Title

FINITE RANGE DROPLET MODEL

Author

Moller, P.

Publication Date

1984-08-01

LBL-18230 c.2

Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

Presented at the 7th International Conference on Atomic Masses and Fundamental Constants (AMCO-7), Darmstadt-Seeheim, Federal Republic of Germany, September 3-7, 1984; and to be published in the Proceedings

FINITE RANGE DROPLET MODEL

P. Möller, W.D. Myers, W.J. Swiatecki, and J. Treiner

August 1984

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF00098

LBL-18230

FINITE RANGE DROPLET MODEL*

P. Möller[†], W. D. Myers, W. J. Swiatecki and J. Treiner[‡]

Nuclear Science Division, Lawrence Berkeley Laboratory
University of California, Berkeley, California 94720

Proceedings of the 7th International Conference
on Atomic Masses and Fundamental Constants (AMCO-7)
3-7 Sept. 1984
Darmstadt-Seeheim
Federal Republic of Germany

*This work was supported by the Director, Office of Energy Research, Division of Nuclear Physics of the Office of High Energy and Nuclear Physics of the U.S. Department of Energy under Contract DE-AC03-76SF00098.

[†]Permanent address: Department of Mathematical Physics, Box 725
S-22007 LUND, SWEDEN

[‡]Permanent address: IPN BP n° 1 97406 ORSAY Cedex, FRANCE

FINITE RANGE DROPLET MODEL*

P. Möller[†], W. D. Myers, W. J. Swiatecki and J. Treiner[‡]

Nuclear Science Division, Lawrence Berkeley Laboratory
University of California, Berkeley, California 94720

Abstract:

A treatment of nuclear masses and deformations is described which combines the Droplet Model with the folding model surface and Coulomb energy integrals. An additional exponential term, inspired by the folding model, but treated here as an an independent contribution with two adjustable parameters, is included. With this term incorporated, the accuracy of the predicted masses and fission barriers was improved significantly, the ability of the Droplet Model to account for isotope shifts in charge radii was retained, and the tendency of the Droplet Model to over-predict the surface-tension squeezing of light nuclei was rectified.

1. Introduction

For almost fifty years the Bethe-Weizsäcker,[1,2]) or Liquid Drop Model (LDM), nuclear mass formula has been spectacularly successful in predicting the binding energy of atomic nuclei. Even in its simplest form the accuracy over the whole periodic table is within a percent or so (10 MeV out of 1000 MeV). The invention of the two-part approach for adding shell corrections[3,4]) and various other refinements (see refs. [5-9])) have led to an order of magnitude improvement in the accuracy (predictions within 1 MeV). In addition, the LDM and its associated refinements have been applied to predictions of nuclear radii, fission barriers, and dynamical situations such as giant monopole and dipole resonances.

The work described here was undertaken in order to combine the features of two different approaches to improving the LDM[10,11]). In ref. [10]) (and in earlier work cited there) a Droplet Model (DM) was developed that introduced the possibility of nuclear compression (or dilatation) and the possibility of a neutron skin for nuclei with a substantial neutron excess. The introduction of these degrees of freedom allowed the LDM expansion of the binding energy in terms $A^{-1/3}$ and I^2 (where $I = (N-Z)/A$) to be carried to one higher order in a consistent way. The folding model approach of ref. [11]) had other virtues. The use of a finite range force for calculating the surface energy automatically generates various corrections necessary for bringing the calculated fission barriers into better agreement

*This work was supported by the Director, Office of Energy Research, Division of Nuclear Physics of the Office of High Energy and Nuclear Physics of the U.S. Department of Energy under Contract DE-AC03-76SF00098.

[†]Permanent address: Department of Mathematical Physics, Box 725
S-22007 LUND, SWEDEN

[‡]Permanent address: IPN BP n° 1 97406 ORSAY Cedex, FRANCE

with the measured values. In addition we have recently begun to investigate the possible importance of exponential terms similar to those associated with the folding integrals[12]).

