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A SEMIEMPIRICAL LIQUID-DROP PLUS SHELL-CORRECTION FORMULA*

P. A. SEEGER

Los Alamos Scientific Laboratory
Los Alamos, New Mexico 87545

and

W. M. HOWARD

Northwestern University, Evanston, Illinois 60201

An atomic mass formula based on the liquid-drop model with shell and deformation energies determined from the Nilsson model and BCS pairing energy has been adjusted to fit simultaneously ground-state binding energies and fission-barrier heights. There are nine free parameters. Calculated mass excesses of 6367 nuclides in the range $20 \leqslant Z \leqslant 120$ and $20 \leqslant N \leqslant 200$ are given in the main table of this issue. Additional calculations are available in a report or on magnetic tape. Differences between calculated and experimental results are shown graphically.

CONTENTS

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DESCRIPTION OF FORMULA

The mass formula used here is based on a separation of the total expression into a smoothly varying (macroscopic) contribution and a fluctuating (microscopic) correction term. The liquid-drop and Nilsson models are used for the respective parts. Nine adjustable parameters are determined by least-squares fitting to 1553 ground-state masses and to 61 fission-barrier heights. The formula is described more fully in Ref. 1, while calculations of ground-state binding energies and particle separation energies are presented in Ref. 2. More complete references to the development are also given in those articles.

The liquid-drop expression[3] includes volume and surface terms, a combined volume and surface asymmetry term in the denominator form,[4] a curvature term, a Coulomb-energy term which includes the effect of surface diffuseness on the effective nuclear radius,[5] a Wigner term, and a small correction for the binding energy of the atomic electrons. Including the microscopic term $S(N,Z,\epsilon_i)$, the complete expression for the binding energy is

$$\begin{aligned} B(Z,A,\epsilon_i) &= \alpha A - \beta(N-Z)^2 A^{-1}[1+\zeta B_s(\epsilon_i)/A^{1/3}]^{-1} \\ &\quad - \gamma A^{2/3} B_s(\epsilon_i) + \phi A^{1/3} B_k(\epsilon_i) - E_c(Z,A,\epsilon_i) \\ &\quad - 35\,|N-Z|/A + 14.33\times 10^{-6} Z^{2.39} + S(N,Z,\epsilon_i). \end{aligned} \tag{1}$$

Shape dependence is indicated explicitly by ϵ_i, which represents any generalized parameterization of nuclear shape. The surface, Coulomb, and curvature-shape dependencies (B_s, B_c, and B_k, respectively) are integrated[1,6] for each shape, and are normalized to unity for a sphere. Ground-state energies are found by maximizing binding energy in a two-parameter (ϵ,ϵ_4) family of shapes[7] and fission barriers in the one-parameter (x) family of idealized liquid-drop saddle-point shapes.[8]

The Coulomb energy includes direct, exchange, and spin-orbit interaction contributions, expanded to fourth order in the ratio of surface diffuseness to radius. The only free parameter is the radius constant r_0.

Calculation of the shell and deformation terms $S(N,Z,\epsilon_i)$ proceeds in three steps: determination of the Nilsson-model levels,[7,9] normalization by the Strutinsky procedure,[10] and calculation of the Bardeen-Cooper-Schrieffer (BCS) ground-state energies.[11] The correction term, which is a sum of a function of Z and of a function of N, scales simply with A. (See Ref. 1 for details.) The neutron potential V_n and proton potential V_p are adjustable parameters. The term S is usually positive in the binding energy because of the maximization with respect to shape; for the nuclides included here, it ranges from -3.6 to $+13.6$ MeV.

USE OF FISSION BARRIERS

An unusual feature of this calculation is the inclusion of fission barriers in the determination of coefficients. We do not have solutions of $S(N,Z,x)$ corresponding to saddle-point shapes, but we believe the microscopic effects are reduced at large deformations. Lacking the appropriate wavefunctions, we cannot form the BCS ground states; we account for even-odd differences by including the traditional $\pm 1/\sqrt{A}$ dependence. This introduces one additional adjustable parameter δ_b. When we denote the stable ground-state shape by $\hat{\epsilon}$ and the metastable saddle-point shape by $\hat{x}$ and subtract each term in Eq. (1), the formula for the barrier height is

$$\begin{aligned} E_b(Z,A) &= \beta(N-Z)^2 A^{-1} \\ &\quad \times \left[\frac{1}{1+\zeta B_s(\hat{x})/A^{1/3}} - \frac{1}{1+\zeta B_s(\hat{\epsilon})/A^{1/3}}\right] \\ &\quad + \gamma A^{2/3}[B_s(\hat{x}) - B_s(\hat{\epsilon})] - \phi A^{1/3}[B_k(\hat{x}) - B_k(\hat{\epsilon})] \\ &\quad + E_c(Z,A,\hat{x}) - E_c(Z,A,\hat{\epsilon}) + S(N,Z,\hat{\epsilon}) \\ &\quad - \delta_b[2 - (Z \bmod 2) - (N \bmod 2)]/\sqrt{A}. \end{aligned} \tag{2}$$

DETERMINATION OF COEFFICIENTS

The fitting procedure involved selecting a value for ζ and iterating between fitting α, β, V_n, V_p, and a linear combination of γ and r_0 to 1553 ground states[12] and fitting ϕ, δ_b, and an independent combination of γ and r_0 to 61 barrier heights.[13-15] The procedure was repeated for various ζ to find the minimum sum of residuals. The resulting values[1] of the nine adjustable parameters are given in the following table.

