eq. (47) below. One then obtains

$$
\begin{aligned}
E_{\rm mac}(Z,N,\text{shape}) = \\
& M_{\rm H}Z + M_{\rm n}N && \text{mass excesses of } Z \text{ hydrogen atoms and } N \text{ neutrons}\\
+\;& \left(-a_1 + J\bar{\delta}^2 - \frac{1}{2}K\bar{\epsilon}^2\right)A && \text{volume energy}\\
+\;& \left(a_2 B_1 + \frac{9}{4}\frac{J^2}{Q}\bar{\delta}^2\frac{B_{\rm s}{}^2}{B_1}\right)A^{2/3} && \text{surface energy}\\
+\;& a_3 A^{1/3} B_{\rm k} && \text{curvature energy}\\
+\;& a_0 A^0 && A^0 \text{ energy}\\
+\;& c_1 \frac{Z^2}{A^{1/3}} B_3 && \text{Coulomb energy}\\
-\;& c_2 Z^2 A^{1/3} B_{\rm r} && \text{volume redistribution energy}\\
-\;& c_4 \frac{Z^{4/3}}{A^{1/3}} && \text{Coulomb exchange correction}\\
-\;& c_5 Z^2 \frac{B_{\rm w} B_{\rm s}}{B_1} && \text{surface redistribution energy}\\
+\;& f_0 \frac{Z^2}{A} && \text{proton form-factor correction to the Coulomb energy}\\
-\;& c_{\rm a}(N-Z) && \text{charge-asymmetry energy}\\
+\;& W\left(|I| + \begin{cases} 1/A \;, & Z \text{ and } N \text{ odd and equal}\\ 0 \;, & \text{otherwise}\end{cases}\right) && \text{Wigner energy}\\
+\;& \begin{cases} \overline{\Delta}_{\rm p} + \overline{\Delta}_{\rm n} - \delta_{\rm np} \;, & Z \text{ and } N \text{ odd}\\ \overline{\Delta}_{\rm p} \;, & Z \text{ odd and } N \text{ even}\\ \overline{\Delta}_{\rm n} \;, & Z \text{ even and } N \text{ odd}\\ 0 \;, & Z \text{ and } N \text{ even}\end{cases} && \text{average pairing energy}\\
-\;& a_{\rm el} Z^{2.39} && \text{energy of bound electrons}
\end{aligned}
\tag{40}
$$

where $A = Z + N$ is the mass number and $I = (N - Z)/A$ is the relative neutron excess. This expression differs from the corresponding one used in our earlier calculations[5] only in the form of the average pairing energy appearing in the next-to-last term. One should note that after minimization the exponential term [Eq. (39)] is present only implicitly in Eq. (40) through its presence in Eq. (49) below. For the average neutron pairing gap $\overline{\Delta}_{\rm n}$, average proton pairing gap

$\overline{\Delta}_{\rm p}$, and average neutron-proton interaction energy $\delta_{\rm np}$ we now use[9,24,42]

$$\overline{\Delta}_{\rm n} = \frac{r_{\rm mac} B_{\rm s}}{N^{1/3}} \tag{41}$$

$$\overline{\Delta}_{\rm p} = \frac{r_{\rm mac} B_{\rm s}}{Z^{1/3}} \tag{42}$$

$$\delta_{\rm np} = \frac{h}{B_{\rm s} A^{2/3}} \tag{43}$$

The zero reference point for the pairing energy now corresponds to even-even nuclei rather than to halfway between even-even and odd-odd nuclei.

The quantities c_1, c_2, c_4, and c_5 are defined by

$$\begin{aligned} c_1 &= \frac{3}{5}\frac{e^2}{r_0} \\ c_2 &= \frac{1}{336}\left(\frac{1}{J}+\frac{18}{K}\right){c_1}^2 \\ c_4 &= \frac{5}{4}\left(\frac{3}{2\pi}\right)^{2/3} c_1 \\ c_5 &= \frac{1}{64Q}{c_1}^2 \end{aligned} \tag{44}$$

In Eq. (40) we have kept only the first term in the expression for the proton form-factor correction to the Coulomb energy, so that f_0 is given by

$$f_0 = -\frac{1}{8}\left(\frac{145}{48}\right)\frac{{r_{\rm p}}^2 e^2}{{r_0}^3} \tag{45}$$

The bulk nuclear asymmetry δ is defined in terms of the neutron density $\rho_{\rm n}$ and proton density $\rho_{\rm p}$ by

$$\delta = \frac{\rho_{\rm n} - \rho_{\rm p}}{\rho_{\rm bulk}} \tag{46}$$

and the *average* bulk nuclear asymmetry is given by

$$\overline{\delta} = \left(I + \frac{3}{16}\frac{c_1}{Q}\frac{Z}{A^{2/3}}\frac{B_{\rm v}B_{\rm s}}{B_1}\right) \Big/ \left(1 + \frac{9}{4}\frac{J}{Q}\frac{1}{A^{1/3}}\frac{{B_{\rm s}}^2}{B_1}\right) \tag{47}$$

The relative deviation in the bulk of the density ρ from its nuclear matter value ρ_0 is defined by

$$\epsilon = -\frac{1}{3}\frac{\rho - \rho_0}{\rho_0} \tag{48}$$

and the *average* relative deviation in the bulk of the density is given by

$$\overline{\epsilon} = \left(Ce^{-\gamma A^{1/3}} - 2a_2\frac{B_2}{A^{1/3}} + L\overline{\delta}^2 + c_1\frac{Z^2}{A^{4/3}}B_4\right)/K \tag{49}$$

The quantity B_1 is the relative generalized surface or nuclear energy in a model that accounts for the effect of the finite range of the nuclear force. It is given by

$$B_1 = \frac{A^{-2/3}}{8\pi^2 {r_0}^2 a^4} \int\!\!\int_V \left(2 - \frac{|\mathbf{r} - \mathbf{r}'|}{a}\right) \frac{e^{-|\mathbf{r}-\mathbf{r}'|/a}}{|\mathbf{r} - \mathbf{r}'|/a} d^3r \, d^3r' \tag{50}$$

where the integration is over the specified sharp-surface deformed *generating* shape of volume V. Since the volume of the generating shape is conserved during deformation we have

$$V = \frac{4\pi}{3} {R_0}^3 \tag{51}$$

where R_0 is the radius of the spherical shape. The relative Coulomb energy B_3 is given by

$$B_3 = \frac{15}{32\pi^2} \frac{A^{-5/3}}{{r_0}^5} \int\!\!\int_V \frac{d^3r \, d^3r'}{|\mathbf{r} - \mathbf{r}'|} \left[1 - \left(1 + \frac{1}{2} \frac{|\mathbf{r} - \mathbf{r}'|}{a_{\mathrm{den}}}\right) e^{-|\mathbf{r}-\mathbf{r}'|/a_{\mathrm{den}}}\right] \tag{52}$$

The quantities B_1 and B_3 are evaluated for $R_0 = r_0 A^{1/3}$. However, in the finite-range droplet model the equilibrium value R_{den} of the equivalent-sharp-surface radius corresponding to the nuclear density is given by the expression

$$R_{\mathrm{den}} = r_0 A^{1/3} (1 + \bar{\epsilon}) \tag{53}$$

Thus, the actual value of the nuclear radius is determined by the balance between Coulomb, compressibility, and surface-tension effects as expressed by Eq. (49). To calculate this balance it is necessary to know the response of the surface-energy and Coulomb-energy terms B_1 and B_3 to size changes. To account for this response we introduce the quantities B_2 and B_4, which are related to the derivatives of B_1 and B_3. These derivatives are evaluated numerically and during this evaluation the radius R of the *generating* shape is varied around the value $r_0 A^{1/3}$.

The quantity B_2, which as mentioned above is related to the derivative of the relative generalized surface energy B_1, is defined by

$$B_2 = \frac{1}{2x_0} \left[\frac{d}{dx} \left(x^2 B_1\right)\right]_{x=x_0} \tag{54}$$

with

$$x = \frac{R}{a} \quad \text{and} \quad x_0 = \frac{r_0 A^{1/3}}{a} \tag{55}$$

The quantity B_4 is related to the derivative of the relative Coulomb energy B_3 and is defined by

$$B_4 = -{y_0}^2 \left[\frac{d}{dy} \left(\frac{B_3}{y}\right)\right]_{y=y_0} \tag{56}$$

with

$$y = \frac{R}{a_{\mathrm{den}}} \quad \text{and} \quad y_0 = \frac{r_0 A^{1/3}}{a_{\mathrm{den}}} \tag{57}$$

For spherical shapes the quantities B_1, B_2, B_3, and B_4 can be evaluated analytically. One obtains

$$\begin{aligned}
B_1^{(0)} &= 1 - \frac{3}{{x_0}^2} + (1 + x_0)\left(2 + \frac{3}{x_0} + \frac{3}{{x_0}^2}\right) e^{-2x_0} \\
B_2^{(0)} &= 1 - \left(1 + 2x_0 - {x_0}^2\right) e^{-2x_0} \\
B_3^{(0)} &= 1 - \frac{5}{{y_0}^2}\left[1 - \frac{15}{8y_0} + \frac{21}{8{y_0}^3} - \frac{3}{4}\left(1 + \frac{9}{2y_0} + \frac{7}{{y_0}^2} + \frac{7}{2{y_0}^3}\right) e^{-2y_0}\right] \\
B_4^{(0)} &= 1 + 5\left[-\frac{3}{{y_0}^2} + \frac{15}{2{y_0}^3} - \frac{63}{4{y_0}^5} + \frac{3}{4}\left(\frac{2}{y_0} + \frac{12}{{y_0}^2} + \frac{32}{{y_0}^3} + \frac{42}{{y_0}^4} + \frac{21}{{y_0}^5}\right) e^{-2y_0}\right]
\end{aligned} \tag{58}$$

The expression B_3 for the relative Coulomb energy yields the energy for an arbitrarily shaped, homogeneously charged, diffuse-surface nucleus to all orders in the diffuseness constant $a_{\rm den}$. The constants in front of the integrals for B_1 and B_3 are chosen so that B_1 and B_3 are 1 for a sphere in the limit in which the range constant a and the diffuseness constant $a_{\rm den}$ are zero, in analogy with the definition of the quantities $B_{\rm s}$ and $B_{\rm C}$ in the standard liquid-drop and droplet models. The quantities B_2 and B_4, which are related to the derivatives of B_1 and B_3, respectively, were introduced above to treat the response of the nucleus to a change in size, resulting from a finite compressibility. The shape-dependent quantities $B_{\rm s}$, $B_{\rm v}$, $B_{\rm w}$, $B_{\rm k}$, and $B_{\rm r}$, which are defined [7] in the standard droplet model, are given by

$$\begin{aligned}
B_{\rm s} &= \frac{A^{-2/3}}{4\pi {r_0}^2}\int_S dS && \text{surface energy} \\
B_{\rm v} &= -\frac{15A^{-4/3}}{16\pi^2 {r_0}^4}\int_S \widetilde{W}(\mathbf{r})\, dS && \text{neutron skin energy} \\
B_{\rm w} &= \frac{225A^{-2}}{64\pi^3 {r_0}^6}\int_S \left[\widetilde{W}(\mathbf{r})\right]^2 dS && \text{surface redistribution energy} \\
B_{\rm k} &= \frac{A^{-1/3}}{8\pi r_0}\int_S \left(\frac{1}{R_1} + \frac{1}{R_2}\right) dS && \text{curvature energy} \\
B_{\rm r} &= \frac{1575A^{-7/3}}{64\pi^3 {r_0}^7}\int_V \left[\widetilde{W}(\mathbf{r})\right]^2 d^3r && \text{volume redistribution energy}
\end{aligned} \tag{59}$$

where

$$\begin{aligned}
W(\mathbf{r}) &= \int_V \frac{1}{|\mathbf{r} - \mathbf{r}'|}\, d^3r' \\
\overline{W} &= \frac{3A^{-1}}{4\pi {r_0}^3}\int_V W(\mathbf{r})\, d^3r \\
\widetilde{W}(\mathbf{r}) &= W(\mathbf{r}) - \overline{W}
\end{aligned} \tag{60}$$

and R_1 and R_2 are the principal radii of curvature.