In the next section we describe how the folding model surface energy and an improved calculation of the Coulomb energy can be incorporated into the DM. Section 3 presents the complete mass formula consisting of DM terms and various other contributions, such as the odd-even mass difference, the Wigner term and the binding of the atomic electrons. A subsequent section is devoted to comparisons between the calculated and measured values of masses, deformations, fission barriers, radii and isotope shifts.

2. Finite Range Droplet Model

In ref. [13]) the general Droplet Model (DM) expression for the energy of a nucleus is written as a function of the neutron skin thickness and bulk density degrees of freedom for arbitrary nuclear shapes. Then the specific form of the DM needed for predicting masses, radii, etc. is obtained by analytic minimization of the energy with respect to these new degrees at freedom. The Finite Range Droplet Model (FRDM) can be derived in exactly the same way. Since the basic elements of the discussion are identical to those in ref. [13]), we will use the same notation here and address only those points where the finite range approach brings in something new. Familiarity with the earlier work will be assumed.

The volume terms are the usual DM ones,

$$[-a_1 + J\bar{\delta}^2 + \frac{1}{2}(K\bar{\varepsilon}^2 - 2L\bar{\varepsilon}\bar{\delta}^2 + M\bar{\delta}^4)]A \quad . \tag{1}$$

The first important difference is that the DM surface energy term, $a_2A^{2/3}(1 + 2\bar{\varepsilon})B_s$ in eq. (35) of ref. [13]) is replaced by an analogous term which can be derived on the basis of the folding model, $a_2A^{2/3}(F_s + 2F_{s2}\bar{\varepsilon})$, where,

$$F_s(\lambda,\text{shape}) = \frac{1}{8\pi^2\lambda^2}\iint (2-\xi)\,\frac{e^{-\xi}}{\xi}\,d\xi_1^3 d\xi_2^3 \quad , \tag{2}$$

$$F_{s2}(\lambda,\text{shape}) = \frac{1}{2\lambda}\frac{d(\lambda^2F_s)}{d\lambda} \quad .$$

In this expression the two volume integrations are over a uniform density distribution of volume $\frac{4}{3}\pi R^3$, and $\lambda = R/a$, $\xi = |\vec{r}_1 - \vec{r}_2|/a$, a = range. Finally, it should be noted that eq. (2) is simply the generalization of the expression, $a_sI_n(r_o,a,A,\text{shape})$, from eq. (2.3) of ref. [11]) that is necessary when adapting the folding approach to the DM where the nuclear volume is allowed to vary.

The DM surface energy also depends on the neutron excess. From studying the derivation in ref. [13]) we were able to determine that this dependence could also be incorporated into the folding model by making the replacement, $Q \rightarrow (F_s/B_s)Q$, where B_s is the usual ratio of the surface area to that of a sphere of equal volume. The quantity B_s also appears in the auxiliary expression, $3\bar{\tau}B_s = 2(I - \bar{\delta})A^{1/3}$, that relates the bulk and global nuclear asymmetries ($\bar{\delta}$ and I) to the average skin thickness $\bar{\tau}$.

The Coulomb energy was calculated using the expression, $c_1Z^2A^{-1/3}(F_c - \bar{\epsilon}F_{c2})$, where the shape dependence is included and the diffuseness correction is calculated exactly by using the folding integral of ref. [11]),

$$F_c(\lambda,\text{shape}) = \frac{15}{32\pi^2\lambda^5} \iint \frac{1}{\xi}\,[1 - (1 + \frac{\xi}{2})e^{-\xi}]d\xi_1^3 d\xi_2^3 \quad ,$$
$$F_{c2}(\lambda,\text{shape}) = -\lambda^2 \frac{d(F_c/\lambda)}{d\lambda} \quad , \tag{3}$$

and $\lambda = R/a_{den}$, $\xi = |\vec{r}_1 - \vec{r}_2|/a_{den}$, a_{den} = range of the density folding function.