The standard deviation of the errors of the calculated binding energies as determined from the ground-state input data[2] is 0.704 MeV. The figure shows that some systematic errors exist. The standard deviation of the errors of the calculated barriers is 0.795 MeV. Statistical tests (χ^2 and F) indicate that none of the input data is inconsistent with the calculated values.

Reference 2 includes tables of calculated binding energies, deformations, etc., of 8001 nuclides. These tables may also be obtained on 12.7-mm magnetic computer tape by sending a blank tape to the authors at the Los Alamos Scientific Laboratory. Please state desired density, parity, and number of tracks.

Mass excesses in the accompanying table are found from binding energies by

$$\Delta M(Z,A) = 7.28922\,Z + 8.07169\,(A-Z) - B(Z,A,\hat{\epsilon}), \text{ in units of MeV.} \tag{3}$$

Values of Coefficients

α = 15.2568 ± 0.0031 MeV, volume-energy coefficient
β = 33.166 ± 0.016 MeV, symmetry-energy coefficient
γ = 17.073 ± 0.028 MeV, surface-energy coefficient
ζ = 3.28 ± 0.21, surface-symmetry-correction coefficient
r_0 = 1.2254 ± 0.0014 fm, nuclear-radius constant
ϕ = −0.76 ± 0.11 MeV, curvature-energy coefficient
V_n = 35.37 ± 0.34 MeV, neutron potential
V_p = 31.08 ± 0.40 MeV, proton potential
δ_b = 9.75 ± 0.77 MeV, barrier pairing-energy coefficient

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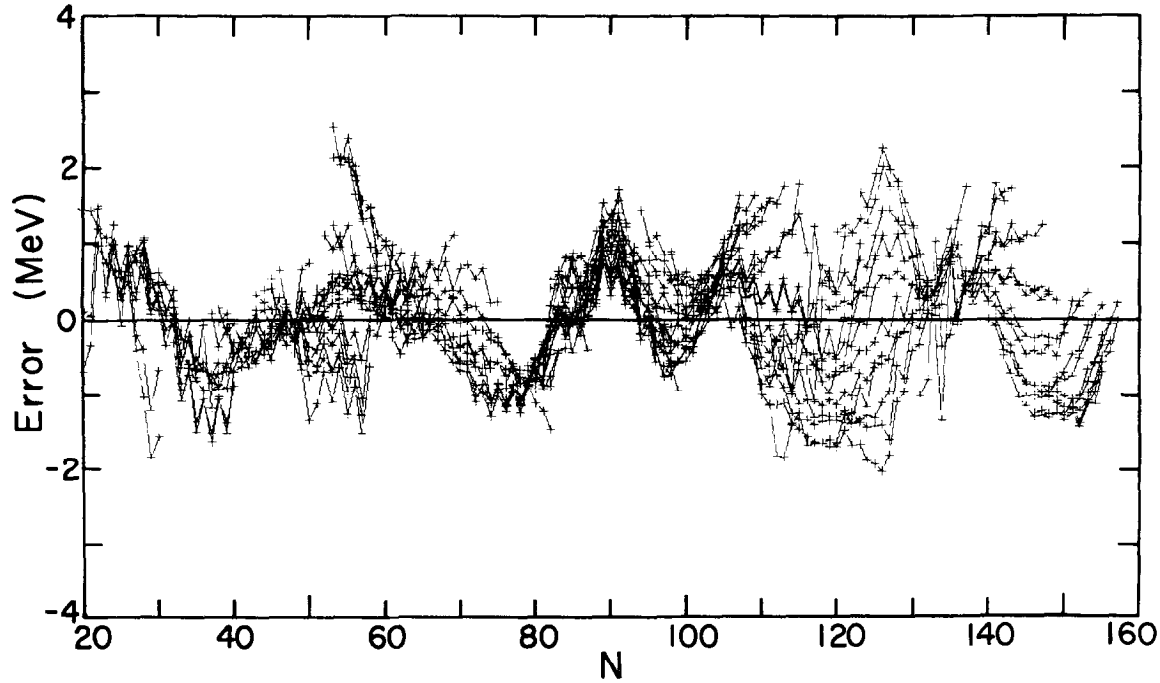

Figure. Residual errors, the differences between calculated ground-state binding energies and the experimental values of Ref. 12, are plotted against neutron number N. Isotopes of each element are connected by lines. Standard deviation is 0.704 MeV; note residual systematic deviations versus both N and Z (for example, near $N = 80$ and near $N = 120$, respectively)