2.4 Values of FRDM macroscopic-model constants

The constants appearing in the expression for the finite-range droplet macroscopic model fall into four categories. The first category, which represents fundamental constants, includes [1,2]

M_{H}	=	7.289034 MeV	hydrogen-atom mass excess
M_{n}	=	8.071431 MeV	neutron mass excess
e^2	=	1.4399764 MeV fm	electronic charge squared

One should note that for consistency we here use the same values for the fundamental constants as in our 1981 mass calculation [1,2]. Results of a more recent evaluation of the fundamental constants appear in Refs. 43 and 44.

The second category, which represents constants that have been determined from considerations other than nuclear masses, includes [1–4]

a_{el}	=	1.433×10^{-5} MeV	electronic-binding constant
K	=	240 MeV	nuclear compressibility constant
r_{p}	=	0.80 fm	proton root-mean-square radius
r_0	=	1.16 fm	nuclear-radius constant
a	=	0.68 fm	range of Yukawa-plus-exponential potential
a_{den}	=	0.70 fm	range of Yukawa function used to generate nuclear charge distribution

The third category, representing those constants whose values were obtained from consideration of odd-even mass differences [9,24,42] and other mass-like quantities, are

r_{mac}	=	4.80 MeV	average pairing-gap constant
h	=	6.6 MeV	neutron-proton interaction constant
W	=	30 MeV	Wigner constant
L	=	0 MeV	density-symmetry constant
a_3	=	0 MeV	curvature-energy constant

It should be noted that the final calculated mass excess is strictly independent of the value used for r_{mac}. This constant affects only the division of the mass excess between a macroscopic part and the remaining microscopic correction. We will therefore not include r_{mac} when we later count the number of constants in our mass model. It is the pairing constant r_{mic} which enters the microscopic model that affects the mass excess. It will be discussed below.

Since $\mu_{\mathrm{th}} = 0$ in our case, Eqs. (6) and (8) can be solved with the experimental data set of 1654 masses with $Z \geq 8$ and $N \geq 8$ [45] and 28 fission-barrier heights to determine the remaining macroscopic constants and the error of our model. Because it is now clear that the measurements of the masses of $^{31-34}$Na that are listed in the 1989 midstream evaluation of Audi [45] are in error, we have made four revisions. For ^{31,32}Na we use early results of mass measurements at TOFI [46]. The final, slightly different values appear in Ref. 47. For ^{33}Na we use results of new measurements at GANIL [48]. The data point for ^{34}Na is excluded.

To present all the macroscopic model constants together we list them here but discuss their adjustment later. These constants are

a_1	=	16.247 MeV	volume-energy constant
a_2	=	22.92 MeV	surface-energy constant
J	=	32.73 MeV	symmetry-energy constant
Q	=	29.21 MeV	effective surface-stiffness constant
a_0	=	0.0 MeV	A^0 constant
c_{a}	=	0.436 MeV	charge-asymmetry constant
C	=	60 MeV	pre-exponential compressibility-term constant
γ	=	0.831	exponential compressibility-term range constant

The pairing constant r_{mic} which enters the microscopic model is also determined in a least-squares minimization with the above 1654 masses, although no barrier heights were included in its determination. Once the value of r_{mic} had been determined the adjustment routines were run again, this time with barriers included, to yield the final values of the constants listed above. The value of r_{mic} will be given in the section on microscopic constants. The resulting error in the FRDM is $\sigma_{\mathrm{th}} = 0.669$ MeV.

For completeness we also specify the mass-energy conversion factor used in the interim 1989 mass evaluation. In this evaluation the relation between atomic mass units and energy is given by [45]

$$1 \ \mathrm{u} = 931.5014 \ \mathrm{MeV} \tag{61}$$

Although a more recent value has been adopted [43,44,49], it is the above value, consistent with the 1989 interim mass evaluation [45], that should be used if our calculated mass excesses in MeV are converted to atomic mass units.

2.5 Finite-range liquid-drop model

In the present version of our model the contribution to the atomic mass excess from the FRLDM macroscopic energy is given by

$$
\begin{aligned}
& E_{\text{mac}}^{\text{FL}}(Z, N, \text{shape}) = \\
& \quad M_{\text{H}} Z + M_{\text{n}} N && \text{mass excesses of } Z \text{ hydrogen atoms and } N \text{ neutrons} \\
& - \; a_{\text{v}} \left(1 - \kappa_{\text{v}} I^2\right) A && \text{volume energy} \\
& + \; a_{\text{s}} \left(1 - \kappa_{\text{s}} I^2\right) B_1 A^{2/3} && \text{surface energy} \\
& + \; a_0 A^0 && A^0 \text{ energy} \\
& + \; c_1 \frac{Z^2}{A^{1/3}} B_3 && \text{Coulomb energy} \\
& - \; c_4 \frac{Z^{4/3}}{A^{1/3}} && \text{Coulomb exchange correction} \\
& + \; f(k_{\text{f}} r_{\text{p}}) \frac{Z^2}{A} && \text{proton form-factor correction to the Coulomb energy} \\
& - \; c_{\text{a}}(N - Z) && \text{charge-asymmetry energy} \\
& + \; W \left(|I| + \begin{cases} 1/A \; , & Z \text{ and } N \text{ odd and equal} \\ 0 \; , & \text{otherwise} \end{cases} \right) && \text{Wigner energy} \\
& + \begin{cases} \overline{\Delta}_{\text{p}} + \overline{\Delta}_{\text{n}} - \delta_{\text{np}} \; , & Z \text{ and } N \text{ odd} \\ \overline{\Delta}_{\text{p}} \; , & Z \text{ odd and } N \text{ even} \\ \overline{\Delta}_{\text{n}} \; , & Z \text{ even and } N \text{ odd} \\ 0 \; , & Z \text{ and } N \text{ even} \end{cases} && \text{average pairing energy} \\
& - \; a_{\text{el}} Z^{2.39} && \text{energy of bound electrons}
\end{aligned}
\tag{62}
$$

This expression differs from the corresponding one used in our earlier calculations [1,2] only in the form of the average pairing energy appearing in the next-to-last term. For the average neutron pairing gap $\overline{\Delta}_{\text{n}}$, average proton pairing gap $\overline{\Delta}_{\text{p}}$, and average neutron-proton interaction energy δ_{np} we now use [9,24,42]

$$\overline{\Delta}_{\text{n}} = \frac{r_{\text{mac}} B_{\text{s}}}{N^{1/3}} \tag{63}$$

$$\overline{\Delta}_{\text{p}} = \frac{r_{\text{mac}} B_{\text{s}}}{Z^{1/3}} \tag{64}$$

$$\delta_{\text{np}} = \frac{h}{B_{\text{s}} A^{2/3}} \tag{65}$$

The zero reference point for the pairing energy now corresponds to even-even nuclei rather than to halfway between even-even and odd-odd nuclei.

In the above expressions the quantities c_1 and c_4 are defined in terms of the electronic charge e and the nuclear-radius constant r_0 by

$$\begin{aligned} c_1 &= \frac{3}{5}\frac{e^2}{r_0} \\ c_4 &= \frac{5}{4}\left(\frac{3}{2\pi}\right)^{2/3} c_1 \end{aligned} \tag{66}$$

The quantity f appearing in the proton form-factor correction to the Coulomb energy is given by

$$f(k_{\rm F}r_{\rm p}) = -\frac{1}{8}\frac{{r_{\rm p}}^2 e^2}{{r_0}^3}\left[\frac{145}{48} - \frac{327}{2880}(k_{\rm F}r_{\rm p})^2 + \frac{1527}{1209600}(k_{\rm F}r_{\rm p})^4\right] \tag{67}$$

where the Fermi wave number is

$$k_{\rm F} = \left(\frac{9\pi Z}{4A}\right)^{1/3}\frac{1}{r_0} \tag{68}$$

The relative neutron excess I is

$$I = \frac{N-Z}{N+Z} = \frac{N-Z}{A} \tag{69}$$

The relative surface energy $B_{\rm s}$, which is the ratio of the surface area of the nucleus at the actual shape to the surface area of the nucleus at the spherical shape, is given by

$$B_{\rm s} = \frac{A^{-2/3}}{4\pi {r_0}^2}\int_S dS \tag{70}$$

The quantity B_1 is the relative generalized surface or nuclear energy in a model that accounts for the effect of the finite range of the nuclear force. It is given by

$$B_1 = \frac{A^{-2/3}}{8\pi^2 {r_0}^2 a^4}\int\!\!\int_V \left(2 - \frac{|\mathbf{r}-\mathbf{r}'|}{a}\right)\frac{e^{-|\mathbf{r}-\mathbf{r}'|/a}}{|\mathbf{r}-\mathbf{r}'|/a} d^3r\, d^3r' \tag{71}$$

The relative Coulomb energy B_3 is given by

$$B_3 = \frac{15}{32\pi^2}\frac{A^{-5/3}}{{r_0}^5}\int\!\!\int_V \frac{d^3r\, d^3r'}{|\mathbf{r}-\mathbf{r}'|}\left[1 - \left(1 + \frac{1}{2}\frac{|\mathbf{r}-\mathbf{r}'|}{a_{\rm den}}\right)e^{-|\mathbf{r}-\mathbf{r}'|/a_{\rm den}}\right] \tag{72}$$

For spherical shapes the quantities B_1 and B_3 can be evaluated analytically. With

$$x_0 = \frac{r_0 A^{1/3}}{a} \quad \text{and} \quad y_0 = \frac{r_0 A^{1/3}}{a_{\rm den}} \tag{73}$$

one obtains

$$\begin{aligned} B_1^{(0)} &= 1 - \frac{3}{{x_0}^2} + (1+x_0)\left(2 + \frac{3}{x_0} + \frac{3}{{x_0}^2}\right)e^{-2x_0} \\ B_3^{(0)} &= 1 - \frac{5}{{y_0}^2}\left[1 - \frac{15}{8y_0} + \frac{21}{8{y_0}^3} - \frac{3}{4}\left(1 + \frac{9}{2y_0} + \frac{7}{{y_0}^2} + \frac{7}{2{y_0}^3}\right)e^{-2y_0}\right] \end{aligned} \tag{74}$$

The expression B_3 for the relative Coulomb energy yields the energy for an arbitrarily shaped, homogeneously charged, diffuse-surface nucleus to all orders in the diffuseness constant $a_{\rm den}$. The constants in front of the integrals for B_1 and B_3 have been chosen so that B_1 and B_3 are 1 for a sphere in the limit in which the range a and diffuseness $a_{\rm den}$ are zero, in analogy with the definition of the quantities $B_{\rm s}$ and $B_{\rm C}$ in the standard liquid-drop model.

2.6 Values of FRLDM macroscopic-model constants

The constants appearing in the expression for the finite-range liquid-drop macroscopic model fall into four categories. The first category, which represents fundamental constants, includes [1,2]

M_{H}	=	7.289034 MeV	hydrogen-atom mass excess
M_{n}	=	8.071431 MeV	neutron mass excess
e^2	=	1.4399764 MeV fm	electronic charge squared

The second category, which represents constants that have been determined from considerations other than nuclear masses, includes [1,2]

a_{el}	=	1.433×10^{-5} MeV	electronic-binding constant
r_{p}	=	0.80 fm	proton root-mean-square radius
r_0	=	1.16 fm	nuclear-radius constant
a	=	0.68 fm	range of Yukawa-plus-exponential potential
a_{den}	=	0.70 fm	range of Yukawa function used to generate nuclear charge distribution

The third category, representing those constants whose values were obtained from consideration of odd-even mass differences [9,24,42] and other mass-like quantities, are

r_{mac}	=	4.80 MeV	average pairing-gap constant
h	=	6.6 MeV	neutron-proton interaction constant
W	=	30 MeV	Wigner constant

It should be noted that the final calculated mass excess is strictly independent of the value used for r_{mac}. This constant affects only the division of the mass excess between the macroscopic part and the remaining microscopic correction. We therefore do not include r_{mac} when we later count the number of constants in our mass model. It is the pairing constant r_{mic} which enters the microscopic model that affects the mass excess. It will be discussed below.