In addition to the revised surface and Coulomb energy expressions with their corresponding dependences on shape (through the folding integrals) and scale (through the terms linear in $\bar{\epsilon}$) we added a new term,

$$-C\,A\,e^{-\gamma A^{1/3}}\bar{\epsilon} \quad , \tag{4}$$

with two new adjustable parameters C and γ.

This type of exponential term, non-analytic in the Droplet Model expansion parameter $A^{-1/3}$, appears in folding-type expressions for the interaction energy. It becomes important quantitatively for nuclear configurations in which portions of the surface approach each other to within the range of the folding function. A well-known example is the proximity potential representing the interaction energy of two nuclei about to come into contact. For a single nucleus this type of term becomes important when the nucleus is small enough so that one side of the nucleus can feel the effect of the surface on the other side (i.e. the absence of nuclear matter beyond a certain distance). The usual Yukawa or Yukawa-exponential folding integrals have in them this type of term, but we found that adding an independent contribution of the type of eq. (4) had striking advantages.

Once the DM has been reformulated along the lines described above, the next step is to minimize the energy with respect to variations in $\bar{\epsilon}$ and $\bar{\delta}$ just as was done in ref. [13]). When the new expressions given above are used the final form of the FRDM part of the mass formula is given by,

$$\begin{aligned}&[-a_1 + J\bar{\delta}^2 + \tfrac{1}{2}(K\bar{\epsilon}^2 - 2L\bar{\epsilon}\bar{\delta}^2 + M\bar{\delta}^4)]A \\ &+ (a_2 + \tfrac{9}{4}(J^2/Q)\bar{\delta}^2(B_s/F_s)^2)A^{2/3}F_s \\ &+ a_3A^{1/3}B_k + a_0 + c_1Z^2A^{-1/3}F_c - c_2Z^2A^{1/3}B_r - c_5Z^2(B_wB_s/F_c) \quad ,\end{aligned} \tag{5}$$

where

$$\bar{\delta} = [I - \tfrac{3}{16}(c_1/Q)ZA^{-2/3}(B_vB_s/F_s)]/[1 + \tfrac{9}{4}(J/Q)A^{-1/3}(B_s^2/F_s)] \tag{6}$$

$$\bar{\epsilon} = [-2a_2A^{-1/3}F_{s2} + C\ e^{-\gamma A^{1/3}} + L\bar{\delta}^2 + c_1Z^2A^{-4/3}F_{c2}]/K \tag{7}$$

3. The Complete Mass Formula

In addition to the FRDM of eqs. (5-7) the expression for the atomic mass defect includes the terms,

$$M_HZ + M_nN - a_{e\ell}Z^{2.39} \quad , \tag{8}$$

where M_H and M_n are the mass defects of the hydrogen atom and of the neutron, respectively. The last term represents the binding energy of the atomic electrons.

Also included are the terms,

$$W\left[|I| + \begin{cases} A^{-1} & , \text{ for } Z = N \text{ odd} \\ 0 & , \text{ otherwise} \end{cases}\right] + \begin{cases} +\ [\Delta A^{-1/2} - \frac{1}{2}\,\delta A^{-1}] & Z \text{ and } N \text{ odd} \\ \frac{1}{2}\,\delta\ A^{-1} & Z \text{ or } N \text{ odd} \\ -\ [\Delta A^{-1/2} - \frac{1}{2}\,\delta A^{-1}] & Z \text{ and } N \text{ even}\ , \end{cases} \tag{9}$$

which are a "Wigner term" and a conventional even-odd correction[10]).

Three other terms that are included are,

$$-c_4Z^{4/3}A^{-1/3} - c_a(N - Z) + f_0 \quad . \tag{10}$$

The first of these is an exchange correction to the Coulomb energy, the second is related to a small charge asymmetry of the nuclear force, and the last is a small correction to the Coulomb energy from the proton form factor[11]).

Finally, we have also included the shell, pairing and zero point energies from ref. [11]),

$$E_{\text{shell}} + E_{\text{pairing}} + E_{\text{zero point}} \quad , \tag{11}$$

but with additional effects added in two regions. For radium and some nearby nuclei we added a correction associated with the octupole degree of freedom originally proposed by Leander,[14]) and in the actinide region we used an analytic approximation (fitted to two points from ref. [11]) and to some later studies we have made) for including the effect of an ϵ_6P_6 term in the single particle potential. The greatest effect this term has is -1.4 MeV and the values we used were taken from the expression,

$$\Delta E_{P_6} = \frac{(Z - 100)^2}{36} + \frac{(N - 150)^2}{50} - 1.4 \text{ MeV} \quad ,$$

when the value is negative. When the quantity on the right hand side is positive ΔE is set to zero.

A preliminary set of values for the various coefficients that enter the final mass formula are,

$$
\begin{array}{llll}
a_1 = 16.2663 \text{ MeV} & r_o = 1.16 \text{ fm} \\
a_2 = 23.0 \text{ MeV} & c_1 = \frac{3}{5}(e^2/r_o) \\
a_o = 2.5 \text{ MeV} & c_2 = \frac{1}{84} c_1^2 (\frac{9}{2K} + \frac{1}{4J}) \\
J = 32.5 \text{ MeV} & c_4 = \frac{5}{4}(3/2\pi)^{2/3} c_1 \\
Q = 29.4 \text{ MeV} & c_5 = \frac{1}{64}(c_1^2/Q) \\
K = 240 \text{ MeV} & \\
C = 230 \text{ MeV} & \gamma = 1.27 \\
a_3 = L = M = 0 & \\
M_H = 7.289034 \text{ MeV} & M_n = 8.071431 \text{ MeV} \\
a_{e\ell} = 1.433 \times 10^{-5} \text{ MeV} & W = 34 \text{ MeV} \\
\Delta = 12 \text{ MeV} & \delta = 20 \text{ MeV} \\
c_a = 0.428 \text{ MeV} & f_o = -\frac{1}{8}(r_p^2 e^2/r_o^3)(\frac{145}{48}) \\
a = 0.68 \text{ fm} & a_{den} = (0.99/\sqrt{2}) \text{ fm} \\
e^2 = 1.4399764 \text{ MeV fm} & r_p = 0.8 \text{ fm}
\end{array}
\qquad (12)
$$

4. Results

Of the preliminary parameters listed in eq. (12) only 9 were actually adjusted in the final fit to masses and fission barriers. These were the primary coefficients a_1, a_2, a_o, J and Q; the two new coefficients C and γ in the phenomenological exponential term, and the Wigner and charge asymmetry coefficients W and c_a. The quantity r_o was not easy to vary because of the way the fitting program was originally organized, and comparisons of measured and calculated charge radii suggest that its value should probably be about 1% larger. The quantity actually minimized was $S = \alpha\sqrt{N_m^{-1}\sum_i (\Delta m_i)^2} + \frac{1}{\sqrt{2}}(1-\alpha)\sqrt{N_b^{-1}\sum_i)\Delta h_i)^2}$, where the sums are over the N_m mass deviations Δm_i and the N_b barrier deviations Δh_i. We used a weight of $\alpha = 0.8$ but found that the fit was rather insensitive to this choice.

The data set to which our fitting procedure was applied consisted of 1323 masses (with N and Z = 8 or greater, and experimental errors less than 1 MeV) from the 1977 compilation of Wapstra and Bos[15]) supplemented by 165 additional masses from ref. [16]) The set of 28 fission barriers was the same as the one used earlier by Möller and Nix[11]).