Since $\mu_{\mathrm{th}} = 0$ in our case, Eqs. (6) and (8) can be solved with the experimental data set of 1654 masses with $Z \geq 8$ and $N \geq 8$ [45] and 28 fission-barrier heights to determine the remaining macroscopic constants and the error of our model. To present all the macroscopic model constants together we list them here but discuss their adjustment later. These constants are

a_{v}	=	16.00126 MeV	volume-energy constant
κ_{v}	=	1.92240 MeV	volume-asymmetry constant
a_{s}	=	21.18466 MeV	surface-energy constant
κ_{s}	=	2.345 MeV	surface-asymmetry constant
a_0	=	2.615 MeV	A^0 constant
c_{a}	=	0.10289 MeV	charge-asymmetry constant

The resulting error in the FRLDM is $\sigma_{\mathrm{th}} = 0.779$ MeV.

2.7 Microscopic model

The shell-plus-pairing correction $E_{\mathrm{s+p}}(Z, N, \mathrm{shape})$ is the sum of the proton shell-plus-pairing correction and the neutron shell-plus-pairing correction, namely

$$E_{\mathrm{s+p}}(Z, N, \mathrm{shape}) = E_{\mathrm{s+p}}^{\mathrm{prot}}(Z, \mathrm{shape}) + E_{\mathrm{s+p}}^{\mathrm{neut}}(N, \mathrm{shape}) \tag{75}$$

We give here the equations for the neutron shell-plus-pairing correction. Completely analogous expressions hold for protons. We have

$$E_{\rm s+p}^{\rm neut}(N,{\rm shape}) = E_{\rm shell}^{\rm neut}(N,{\rm shape}) + E_{\rm pair}^{\rm neut}(N,{\rm shape}) \tag{76}$$

Both terms are evaluated from a set of calculated single-particle levels. As before, the shell correction is calculated by use of Strutinsky's method [25,26]. Thus

$$E_{\rm shell}^{\rm neut}(N,{\rm shape}) = \sum_{i=1}^{N} e_i - \widetilde{E}^{\rm neut}(N,{\rm shape}) \tag{77}$$

where e_i are calculated single-particle energies and $\widetilde{E}^{\rm neut}(N,{\rm shape})$ is the smooth single-particle energy sum calculated in the Strutinsky method. The pairing correction is the difference between the pairing correlation energy and the average pairing correlation energy, namely

$$E_{\rm pair}^{\rm neut}(N,{\rm shape}) = E_{\rm p.c.}^{\rm neut}(N,{\rm shape}) - \widetilde{E}_{\rm p.c.}^{\rm neut}(N,{\rm shape}) \tag{78}$$

where $E_{\rm p.c.}^{\rm neut}(N,{\rm shape})$ is given by Eq. (103) below and $\widetilde{E}_{\rm p.c.}^{\rm neut}(N,{\rm shape})$ is given by Eq. (110) below. For the pairing correction we now use the Lipkin-Nogami [21–23] version of the BCS method, which takes into account the lowest-order correction to the total energy of the system associated with particle-number fluctuation.

The single-particle potential felt by a nucleon is given by

$$V = V_1 + V_{\rm s.o.} + V_{\rm C} \tag{79}$$

The first term is the spin-independent nuclear part of the potential, which is calculated in terms of the folded-Yukawa potential

$$V_1(\mathbf{r}) = -\frac{V_0}{4\pi {a_{\rm pot}}^3}\int_{\rm V} \frac{e^{-|\mathbf{r}-\mathbf{r}'|/a_{\rm pot}}}{|\mathbf{r}-\mathbf{r}'|/a_{\rm pot}} d^3r' \tag{80}$$

where the integration is over the volume of the generating shape, whose volume is held fixed at $\frac{4}{3}\pi {R_{\rm pot}}^3$ as the shape is deformed. The potential radius $R_{\rm pot}$ is given by

$$R_{\rm pot} = R_{\rm den} + A_{\rm den} - B_{\rm den}/R_{\rm den} \tag{81}$$

with

$$R_{\rm den} = r_0 A^{1/3}(1+\overline{\epsilon}) \tag{82}$$

Values of the model constants $A_{\rm den}$ and $B_{\rm den}$ will be given later. The potential depth $V_{\rm p}$ for protons and potential depth $V_{\rm n}$ for neutrons are given by

$$V_{\rm p} = V_{\rm s} + V_{\rm a}\overline{\delta} \tag{83}$$

$$V_{\rm n} = V_{\rm s} - V_{\rm a}\overline{\delta} \tag{84}$$

The average bulk nuclear asymmetry $\overline{\delta}$ appearing in Eqs. (83) and (84) and average relative deviation $\overline{\epsilon}$ in the bulk of the density appearing in Eq. (82) are given by the droplet model and thus depend on the values of the droplet-model constants. The FRDM macroscopic constants are determined in a nonlinear least-squares adjustment, which requires about 1000 steps to find the optimum constants. In principle, these constants should then be used in the determination of the single-particle potential, the potential-energy surfaces should be recalculated with the new constants, a new mass calculation should be performed, and a new set of macroscopic constants should be determined, with this iteration repeated until convergence. Because the calculation of potential-energy surfaces is extremely time-consuming, only one iteration has been performed.

Furthermore, in determining the single-particle potential we have used the following early forms[50] of the droplet model expressions for $\bar{\delta}$ and $\bar{\epsilon}$:

$$\bar{\delta} = \left(I + \frac{3}{8}\frac{c_1}{Q}\frac{Z^2}{A^{5/3}} \right) / \left(1 + \frac{9}{4}\frac{J}{Q}\frac{1}{A^{1/3}} \right) \tag{85}$$

$$\bar{\epsilon} = \left(-\frac{2a_2}{A^{1/3}} + L\bar{\delta}^2 + c_1 \frac{Z^2}{A^{4/3}} \right) / K \tag{86}$$

The range

$$a_{\rm pot} = 0.8 \text{ fm} \tag{87}$$

of the Yukawa function in Eq. (80) has been determined from an adjustment of calculated single-particle levels to experimental data in the rare-earth and actinide regions[34]. It is kept constant for nuclei throughout the periodic system.

The spin-orbit potential is given by the expression

$$V_{\rm s.o.} = -\lambda \left(\frac{\hbar}{2m_{\rm nuc}c} \right)^2 \frac{\boldsymbol{\sigma} \cdot \nabla V_1 \times \boldsymbol{p}}{\hbar} \tag{88}$$

where λ is the spin-orbit interaction strength, $m_{\rm nuc}$ is the nucleon mass, $\boldsymbol{\sigma}$ represents the Pauli spin matrices, and $\boldsymbol{p}$ is the nucleon momentum.

The spin-orbit strength has been determined from adjustments to experimental levels in the rare-earth and actinide regions. It has been shown[1,14,34] that many nuclear properties throughout the periodic system are well reproduced with λ given by a function linear in A through the values determined in these two regions. This gives

$$\lambda_{\rm p} = 6.0 \left(\frac{A}{240} \right) + 28.0 = 0.025A + 28.0 = k_{\rm p}A + l_{\rm p} \tag{89}$$

for protons and

$$\lambda_{\rm n} = 4.5 \left(\frac{A}{240} \right) + 31.5 = 0.01875A + 31.5 = k_{\rm n}A + l_{\rm n} \tag{90}$$

for neutrons.

Finally, the Coulomb potential for protons is given by

$$V_{\rm C}(\mathbf{r}) = e\rho_{\rm c} \int_{\rm V} \frac{d^3r'}{|\mathbf{r} - \mathbf{r}'|} \tag{91}$$

where the charge density $\rho_{\rm c}$ is given by

$$\rho_{\rm c} = \frac{Ze}{\frac{4}{3}\pi A {r_0}^3} \tag{92}$$

The number of basis functions used in our calculations is

$$N_{\rm bas} = 12 \tag{93}$$

The overall curvature of the basis functions is chosen to yield

$$\hbar\omega_0 = C_{\rm cur}/A^{1/3} \tag{94}$$

with

$$C_{\rm cur} = 41 \ \text{MeV} \tag{95}$$

2.8 Microscopic pairing models

Because of its basic simplicity, the BCS pairing model [51–54] has been the pairing model of choice in most previous nuclear-structure calculations [1,2,29,55]. However, a well-known deficiency of the BCS model is that for large spacings between the single-particle levels at the Fermi surface, no non-trivial solutions exist. In practical applications, these situations occur not only at magic numbers, but also, for example, for deformed actinide nuclei at neutron numbers $N = 142$ and 152. By taking into account effects associated with particle-number fluctuations, the Lipkin-Nogami approximation [21–23] goes beyond the BCS approximation and avoids such collapses.

In solving the pairing equations for neutrons or protons in either the BCS or Lipkin-Nogami model, we consider a constant pairing interaction G acting between $N_2 - N_1 + 1$ doubly degenerate single-particle levels, which are occupied by $N_{\rm int}$ nucleons. This interaction interval starts at level N_1, located below the Fermi surface, and ends at level N_2, located above the Fermi surface. With the definitions we use here, the levels are numbered consecutively starting with number 1 for the level at the bottom of the well. Thus, for even particle numbers, the last occupied levels in the neutron and proton wells are $N/2$ and $Z/2$, respectively.

The level pairs included in the pairing calculation are often chosen symmetrically around the Fermi surface. However, for spherical nuclei it is more reasonable to require that degenerate spherical states have equal occupation probability. This condition cannot generally be satisfied simultaneously with a symmetric choice of levels in the interaction region. We therefore derive the pairing equations below for the more general case of arbitrary N_1 and N_2.

In the Lipkin-Nogami pairing model [21–23] the pairing gap Δ, Fermi energy λ, number-fluctuation constant λ_2, occupation probabilities ${v_k}^2$, and shifted single-particle energies ϵ_k are determined from the $2(N_2 - N_1) + 5$ coupled nonlinear equations

$$N_{\rm tot} = 2 \sum_{k=N_1}^{N_2} {v_k}^2 + 2(N_1 - 1) \tag{96}$$

$$\frac{2}{G} = \sum_{k=N_1}^{N_2} \frac{1}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}} \tag{97}$$

$${v_k}^2 = \frac{1}{2}\left[1 - \frac{\epsilon_k - \lambda}{\sqrt{(\epsilon_k - \lambda)^2 + \Delta^2}}\right], \quad k = N_1, N_1 + 1, \ldots, N_2 \tag{98}$$

$$\epsilon_k = e_k + (4\lambda_2 - G){v_k}^2, \quad k = N_1, N_1 + 1, \ldots, N_2 \tag{99}$$

$$\lambda_2 = \frac{G}{4}\left[\frac{\left(\sum_{k=N_1}^{N_2} {u_k}^3 v_k\right)\left(\sum_{k=N_1}^{N_2} u_k {v_k}^3\right) - \sum_{k=N_1}^{N_2} {u_k}^4 {v_k}^4}{\left(\sum_{k=N_1}^{N_2} {u_k}^2 {v_k}^2\right)^2 - \sum_{k=N_1}^{N_2} {u_k}^4 {v_k}^4}\right] \tag{100}$$

where

$${u_k}^2 = 1 - {v_k}^2 \ , \quad k = N_1, N_1 + 1, \ldots, N_2 \tag{101}$$

The quasi-particle energies E_k of the odd nucleon in an odd-A nucleus are now given by [22]

$$E_k = \left[(\epsilon_k - \lambda)^2 + \Delta^2\right]^{1/2} + \lambda_2, \quad k = N_1, N_1 + 1, \ldots, N_2 \tag{102}$$

In the Lipkin-Nogami model it is the sum $\Delta + \lambda_2$ that is identified with odd-even mass differences [22]. We denote this sum by $\Delta_{\rm LN}$.

The pairing-correlation energy plus quasi-particle energy in the Lipkin-Nogami model is given by

$$E_{\mathrm{p.c.}} = \sum_{k=N_1}^{N_2} (2{v_k}^2 - n_k)e_k - \frac{\Delta^2}{G} - \frac{G}{2}\sum_{k=N_1}^{N_2}(2{v_k}^4 - n_k) - 4\lambda_2 \sum_{k=N_1}^{N_2} {u_k}^2{v_k}^2 + E_i\theta_{\mathrm{odd},N_{\mathrm{tot}}} \tag{103}$$

where e_k are the single-particle energies and n_k, with values 2, 1, or 0, specify the sharp distribution of particles in the absence of pairing. The quasi-particle energy E_i for the odd particle occupying level i is given by Eq. (102), and $\theta_{\mathrm{odd},N_{\mathrm{tot}}}$ is unity if N_{tot} is odd and zero if N_{tot} is even.

2.9 Effective-interaction pairing-gap models

In microscopic pairing calculations the pairing strength G for neutrons and protons can be obtained from effective-interaction pairing gaps $\Delta_{G_{\mathrm{n}}}$ and $\Delta_{G_{\mathrm{p}}}$ given by [9]

$$\Delta_{G_{\mathrm{n}}} = \frac{r_{\mathrm{mic}}B_{\mathrm{s}}}{N^{1/3}} \tag{104}$$

$$\Delta_{G_{\mathrm{p}}} = \frac{r_{\mathrm{mic}}B_{\mathrm{s}}}{Z^{1/3}} \tag{105}$$

The dependence of the pairing strength G on the corresponding effective-interaction pairing gap Δ_G is obtained from the microscopic equations by assuming a constant level density for the average nucleus in the vicinity of the Fermi surface. This allows the sums in the equations to be replaced by integrals. The average level density of doubly degenerate levels is taken to be

$$\widetilde{\rho} = \frac{1}{2}\widetilde{g}(\widetilde{\lambda}) \tag{106}$$

where $\widetilde{g}$ is the smooth level density that is obtained in Strutinsky's shell-correction method and $\widetilde{\lambda}$ is the Fermi energy of the smoothed single-particle energy [29,56]. Thus, we can make the substitution

$$\sum_{k=N_1}^{N_2} f(e_k - \lambda) \Longrightarrow \widetilde{\rho}\int_{y_1}^{y_2} f(x)dx \tag{107}$$

where

$$\begin{aligned} y_1 &= \frac{-\frac{1}{2}N_{\mathrm{tot}} + N_1 - 1}{\widetilde{\rho}} \\ y_2 &= \frac{-\frac{1}{2}N_{\mathrm{tot}} + N_2}{\widetilde{\rho}} \end{aligned} \tag{108}$$

The gap equation (97) can now be evaluated for an *average* nucleus, with the result

$$\begin{aligned} \frac{1}{G} &= \frac{1}{2}\widetilde{\rho}\int_{y_1}^{y_2}\frac{dx}{\sqrt{x^2+{\Delta_G}^2}} \\ &= \frac{1}{2}\widetilde{\rho}\left[\ln\left(\sqrt{{y_2}^2+{\Delta_G}^2}+y_2\right) - \ln\left(\sqrt{{y_1}^2+{\Delta_G}^2}+y_1\right)\right] \end{aligned} \tag{109}$$

From this expression, the pairing strength G in the BCS model can be determined in any region of the nuclear chart.

The same expression may also be used in the Lipkin-Nogami case, but some reinterpretations are necessary. It is now the energies ϵ_k occurring in Eq. (97) that are assumed to be equally spaced. These are not precisely the single-particle energies e_k but are related to them by Eq. (99). Thus, in order for ϵ_k to be equally spaced, the single-particle energies e_k must be shifted downward by the amounts $(4\lambda_2 - G){v_k}^2$. Since the occupation probability ${v_k}^2$ is approximately unity far below the Fermi surface and zero far above, the corresponding single-particle energy distribution is approximately uniform far above and far below the Fermi surface but spread apart by the additional amount $4\lambda_2 - G$ close to the Fermi surface. Although this decrease in level density near the Fermi surface is accidental, it is in approximate accord with the ground-state structure of real nuclei, since the increased stability associated with ground-state configurations is due to low level densities near the Fermi surface[24,56].

In the Lipkin-Nogami model, it is the quantity $\Delta + \lambda_2$ that is associated with odd-even mass differences, whereas in the BCS model it is Δ only that should be directly compared to the experimental data. This leads to the expectation that there is a related difference between $\Delta_G^{\rm LN}$ and $\Delta_G^{\rm BCS}$, the effective-interaction pairing gaps associated with the LN and BCS models, respectively. Since we determine the constants of the model for $\Delta_G^{\rm LN}$ directly from least-squares minimization, it is not necessary to specify exactly such a relationship. However, the above observation is of value as a rough rule of thumb, and to remind us to expect that the effective-interaction pairing gaps in the BCS and LN models are of somewhat different magnitude.

The expression for the *average* pairing correlation energy plus quasi-particle energy $\widetilde{E}_{\rm p.c.}$ in the Lipkin-Nogami model is obtained in a similar manner as the expression for the pairing matrix element G. For the average pairing correlation energy plus quasi-particle energy in the Lipkin-Nogami model we then obtain

$$\begin{aligned}\widetilde{E}_{\rm p.c.} \;=\;& \frac{1}{2}\widetilde{\rho}\left[(y_2 - G)\left(y_2 - \sqrt{{y_2}^2 + {\Delta_G}^2}\right) + (y_1 - G)\left(y_1 + \sqrt{{y_1}^2 + {\Delta_G}^2}\right)\right] \\ & + \frac{1}{4}(G - 4\widetilde{\lambda}_2)\widetilde{\rho}\Delta_G\left[\tan^{-1}\left(\frac{y_2}{\Delta_G}\right) - \tan^{-1}\left(\frac{y_1}{\Delta_G}\right)\right] + \overline{\Delta}\theta_{{\rm odd},N_{\rm tot}} \qquad (110)\end{aligned}$$

where the average pairing gap $\overline{\Delta}$ is given by Eqs. (41) and (42) or Eqs. (63) and (64).

The expression for $\widetilde{\lambda}_2$ for an average nucleus is fairly lengthy. It is given by

$$\widetilde{\lambda}_2 = \frac{G}{4}\left(\frac{A - C}{B - C}\right) \qquad (111)$$

where

$$\begin{aligned}A \;&=\; \left(\frac{\widetilde{\rho}\Delta_G}{4}\right)^2\left\{\left(\frac{2}{G\widetilde{\rho}}\right)^2 - \left[\ln\left(\frac{\sqrt{{y_2}^2 + {\Delta_G}^2}}{\sqrt{{y_1}^2 + {\Delta_G}^2}}\right)\right]^2\right\} \\ B \;&=\; \frac{{\Delta_G}^2\widetilde{\rho}^2}{16}\left[\tan^{-1}\left(\frac{y_2}{\Delta_G}\right) - \tan^{-1}\left(\frac{y_1}{\Delta_G}\right)\right]^2 \\ C \;&=\; \frac{\widetilde{\rho}\Delta_G}{32}\left[\Delta_G\left(\frac{y_2}{{y_2}^2 + {\Delta_G}^2} - \frac{y_1}{{y_1}^2 + {\Delta_G}^2}\right) + \tan^{-1}\left(\frac{y_2}{\Delta_G}\right) - \tan^{-1}\left(\frac{y_1}{\Delta_G}\right)\right] \qquad (112)\end{aligned}$$

One should note that the pairing strength G depends on the interval (N_1, N_2) over which the pairing force is active. However, in our formulation we do not use G as a primary constant. Instead, we use the effective-interaction pairing gaps $\Delta_{G_{\rm n}}$ and $\Delta_{G_{\rm p}}$, which are independent of the choice of interaction interval (N_1, N_2). We choose the pairing interaction interval so that at least all levels up to 5 MeV above the Fermi surface are included. It has sometimes been asked whether particles scattered into the continuum by the pairing force would escape from the nucleus if the interaction interval includes unbound states. Of course not! The superfluid state is the *most bound* configuration. The single-particle picture does not give the true nuclear ground or excited states; it only serves as the set of basis functions for the pairing calculation. Instead, the quasi-particle energies obtained in the pairing calculation represent a subset of all possible excited states. If, in an excited nucleus, the quasi-particle energies are lower than the particle separation energies no nucleons escape.

2.10 Shell correction

The Strutinsky shell-correction method [25,26] requires two additional constants, the order p and the range $\gamma_{\rm S}$. The shell correction should be insensitive to these quantities within a certain range of values. Their values can therefore be determined in principle by requiring the plateau condition to be fulfilled. We have found that for heavy nuclei this condition is indeed fulfilled, with the shell correction for nuclear ground-state shapes insensitive to the values of these two constants. However, for light nuclei this is no longer the case. Here the shell correction may vary by several MeV for a reasonable range of values of the range $\gamma_{\rm S}$. Moreover, the shell correction often does not exhibit any plateau. This probably indicates a gradual breakdown of the shell-correction method as one approaches the very lightest region of nuclei, where the number of single-particle levels is small.

In the present calculation we choose

$$p = 8 \tag{113}$$

for the order in the Strutinsky shell-correction method. The corresponding range $\gamma_{\rm S}$ is given by

$$\gamma_{\rm S} = C_{\rm S}\hbar\omega_0 B_{\rm s} \tag{114}$$

with

$$C_{\rm S} = 1.0 \tag{115}$$

and $B_{\rm s}$ given by Eq. (70). This choice lowers the error of the mass model to 0.669 MeV from 0.734 MeV obtained with the same range coefficient but no dependence on surface area in a sixth-order correction.

The version of the Strutinsky method [25,26] that we use here was originally proposed for infinite single-particle wells. For finite wells the calculated shell correction diverges to $+\infty$ as the number of basis functions approaches $+\infty$. This difficulty is avoided by using only a limited number of basis functions. It has been found that the calculated shell correction is approximately independent of $N_{\rm bas}$ in the range $8 \lesssim N_{\rm bas} \lesssim 13$ [29].

One may expect the Strutinsky method to be less accurate for light nuclei than for heavy nuclei because the smooth, average quantities calculated in the Strutinsky method are less accurately determined from the few levels occurring in light nuclei. One could also ask if the method is less accurate near the drip lines than close to β stability because the truncated single-particle level spectrum that we use deviates more from a realistic single-particle spectrum near the drip lines than near β-stable nuclei. Below, where we study the reliability of the model for light nuclei and for nuclei far from β stability, we find that the model error does indeed grow as the size of the nuclear system decreases. However, we find no obvious increase in the model error for today's known nuclei that are the furthest from β stability. The reliability of the Strutinsky method for the folded-Yukawa single-particle potential is further discussed in the appendix of Ref. 29.

2.11 Zero-point energy

As a final step in the calculation of nuclear ground-state masses a zero-point energy is added to the calculated potential energy at the ground-state shape. As mentioned above, we now add only a zero-point energy for the fission, or ϵ_2, mode. In the harmonic approximation this zero-point energy E_{zp} is given by

$$E_{\mathrm{zp}} = \frac{1}{2}\hbar\omega_\epsilon \tag{116}$$

where

$$\omega_\epsilon = (C_\epsilon/B_\epsilon)^{1/2} \tag{117}$$

Here C_ϵ is the potential-energy stiffness constant and B_ϵ is the inertia associated with motion in the ϵ_2 direction. Details of their calculation are given in Ref. 1. The angular frequency ω_ϵ is related to that corresponding to irrotational flow by

$$\omega_\epsilon = \mathcal{K}\omega_\epsilon^{\mathrm{ir}} \tag{118}$$

The constant $\mathcal{K}$ has been previously determined by requiring that for a spherical shape the inertia B_ϵ equal the inertia determined from an adjustment to spontaneous-fission half-lives for actinide nuclei [1,57].

2.12 Values of microscopic-model constants

The constants appearing in the expressions occurring in the microscopic shell-plus-pairing calculation fall into four categories. The first category, which represents fundamental constants, includes

m_{nuc}	=	938.90595 MeV	nucleon mass
$\hbar c$	=	197.32891 MeV fm	Planck's constant multiplied by the speed of light and divided by 2π
e^2	=	1.4399764 MeV fm	electronic charge squared

The electronic charge squared has already been counted among the macroscopic constants.

The second category, which represents constants that have been determined from considerations other than nuclear masses, includes [1,2,29]

C_{cur}	=	41 MeV	basis curvature constant
V_{s}	=	52.5 MeV	symmetric potential-depth constant
V_{a}	=	48.7 MeV	asymmetric potential-depth constant
A_{den}	=	0.82 fm	potential radius correction constant
B_{den}	=	0.56 fm^2	potential radius curvature-correction constant
a_{pot}	=	0.8 fm	potential diffuseness constant
k_{p}	=	0.025	proton spin-orbit A coefficient
l_{p}	=	28.0	proton spin-orbit constant
k_{n}	=	0.01875	neutron spin-orbit A coefficient
l_{n}	=	31.5	neutron spin-orbit constant
$\mathcal{K}$	=	0.33	zero-point-energy constant

The third category, representing those constants whose values were obtained from consideration of mass-like quantities, are

N_{bas}	=	12	number of basis functions
p	=	8	order of Strutinsky shell correction
C_{S}	=	1.0	Strutinsky range coefficient

The fourth category, representing those constants whose values were obtained from a least-squares adjustment simultaneously with the macroscopic constants of the FRDM, includes only one microscopic constant, namely

$r_{\rm mic}$	=	3.2 MeV	LN effective-interaction pairing-gap constant

In addition, the following droplet-model constants, which have been determined in an earlier study [50], are used in the expressions for the *average* bulk nuclear asymmetry $\overline{\delta}$ and *average* relative deviation $\overline{\epsilon}$ in the bulk density that are used to calculate $V_{\rm p}$, $V_{\rm n}$, and $R_{\rm den}$ in Eqs. (83), (84), and (82), respectively:

a_2	=	22.00 MeV	surface-energy constant
J	=	35 MeV	symmetry-energy constant
L	=	99 MeV	density-symmetry constant
Q	=	25 MeV	effective surface-stiffness constant
K	=	300 MeV	compressibility constant
r_0	=	1.16 fm	nuclear-radius constant

Insertion of these values and the value of e^2 on which c_1 depends in Eqs. (85) and (86) leads to

$$\overline{\delta} = \frac{(N-Z)/A + 0.0112 Z^2/A^{5/3}}{1 + 3.15/A^{1/3}} \tag{119}$$

$$\overline{\epsilon} = -\frac{0.147}{A^{1/3}} + 0.330\overline{\delta}^2 + \frac{0.00248 Z^2}{A^{4/3}} \tag{120}$$

One could in principle carry through the iterations discussed above to obtain a consistent set of droplet-model constants for the macroscopic part and for the single-particle potential, but the required computational effort would be extensive. However, the value of r_0 is precisely the same as that used in the macroscopic model.

3 Enumeration of constants

It is always of interest to have a clear picture of exactly what constants enter a model. Naturally, anyone who sets out to verify a calculation by others or uses a model for new applications needs a complete specification of the model, for which a full specification of the constants and their values is an essential part. Also, when different models are compared it is highly valuable to fully understand exactly what constants enter the models. Unfortunately, discussions of model constants are often incomplete, misleading, and/or erroneous. For example, in Table A of Ref. 58 the number of parameters of the mass model of Spanier and Johansson [59] is listed as 12. However, in the article [59] by Spanier and Johansson the authors themselves list in their Table A 30 parameters plus 5 magic numbers that are not calculated within the mass model and must therefore be considered parameters, for a total of at least 35 parameters.

We specify here *all* the constants that enter our model, rather than just those that in the final step are adjusted to experimental data by a least-squares procedure. We also include such constants as the number of basis functions used and fundamental constants like the electronic charge and Planck's constant.

Table 1: Constants in the FRDM. The third column gives the number of constants adjusted to nuclear masses or mass-like quantities such as odd-even mass differences or fission-barrier heights. The fourth column gives the number of constants determined from other considerations.

Constants	Comment	Mass-like	Other
M_{H}, M_{n}, e^2	Macroscopic fundamental constants	0	3
a_{el}, r_0, r_{p}, a, a_{den}, K	Macroscopic constants from considerations other than mass-like data	0	6
L, a_3, W, h	Macroscopic constants obtained in prior adjustments to mass-like data	4	0
a_1, a_2, J, Q, a_0, C, γ, c_{a}	Macroscopic constants determined by current least-squares adjustments	8	0
$\hbar c$, m_{nuc}	Microscopic fundamental constants	0	2
V_{s}, V_{a}, A_{den}, B_{den}, C_{cur}, k_{p}, l_{p}, k_{n}, l_{n}, a_{pot}, $\mathcal{K}$	Microscopic constants	0	11
N_{bas}, p, C_{S}	Microscopic constants determined from considerations of mass-like quantities	3	0
r_{mic}	Microscopic constant determined by current least-squares adjustments	1	0
a_1, a_2, J, K, L, Q	Droplet-model constants that enter the single-particle potential (see discussion in text)	0	0
Subtotals		16	22
Total			38

3.1 Constants in the FRDM

The discussion in the previous section allows us to enumerate the constants in the FRDM model in Table 1. From this list we see that the macroscopic-microscopic method requires relatively few constants. One feature of the model gives rise to a small complication when counting the number of constants. Droplet-model constants occur also in the determination of the single-particle potential. However, a different set of constants is used here because, as discussed above, one does not know what the optimum values are until the calculation has been completed. In principle, the calculation should be repeated with the new droplet-model constants defining the single-particle potential until convergence is obtained. In Table 1 we have counted the number of constants as if this procedure had been carried out.

However, since the droplet-model constants used in the present calculations are different in the microscopic part and in the macroscopic part, different counting schemes could also be employed. Since the droplet-model constants used in the microscopic expressions are obtained from four primary constants [50] and nuclear masses were used only to give rough estimates of these constants, one may not wish to regard them as determined from mass-like quantities. One of the four primary constants is the nuclear radius constant r_0, which has the same value as we use in our macroscopic model. Therefore, only three remain that could be considered as additional FRDM constants. With this classification scheme the number of constants adjusted

Table 2: Constants in the FRLDM. The third column gives the number of constants adjusted to nuclear masses or mass-like quantities such as odd-even mass differences or fission-barrier heights. The fourth column gives the number of constants determined from other considerations.

Constants	Comment	Mass-like	Other
M_{H}, M_{n}, e^2	Macroscopic fundamental constants	0	3
a_{el}, r_0, r_{p}, a, a_{den}	Macroscopic constants from considerations other than mass-like data	0	5
W, h	Macroscopic constants obtained in prior adjustments to mass-like data	2	0
a_{v}, κ_{v}, a_{s}, κ_{s}, a_0, c_{a}	Macroscopic constants determined by current least-squares adjustments	6	0
$\hbar c$, m_{nuc}	Microscopic fundamental constants	0	2
V_{s}, V_{a}, A_{den}, B_{den}, C_{cur}, k_{p}, l_{p}, k_{n}, l_{n}, a_{pot}, $\mathcal{K}$	Microscopic constants	0	11
N_{bas}, p, C_{S}, r_{mic}	Microscopic constants determined from considerations of mass-like quantities	4	0
a_1, a_2, J, K, L, Q	Droplet-model constants that enter the single-particle potential (see discussion in text)	3	0
Subtotals		15	21
Total			36

to mass-like quantities remains 16 and the total number of constants in the model increases from 38 to 41. Alternatively, if we do count the three primary constants as adjusted to nuclear masses, the total number of FRDM constants is 41, while the number adjusted to mass-like quantities increases from 16 to 19.

3.2 Constants in the FRLDM

The constants in the FRLDM, which are either identical to or similar to the constants in the FRDM, are enumerated in Table 2. We mentioned in the discussion of the FRDM constants that the six constants in the last line of Table 1 would converge to the values of the same constants listed earlier in the table after a sufficient number of iterations. In the FRDM these constants therefore need not be regarded as additional constants. In contrast, in the FRLDM they must be regarded as constants obtained from adjustments to mass-like quantities. However, as mentioned in the discussion of the FRDM constants, these constants are all obtained from three primary constants, so we only include three in this category.

4 Results

4.1 Determination of ground-state shapes and masses

The adjustment of constants in the macroscopic model is simplified enormously because the ground-state shape and fission saddle-point shape are approximately independent of the precise values of these constants when they are varied within a reasonable range[60]. We therefore calculate the ground-state deformation with one set of constants and subsequently determine the various terms in the mass expression at this deformation. The constants of the macroscopic model can then be adjusted, with the nuclear shapes remaining fixed.

A significant advantage of this approach is that the effect of new features can often be investigated without repeating the entire calculation from the beginning, which would take about 100 hours of CRAY-1 CPU time. For example, when we investigated different pairing models and determined the optimum value of the pairing constant, we needed to recalculate only the pairing-energy term for each of the 8979 nuclei in our study. Since we have in the initial part of the calculation determined ground-state shapes and stored the corresponding ground-state single-particle levels for all nuclei on disc, we need only read in the single-particle levels, do the pairing calculation, and readjust the model constants to obtain the effect of a new pairing model or new pairing-model constant. Such a study takes only about 20 minutes of CRAY-1 CPU time.

Our determination of mass-model constants and ground-state nuclear masses involves several steps. We first briefly list these steps and then continue with a more extensive discussion.

1. Potential-energy surfaces are calculated versus ϵ_2 and ϵ_4. In this calculation, which was actually performed already in 1987, the FRLDM as defined in Ref. 3 is used, except that for the pairing calculations the BCS approximation is used instead of the LN approximation. From these potential-energy surfaces the ground-state ϵ_2 and ϵ_4 deformations are determined.

2. The ground-state energy is minimized with respect to ϵ_3 and also with respect to ϵ_6 for fixed values of ϵ_2 and ϵ_4.

3. When the resulting ground-state shapes have been determined, single-particle levels are calculated for each nucleus at the appropriate deformation and stored on disc. The shell-plus-pairing correction is also calculated and stored on disc at this time. The shell-plus-pairing correction is then available for use in the calculation of ground-state masses and in the determination of macroscopic-model constants. It is the only microscopic quantity required for the mass adjustment.

4. Now that the ground-state shapes have been determined, the various shape-dependent functions that occur in the macroscopic energy are evaluated at each appropriate ground-state shape and stored on disc.

5. Analogous steps to those above for masses are carried out also for 28 fission-barrier heights.

6. Least-squares adjustments are now performed, with the nuclear masses weighted 80% and the fission-barrier heights weighted 20%. The macroscopic-model constants are determined and the ground-state masses and the fission barriers are calculated.

7. Finally, when the ground-state shapes and masses and fission-barrier heights are known, other properties such as β-decay half-lives, β-delayed neutron-emission and fission probabilities, and Q values for α decay are calculated.

For the major portion of the potential-energy-surface calculation we have chosen the following grid:

$$\epsilon_2 = -0.50\ (0.05)\ 0.50, \qquad \epsilon_4 = -0.16\ (0.04)\ 0.16 \tag{121}$$

When the ground-state minimum is outside this grid we have used instead the expanded, but less-dense grid:

$$\epsilon_2 = -1.0\ (0.1)\ 1.0, \qquad \epsilon_4 = -0.28\ (0.07)\ 0.28 \tag{122}$$

For large values of ϵ_4 the nuclear shapes develop somewhat unnatural wiggles. These wiggles can be removed and the energy lowered by use of higher multipoles in the specification of the nuclear shape [30,61]. We include in the first step of our calculations one higher multipole, namely ϵ_6. However, since in this step we want to consider only two independent shape coordinates, we determine ϵ_6 at each value of ϵ_2 and ϵ_4 by minimizing the macroscopic potential energy for ^{240}Pu. For heavy nuclei the value of ϵ_6 obtained in such a minimization is approximately independent of the nucleus considered. On the other hand, for very light nuclei minimization with respect to ϵ_6 (and in some cases with respect to ϵ_4) leads to values corresponding to unphysical shapes. These arise because if the distance across a wiggle on the nuclear surface is of the order of the range of the Yukawa-plus-exponential folding function, the nuclear energy increases very little but the Coulomb energy decreases strongly with increasing deformation. For ϵ_6 we avoid this difficulty by minimizing the energy for ^{240}Pu, which is sufficiently large that also with ϵ_6 distortions included the wiggles on the surface are larger than the range of the Yukawa-plus-exponential function. In the light region we avoid unphysical values of ϵ_4 by including only a physical range of values in our grid.

We use the single-particle states of the folded-Yukawa single-particle potential to calculate the shell-plus-pairing corrections at each grid point. Although the constants of the single-particle potential depend on Z and N, for the determination of the ground-state values of ϵ_2 and ϵ_4 we use the same set of calculated levels for a region of neighboring nuclei, since it is too time-consuming to repeat the diagonalization for each value of Z and N. However, when the same levels are used for a moderately large region of nuclei, the shell correction for a magic nucleus calculated in this way may differ by 1 MeV or more from the shell correction calculated with the single-particle potential appropriate to that particular nucleus.

To overcome this difficulty we proceed by first noting that most constants of the single-particle potential have been determined for nuclei close to line of β-stability. Because of this and because the radius of the single-particle potential is one of its most important constants, we reduce the Z and N dependence of the constants of the microscopic model to an A dependence only. We next divide the nuclear chart into regions of suitable size, choosing for each region one set of single-particle constants. The regions are centered about the mass numbers $A = 16$, 20, 40, 60, 80, 100, 120, 140, 160, 180, 200, 220, 240, 260, 280, 300, 320, and 340. The individual values of Z and N for each region are taken to be the closest integers corresponding to Green's approximation [62] to the line of β stability, namely

$$N - Z = \frac{0.4A^2}{A + 200} \tag{123}$$

For each nucleus with a mass number different from one of these central mass numbers we calculate the microscopic corrections for *two* sets of constants. For example, nuclei with $201 \leq A \leq 239$ are included in the $A = 220$ calculation and nuclei with $221 \leq A \leq 259$ are included in the $A = 240$ calculation. To determine $E_{\mathrm{s+p}}$ for, say, a nucleus with $A = 225$ we linearly interpolate on the ϵ_2–ϵ_4 grid in terms of A between the result for $A = 220$ and the result for $A = 240$. We find that such an interpolation gives results that agree to within a few-hundred keV with those obtained with a single-particle potential appropriate to the specific nuclei concerned.

Once the ground-state values of ϵ_2 and ϵ_4 are determined from the minimum of $E_{\mathrm{s+p}}$ in this way, the shell-plus-pairing corrections are recalculated at these ground-state shapes with the exact single-particle potential appropriate to each of the 8979 nuclei. The slight approximation made in calculating the potential-energy surfaces affects only the calculation of the *shape* and has a negligible effect on the final energy.

After the ground-state ϵ_2 and ϵ_4 deformations are determined, we investigate the stability of the ground state with respect to ϵ_3 and ϵ_6 shape degrees of freedom. Rather than simultaneously

Table 3: Determination of the pairing constant r_{mic}. See text for explanation of the listed quantities.

r_{mic} (MeV)	σ_{th} Mass model (MeV)	rms Δ_{LN} (MeV)	rms $\Delta_{\mathrm{th.mass}}$ (MeV)	rms S_{n} (MeV)
3.1	0.6746	0.1740	0.2035	0.409
3.2	0.6694	0.1691	0.2044	0.411
3.3	0.6695	0.1675	0.2091	0.416
3.5	0.6733	0.1745	0.2287	0.432

varying all shape degrees of freedom, we instead vary ϵ_3 and ϵ_6 separately, with ϵ_2 and ϵ_4 held fixed at the values previously determined. When ϵ_3 is varied ϵ_6 is set equal to the value used in the original minimization with respect to ϵ_2 and ϵ_4, and when ϵ_6 is varied ϵ_3 is set equal to zero. The deeper of the two minima obtained in these two minimizations is selected as the ground state. The importance of the ϵ_3 and ϵ_6 shape degrees of freedom is discussed further in Ref. 10. Because surface wiggles should not become too small relative to the range in the Yukawa-plus-exponential function, the ϵ_6 minimization is carried out only for nuclei with $A > 60$.

After the ground-state shapes are determined, the shell-plus-pairing corrections and shape-dependent macroscopic functions are calculated and stored on disc. The programs that use this information to determine the macroscopic-model constants and calculate ground-state masses are then run. Although the least-squares adjustment is a nonlinear one, it takes only a few minutes to find the optimum constant set in an 8-constant variation and to calculate the final mass table. At this point it is relatively simple to investigate alternative model assumptions. As an example, we discuss the results of one such investigation concerning the effect of varying the microscopic pairing constant r_{mic}.

In our earlier pairing-model studies [9] we determined r_{mic} in Eqs. (104) and (105) by minimizing the rms deviation between pairing gaps calculated in the LN model and experimental pairing gaps. An alternative possibility is to find r_{mic} by minimizing the error in the *mass model*. Because our change in the order of the Strutinsky shell correction does influence slightly the pairing calculations through the determination of G from the effective-interaction pairing gap Δ_G, a small change in r_{mic} could in principle be required to obtain an optimum pairing calculation. In a study of how the model error σ_{th} and the rms errors of the Lipkin-Nogami pairing gap Δ_{LN}, the theoretical-mass pairing gap $\Delta_{\mathrm{th.mass}}$, and the neutron separation energy S_{n} depend on r_{mic}, we first calculate the ground-state shell-plus-pairing corrections for several values of r_{mic}. For each of these values we then determine a set of macroscopic-model constants and generate a full-fledged mass table. In this process we also obtain microscopic pairing quantities and neutron separation energies and compare with experimental values. Recall that Δ_{LN} is the sum of the pairing gap Δ and the number fluctuation constant λ_2 that occur in the Lipkin-Nogami equations. The pairing gap $\Delta_{\mathrm{th.mass}}$ is determined from odd-even *theoretical* mass differences. The results are summarized in Table 3.

Ideally, the minimum deviation should occur for all quantities at the same value of r_{mic}, which is almost but not quite the case. As seen in Table 3, all minima are close to the mass-model minimum at $r_{\mathrm{mic}} = 3.2$ MeV. We therefore choose this value of r_{mic} for our microscopic pairing calculations. Experimental pairing gaps determined from odd-even mass differences contain large errors arising from non-smooth contributions to the mass surface other than pairing effects, for example, from shape transitions and gaps in the deformed single-particle level spectra. Since such contributions are equally present in $\Delta_{\rm exp}$ and $\Delta_{\rm th.mass}$, they should cancel out approximately in the difference between these two quantities, if the mass model errors were sufficiently small. Consequently, the other non-smooth contributions to the mass surface are not expected to affect an rms minimization of $\Delta_{\rm th.mass}$. It is therefore of interest to note that our chosen value of $r_{\rm mic}$ is intermediate between what would have been obtained from considering $\Delta_{\rm th.mass}$ and $\Delta_{\rm LN}$ deviations.

The FRDM, which includes Coulomb redistribution effects, is now our preferred nuclear mass model. Relative to the work described in Ref. 10, the following further improvements have been incorporated into the model. First, it was found that the γ zero-point energy could not be calculated with sufficient accuracy in our current model. It is therefore no longer included, whereas the ϵ_2 zero-point energy is still retained. Second, we have also returned to our original choice of basis functions corresponding to 12 oscillator shells for all A values, instead of using somewhat fewer basis functions for lighter nuclei [10]. Third, we now use an eighth-order Strutinsky shell-correction with range $\gamma_{\rm S} = 1.0\hbar\omega_0 B_{\rm s}$ instead of our earlier choice of a sixth-order Strutinsky shell correction with the same range coefficient but no dependence on surface area. The change in zero-point energy reduced the error in the calculated neutron separation energies from 0.551 MeV to 0.444 MeV and the error in the calculated masses from 0.778 MeV [10] to 0.773 MeV. The second and third improvements further reduced the separation-energy error to 0.411 MeV and the mass-model error to 0.669 MeV. The rms error for $\Delta_{\rm th.mass}$ has decreased in a similar manner as the error in $S_{\rm n}$. Although the effect of the mass-model improvements on $\Delta_{\rm LN}$ is small, the effect on $\Delta_{\rm th.mass}$ is dramatic. Relative to our earlier pairing calculation [9], the improvement is more than 20%. It is no accident that both $S_{\rm n}$ and $\Delta_{\rm th.mass}$ showed similar improvements. Both are determined from mass differences between nearby masses, and such differences dramatically improved when the inaccurate γ zero-point energies were excluded from the calculations. The constants of the final model were presented in an earlier section.

As seen in Table 3, the error in our mass model is now 0.669 MeV. We have also performed a mass calculation with the FRLDM as the macroscopic model and identical shell-plus-pairing corrections as in the FRDM calculation. For the FRLDM the corresponding error is 0.779 MeV, which is 16% higher.

Figure 1 shows the results of the FRDM calculation. As usual, the top part shows the differences between measured masses and the spherical macroscopic FRDM contributions plotted against the neutron number N, with isotopes of a particular element connected by a line. These experimental microscopic corrections are to be compared with the calculated microscopic corrections plotted in the middle part of the figure. When the macroscopic and microscopic parts of the mass calculation are combined and subtracted from the measured masses, the deviations in the bottom part of the figure remain. The trends of the error in the heavy region suggest that this mass model should be quite reliable for nuclei beyond the current end of the periodic system. This has been made all the more plausible by simulations discussed in Sec. 4.3 on extrapability. When ϵ_3 and ϵ_6 shape degrees of freedom are included in the mass calculations, it becomes clear that the FRLDM, which does not treat Coulomb redistribution effects, is deficient in the heavy-element region, as is seen in Fig. 2. Thus, our preferred mass model is now the FRDM, which includes compressibility effects and the associated Coulomb redistribution.

4.2 Compressibility

We have earlier [4] studied how the discrepancy between measured masses and calculated masses depends on the compressibility constant K and on the new exponential term. In this earlier investigation we used the 1984 version of the FRDM [5]. We found that the minimum error occurred for $K = 324$ MeV. For this value the rms deviation between calculated and experimental masses was 0.666 MeV. For the conventional value $K = 240$ MeV the rms error was only marginally higher, namely 0.676 MeV. Because of the relative insensitivity of the rms error to the value of the compressibility constant K we retained [4] the historical value $K = 240$ MeV, as we also do here.

It is of interest to investigate the sensitivity of the model error to K also in the current version of the model. In Fig. 3 the solid circles connected by a solid line show the theoretical error in the mass model as a function of $1/K$. For each value of K the constants in the model are determined by minimizing the same weighted sum of barrier and mass errors that is referred to under point 6 in Sec. 4.1. However, only the theoretical error in the mass model itself is plotted. The arrow at $K = 243$ MeV indicates the optimum value of K obtained when the compressibility coefficient is varied along with the other constants. Thus, in our current model we obtain in a least-squares minimization a compressibility coefficient that is close to the value $K = 240$ MeV that was adopted from other considerations, but the determination is clearly subject to a large uncertainty.

We also investigate how the error for nuclei with $N \geq 65$ depends on K. This dependence is shown as solid squares connected by a long-dashed line. The model constants have the same values as obtained from the adjustments corresponding to the solid circles. Thus, *no new adjustment* is performed to this limited region of nuclei; we only investigate the behavior of the error associated with this region.

Finally, we show as open circles connected by a short-dashed line the result obtained in an adjustment without the exponential term. Here the minimum of the weighted sum of mass and barrier errors occurs at $K = 451$ MeV. The minimum of the function actually plotted, which is the mass error only, occurs at a slightly higher value of K.

The relatively low curvature of the solid curve shows that K cannot be reliably determined from an adjustment to nuclear masses. The conventional droplet model value $K = 240$ MeV is consistent with the result we obtain in a least-squares adjustment to masses and fission barrier heights, but from the adjustment alone one would not be able to rule out that K has some other value in the range from somewhat below 200 MeV to about 500 MeV.

The long-dashed curve shows that heavy nuclei in particular disfavor values of K close to infinity. For heavy nuclei with $N \geq 65$ the error in the FRDM increases by 25% from its minimum value as K approaches $+\infty$, whereas the increase is only 8% when all nuclei are considered. This observation has been made earlier and was taken as evidence for a Coulomb redistribution effect [10].

The short-dashed curve giving the results without an exponential term in the mass model is moderately incompatible with a compressibility coefficient close to 240 MeV and completely rules out a significantly lower value. However, our preferred treatment of the compressibility is the formulation that includes the exponential term, in which treatment the restrictions on K are the much less severe ones given above.

4.3 Extrapability

One test of the reliability of a nuclear mass model is to compare deviations between measured and calculated masses in new regions of nuclei that were not considered when the constants of the model were determined to deviations in the original region. This type of analysis was used earlier by Haustein [63]. However, we here considerably modify his approach. In addition to examining the raw differences between measured and calculated masses, we use these differences to determine the *model* mean discrepancy μ_{th} from the true masses and the *model* standard deviation σ_{th} around this mean, for new regions of nuclei. Whereas the raw differences do not show the true behavior of the theoretical error because errors in the measurements contribute to these differences, by use of the ideas developed in Sec. 2.1 we are able to estimate the *true* mean μ_{th} and standard deviation σ_{th} of the theoretical error term e_{th}.

Since our new mass model was developed only recently, we cannot test its reliability in new regions of nuclei because sufficiently many new data points are not available. Therefore, we

Table 4: Comparison of errors of two different mass calculations. The errors are tabulated both for the region in which the constants were originally adjusted and for a set of new nuclei that were not taken into account in the determination of the constants of the mass models. The error ratio is the ratio between the numbers in columns 8 and 3.

	Original nuclei		New nuclei					
Model	rms (MeV)	$\sigma_{\rm th}$ (MeV)	$N_{\rm nuc}$	rms (MeV)	$\mu_{\rm th}$ (MeV)	$\sigma_{\rm th}$ (MeV)	$\sigma_{\rm th;\mu=0}$ (MeV)	Error ratio
FRLDM (1981)	0.835	0.831	351	0.911	−0.321	0.826	0.884	1.06
FRDM (1992)	0.673	0.671	351	0.735	−0.004	0.686	0.686	1.02

have resorted to a simple simulation, in which we adjusted the constants in the model to the same experimental data set that was used in our 1981 mass calculation [1,2]. Consequently, this calculation is not completely identical to the one on which Fig. 1 is based. The differences between the 351 new masses that are now measured [45] and the calculated masses are plotted *versus* the number of neutrons from β-stability in Fig. 4. We observe no systematic increase in the error with increasing number of neutrons from β-stability. For the new region of nuclei the square root of the second central moment is 0.686 MeV, compared to 0.671 MeV in the region where the parameters were adjusted, representing an increase of only 2%. In contrast, mass models based on postulated shell-correction terms and on a correspondingly larger number of constants normally diverge outside the region where the constants were determined [11,12].

To study more quantitatively how the error depends upon the distance from β-stability, we introduce bins in the error plot sufficiently wide to contain about 10–20 points and calculate the mean error and standard deviation about the mean for each of these bins by use of the methods described in Sec. 2.1. The results for our 1981 FRLDM and for our 1992 FRDM, but adjusted only to the same data set as was used in our 1981 calculation, are shown in Fig. 5. For each model the central, *light*-gray band representing the original error region extends one (global) standard deviation $\sigma_{\rm th}$ on each side of zero. The solid dots connected by a thick black line represent the mean of the error $\mu_{\rm th}$ for nuclei that were not considered when the constants in the model were determined. The thin black lines represent the standard deviation for each bin. The *dark*-gray areas indicate regions for which the individual bin deviations are not contained within the original global error. The properties of the two models displayed in Figs. 5 are summarized in Table 4.

To test the reliability of the FRDM for extrapolation beyond the heaviest known elements we have performed a rather severe test in which we adjust the constants in the model only to data in the region $Z, N \geq 28$ and $A \leq 208$. There are 1110 known masses in this region compared to 1654 in the region $Z, N \geq 8$ used in our standard adjustment. Thus, about one third of all known masses are excluded, with nuclei removed from both ends of the region of adjustment. We then apply the model with these constants to the calculation of all known masses in our standard region and compare the results to our standard model in Fig. 6. The error for the known nuclei is now 0.745 MeV, compared to 0.669 MeV with our standard model adjusted to all known nuclei. Although there is a noticeable increase of the error in the regions that were not included in the adjustment, an inspection of Fig. 6 indicates that the increased error in the heavy region is not due to a systematic divergence of the mean error, but rather to a somewhat larger scatter in the error.

In our standard model the mass excesses of $^{272}110$ and $^{288}110$ are 133.82 MeV and 165.68 MeV, respectively. In our restricted adjustment we obtain 133.65 MeV and 166.79 MeV, respectively. Thus, although $^{288}110$ is 80 units in A away from the last nucleus included in the restricted adjustment, the mass obtained in this numerical experiment is only about 1 MeV different from that obtained in the calculation whose constants were adjusted to nuclei up to 50 units in A closer to the superheavy region. Since our standard calculation is adjusted so much closer to the superheavy region than is the numerical experiment, we feel that it should be accurate to about an MeV in the superheavy region. Since models with and without Coulomb redistribution energies often differ by considerably more, the masses of superheavy elements could provide very strong further confirmation of the existence of Coulomb redistribution effects. A suitable nucleus for such a test is $^{272}110$. The FRDM, which includes Coulomb-redistribution effects, predicts a mass excess of 133.82 MeV for this nucleus, whereas the FRLDM, which does not include Coulomb-redistribution effects, predicts 136.61 MeV.

Figure 1 shows that as the lighter region is approached the error gradually increases in a systematic way. We have explored this possibility by first determining the model error for limited regions of nuclei by use of Eq. (9). We select $A = 25(25)250$ as centerpoints of the regions and define each region to extend from $A_{\rm center} - 24$ to $A_{\rm center} + 25$. The errors in these restricted regions are shown as solid circles in Fig. 7. Since the trend of the error looks approximately like c/A^{α} we have determined the parameters of this assumed error function by use of the maximum-likelihood equations (15) and (16). We find $c = 8.62$ MeV and $\alpha = 0.57$. The error function corresponding to these parameters is plotted as a solid line.

4.4 Fission barriers

Calculated heights of the outer peak in the fission barrier are compared to measured values in Table 5. The results are also shown graphically in Fig. 8. Extensive fission studies based on earlier and current versions of the models discussed here are presented in Refs. 30, 31, 33, and 64–69.

4.5 Ground-state masses and deformations

In the Table we tabulate our calculated ground-state deformations in the ϵ parameterization, the corresponding coefficients β in a spherical-harmonics expansion, the atomic mass excesses and microscopic energies calculated in both the FRDM and FRLDM, and experimental masses and associated errors that were used in the adjustment of model constants.

To give an overview, the tabulated FRDM quantities are plotted versus N and Z in the form of color contour diagrams. The calculated ground-state deformations ϵ_2, ϵ_3, ϵ_4, and ϵ_6 are shown in Figs. 9–12, and the corresponding coefficients β_2, $|\beta_3|$, β_4, and β_6 are shown in Figs. 13–16. We observe some features that are by now well-known. For example, the absolute value of the quadrupole deformation ϵ_2 increases by about 0.05 for each deformed region below the actinide region. Oblate deformations occur in transition regions on the heavy side of most deformed regions. The hexadecapole deformation ϵ_4 is large and negative in the beginning of deformed regions and large and positive in the end of deformed regions. The coefficients β_3, β_4, and β_6 have the opposite sign from the corresponding ϵ deformations, whereas β_2 has the same sign as ϵ_2 but is roughly 10% larger.

The microscopic energy $E_{\rm mic}$ is plotted in Fig. 17. The familiar doubly magic regions around $^{100}_{50}{\rm Sn}_{50}$, $^{132}_{50}{\rm Sn}_{82}$, and $^{208}_{82}{\rm Pb}_{126}$ stand out clearly. The center of the superheavy region is located at $^{294}115_{179}$. The large negative microscopic correction originating in the superheavy region extends a significant distance towards the southwest and reaches into the deformed actinide region. It is these large, negative microscopic corrections that have made possible the extension of the known elements as far as $^{266}_{109}{\rm Mt}_{157}$. As is seen in Figs. 18 and 19, the largest effects of ϵ_3 and ϵ_6 in experimentally accessible regions occur around $^{222}_{88}{\rm Ra}_{134}$ and $^{252}_{100}{\rm Fm}_{152}$, respectively.

Table 5: Comparison of experimental and calculated fission-barrier heights for 28 nuclei.

Z	N	A	Experimental barrier (MeV)	Calculated barrier (MeV)	Discrepancy (MeV)
48	61	109	34.00	35.69	−1.69
66	94	160	27.40	27.88	−0.48
76	110	186	23.40	21.21	2.19
	112	188	24.20	21.07	3.13
80	118	198	20.40	19.16	1.24
84	126	210	20.95	21.81	−0.86
	128	212	19.50	19.69	−0.19
88	140	228	8.10	8.41	−0.31
90	138	228	6.50	7.43	−0.93
	140	230	7.00	7.57	−0.57
	142	232	6.30	7.63	−1.33
	144	234	6.65	7.44	−0.79
92	140	232	5.40	6.61	−1.21
	142	234	5.80	6.79	−0.99
	144	236	5.75	6.65	−0.90
	146	238	5.90	4.89	1.01
	148	240	5.80	5.59	0.21
94	144	238	5.30	4.85	0.45
	146	240	5.50	4.74	0.76
	148	242	5.50	5.25	0.25
	150	244	5.30	5.78	−0.48
	152	246	5.30	6.27	−0.97
96	146	242	5.00	4.24	0.76
	148	244	5.00	5.05	−0.05
	150	246	4.70	5.69	−0.99
	152	248	5.00	6.07	−1.07
	154	250	4.40	5.51	−1.11
98	154	252	4.80	5.31	−0.51

In Fig. 20 we show the discrepancy between experimental and calculated masses in the form of a contour diagram versus N and Z. Above $N \approx 65$ there are only a few nuclei with an error marginally larger than 1 MeV. The noticeable errors near $Z = 40$, $N = 56$ are probably related to the unique[14] shell structure in this region and the reinforcement of the $N = 56$ shell closure for proton number $Z = 40$ and proton numbers just below. Such proton-neutron interactions are not accurately described within any simple single-particle effective-interaction framework.

5 Acknowledgements

We are grateful to G. Audi for permission to use the results of his unpublished 1989 midstream atomic mass evaluation and to Hu Ji-min for his perceptive comments on an early version of our manuscript. This work was supported by the U. S. Department of Energy. One of us (P. M.) would like to acknowledge through a historical note the hospitality and support received during the course of this work. The main sponsor of the mass-model work during the years 1985–1993 has been the Los Alamos National Laboratory, but numerous other institutions have also been involved. During visits to Lawrence Berkeley Laboratory in the summers of 1981 and 1982 and in the 1983–84 academic year the finite-range droplet model was developed [5]. Systematic work on an improved mass model started during visits to Los Alamos National Laboratory in 1985–87, and interim results were published a year later [3,4]. The calculation of contour maps and the corresponding ground-state deformations ϵ_2 and ϵ_4 for 8979 nuclei was sponsored by Lawrence Livermore National Laboratory in the fall of 1987. The Lipkin-Nogami pairing code was developed as part of a contract with Idaho National Engineering Laboratory in 1988. In 1990 a completely new code for the FRDM was written during a summer visit to Lund University. Whereas the previous code would run only on Cray and CDC computers the new code could run on any workstation. Thus, we were able to carry out the minimization of the potential energy with respect to ϵ_3 and ϵ_6 without substantial charges on available workstation clusters. Initial minimization calculations were carried out during the visit to Lund University. These were continued in the fall of 1990 during a visit to Institut für Kernchemie, Mainz, which visit was also sponsored by Gesellschaft für Schwerionenforschung, Darmstadt. The model development and calculations were brought to their current stage at Los Alamos National Laboratory in 1991 [9,10,12] and in 1992 [11]. This publication was put together at Los Alamos in the summer of 1993, with final editorial changes made at Los Alamos in the summer and fall of 1994.

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Figure captions

Fig. 1 Comparison of experimental and calculated microscopic energies $E_{\rm mic}$ for 1654 nuclei, for a macroscopic model corresponding to the FRDM. The bottom part showing the difference between these two quantities is equivalent to the difference between measured and calculated ground-state masses. There are almost no systematic errors remaining for nuclei with $N \geq 65$, for which region the error is only 0.448 MeV. The results shown in this figure represent our new mass model. The lines are drawn through isotope chains.

Fig. 2 Analogous to Fig. 1, but for the FRLDM, which contains no Coulomb-redistribution terms. This leads to the systematic negative errors in the heavy region, which indicate that the calculated masses are systematically too high.

Fig. 3 Relation between the compressibility coefficient K and the mass-model error. Calculated values are indicated by symbols, which are connected by curves to guide the eye. In our standard FRDM, which is our preferred model, the error depends only relatively weakly on the compressibility coefficient in the range 200 MeV $\lesssim K \lesssim$ 500 MeV, as is shown by the solid circles. Without the exponential term a relatively high compressibility coefficient would be required. The error in the heavy region, shown by the solid squares, indicates that heavy nuclei, in particular, do not favor very large values of K. For heavy nuclei with $N \geq 65$ the model error increases by 25% from its minimum value as K approaches $+\infty$, whereas the increase is only 8% when all nuclei are considered.

Fig. 4 Calculation showing the reliability of the FRDM in new regions of nuclei. Here we use a smaller set of measured masses to determine the constants of the model than in the full calculation shown in Fig. 1. The errors for nuclei not included in the adjustment are displayed in this figure. The error is only 2% larger in the new region compared to that in the region where the constants were determined. The two largest deviations occur for ^{23}O and ^{24}O, which probably indicates that this region of light very neutron-rich nuclei is outside the range of model applicability. Proton number 8 is the lowest value of Z that we consider in this model. For the position of the line of β stability we use Green's approximation given by Eq. (123). This equation is solved for each proton number Z assuming A and N are floating-point numbers. Thus, the points in this figure are located at non-integral values of N.

Fig. 5 Comparison of the error behavior for two models applied to new nuclei *versus* the number of neutrons from β-stability. See text for details.

Fig. 6 Test of extrapability of the FRDM towards the superheavy region. The top part of the figure shows the error of the standard FRDM. In the lower part the error was obtained from a mass model whose constants were determined from adjustments to the restricted set of nuclei with $Z, N \geq 28$ and $A \leq 208$. In the light region of nuclei there is no noticeable divergence of the results obtained in the restricted adjustment. In the heavy region there is some increase in the spread of the error, but no systematic divergence of the mean error. Based on the more detailed discussion in the text we deduce that our calculated masses for the superheavy elements are accurate to about one MeV.

Fig. 7 Error in the mass calculation as a function of mass number A. The theoretical error has been determined for limited regions throughout the periodic system.

The error represented by each solid circle is based on nuclei in a region that extends 24 mass units below the circle and 25 mass units above the circle. The points are well approximated by the function 8.62 MeV/$A^{0.57}$.

Fig. 8 Comparison of experimental and calculated fission-barrier heights for 28 nuclei. Isotopes are connected by lines.

Fig. 9 Calculated ground-state values of $|\epsilon_2|$ for 7969 nuclei with $N < 200$. Oblate shapes are indicated with horizontal black lines. About 14 deformed regions stand out, bordered or partially bordered by blue lines corresponding to magic nucleon numbers. The magnitude of the deformation in the deformed regions increases by about 0.05 with successively lighter regions or as one goes from neutron-rich to proton-rich regions. Highly deformed superheavy nuclei with $N \geq 178$ usually have very low fission barriers, and should consequently have spontaneous-fission half-lives that are too short to be detectable.

Fig. 10 Calculated ground-state values of ϵ_3 for 7969 nuclei with $N < 200$. Most nuclei in the investigated region inside the black line are stable with respect to mass-asymmetric octupole deformations; only 640 nuclei are unstable with respect to these deformations. The largest effects of experimental significance are centered around ${}^{222}_{88}\mathrm{Ra}_{134}$.

Fig. 11 Calculated ground-state values of ϵ_4 for 7969 nuclei with $N < 200$. Characteristically, the values are large and negative in the beginning of major deformed regions and large and positive in the end of major deformed regions. In accordance with this general trend, ϵ_4 is large and positive near the rock of stability in the vicinity of ${}^{272}110$ near the end of the deformed "actinide" region.

Fig. 12 Calculated ground-state values of ϵ_6 for 7969 nuclei with $N < 200$. The behavior of ϵ_6 is less regular than that of the lower, even multipole distortions.

Fig. 13 Calculated ground-state values of $|\beta_2|$ for 7969 nuclei with $N < 200$, which have been obtained by use of the transformation (38) from the ϵ deformations. Oblate shapes are indicated by horizontal black lines. Comments given in Fig. 9 also apply here.

Fig. 14 Calculated ground-state values of $|\beta_3|$ for 7969 nuclei with $N < 200$, which have been obtained by use of the transformation (38) from the ϵ deformations.

Fig. 15 Calculated ground-state values of β_4 for 7969 nuclei with $N < 200$, which have been obtained by use of the transformation (38) from the ϵ deformations. Comments given in Fig. 11 also apply here, but note that the sign of β_4 is opposite that of ϵ_4 when significant deformations develop.

Fig. 16 Calculated ground-state values of β_6 for 7969 nuclei with $N < 200$, which have been obtained by use of the transformation (38) from the ϵ deformations. Comments given in Fig. 12 also apply here, but note that the sign of β_6 is opposite that of ϵ_6 when significant deformations develop.

Fig. 17 Calculated ground-state microscopic energies E_{mic} for 7969 nuclei with $N < 200$. Well-known doubly magic regions at ${}^{100}_{50}\mathrm{Sn}_{50}$, ${}^{132}_{50}\mathrm{Sn}_{82}$, and ${}^{208}_{82}\mathrm{Pb}_{126}$ stand out clearly. The minimum in the superheavy region is offset somewhat from ${}^{298}114_{184}$ and is located instead at ${}^{294}115_{179}$. An interesting feature, also present in our first mass calculation[2,14], is the rock of stability at ${}^{272}_{109}\mathrm{Mt}_{163}$.

Fig. 18 Calculated ground-state octupole instability for 7969 nuclei with $N < 200$. Only 640 nuclei exhibit any instability with respect to this shape degree of freedom. The largest effect in the experimentally accessible region is -1.41 MeV for ${}^{222}_{89}\mathrm{Ac}_{133}$.

Fig. 19 Calculated ground-state hexacontatetrapole instability for 7969 nuclei with $N < 200$. The instability is relative to the energy corresponding to the macroscopic equilibrium value of ϵ_6, with ϵ_3 set equal to zero. The largest effect is -1.29 MeV for ${}^{251}_{99}\mathrm{Es}_{152}$.

Fig. 20 Discrepancy between measured and calculated masses. Above $N = 65$ only a few discrepancies are marginally more than 1 MeV. There is a gradual increase of the error towards the light region. The large, fluctuating error near $N = 60$ is probably due to deviations between our simple effective interaction and the true nuclear force. It is well-known that for $Z \approx 40$ there is a re-enforcement of the $N = 56$ sub-shell closure. Such effects cannot be described within the framework of a single-particle model.

EXPLANATION OF TABLE

Table. Calculated Nuclear Ground-State Masses and Deformations, Compared to Experimental Masses Where Available

Z	Proton number. The mass table is ordered by increasing proton number. The corresponding chemical symbol of each named element is given in parentheses.
N	Neutron number
A	Mass number
ϵ_2	Calculated ground-state quadrupole deformation in the Nilsson perturbed-spheroid parameterization
ϵ_3	Calculated ground-state octupole deformation in the Nilsson perturbed-spheroid parameterization
ϵ_4	Calculated ground-state hexadecapole deformation in the Nilsson perturbed-spheroid parameterization
ϵ_6	Calculated ground-state hexacontatetrapole deformation in the Nilsson perturbed-spheroid parameterization. The value in this column is used in the mass calculation. If $\epsilon_3 \neq 0$ then ϵ_6 was not varied but was instead held fixed at the value that minimizes the macroscopic energy for ^{240}Pu.
$\epsilon_6^{\mathrm{sym}}$	Calculated ground-state hexacontatetrapole deformation in the Nilsson perturbed-spheroid parameterization for $\epsilon_3 = 0$. This is the optimum value of ϵ_6 when mass asymmetry is *not* considered. It is provided for use in computer codes or other applications that cannot take into account mass-asymmetric shapes.
β_2	Calculated quadrupole deformation of the nuclear ground-state expressed in the spherical-harmonics expansion defined by Eq. (37)
β_3	Calculated octupole deformation of the nuclear ground-state expressed in the spherical-harmonics expansion defined by Eq. (37)
β_4	Calculated hexadecapole deformation of the nuclear ground-state expressed in the spherical-harmonics expansion defined by Eq. (37)
β_6	Calculated hexacontatetrapole deformation of the nuclear ground-state expressed in the spherical-harmonics expansion defined by Eq. (37)
E_{mic}	Calculated ground-state microscopic energy, given by the difference between the calculated ground-state atomic mass excess and the spherical macroscopic energy calculated from Eq. (40), in our preferred model, the FRDM
M_{th}	Calculated ground-state atomic mass excess, in our preferred model, the FRDM
M_{exp}	Experimental ground-state atomic mass excess in the 1989 midstream evaluation of Audi [45], with four revisions
σ_{exp}	Experimental error associated with the ground-state atomic mass excess in the 1989 midstream evaluation of Audi [45], with four revisions
$E_{\mathrm{mic}}^{\mathrm{FL}}$	Calculated ground-state microscopic energy, given by the difference between the calculated ground-state atomic mass excess and the spherical macroscopic energy calculated from Eq. (62), in the FRLDM
$M_{\mathrm{th}}^{\mathrm{FL}}$	Calculated ground-state atomic mass excess, in the FRLDM

Absence of an entry in ϵ_3, $\epsilon_6^{\mathrm{sym}}$, and β_3 means that the ground state is symmetric in shape.

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