The r.m.s. deviation that we obtained was 0.676 MeV for the masses and 1.135 Mev for the fission barriers. The upper part of fig. 1 compares the measured and calculated deviations from the smooth part of the mass formula (the shell effect). The bottom part of fig. 1 displays the difference between the two, which is also the difference between calculated and measured atomic masses . There is no systematic long-range structure (either along or across the valley of beta-stability) as far as we can tell. The measured and calculated fission barriers are compared in fig. 2.

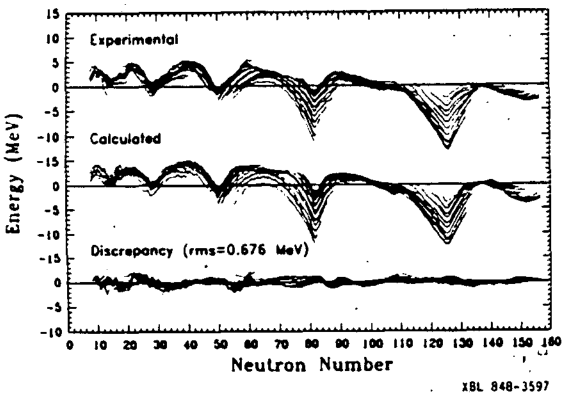


Fig. 1 Comparison of measured and calculated ground-state shell effects for 1488 nuclides.

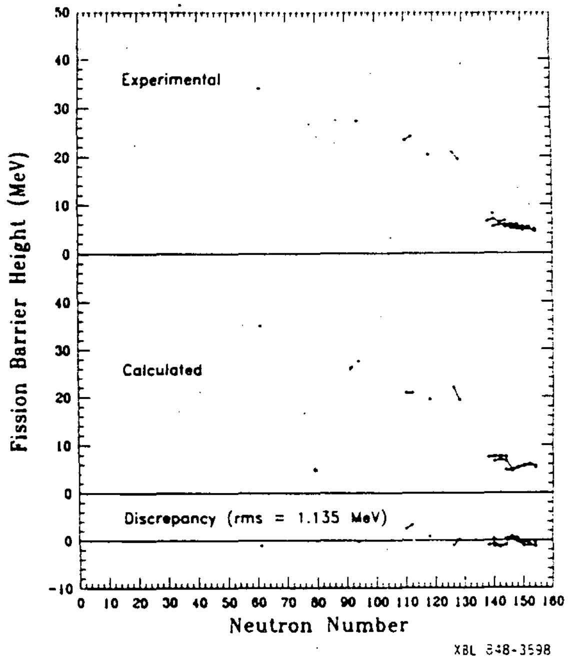
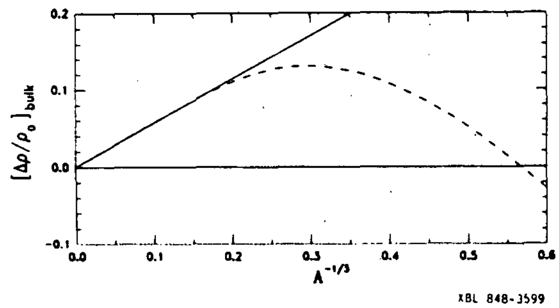


Fig. 2 Comparison of measured and calculated fission-barrier heights for 28 nuclei.

The key to the substantially improved results we have obtained here seems to be the empirical, exponential term of eq. (4). We had hoped that all finite range effects would be adequately represented by the folding model surface energy expression but this was not the case. Fig. 3 serves to illustrate this point. The quantity plotted here versus $A^{-1/3}$ is $(\Delta\rho/\rho_0)_{bulk}$, which is the fractional deviation of the central density of a nucleus from the nuclear matter value. For the idealized case of N = Z nuclei without Coulomb energy the FRDM expression for this quantity is,

$$(\Delta\rho/\rho_0)_{bulk} = 6(a_2/K)A^{-1/3}F_{s2} - 3(C/K)e^{-\gamma A^{1/3}} \quad . \tag{13}$$

The solid line in the figure is the old DM prediction obtained by keeping only the first term and setting $F_{s2} = 1$. Inclusion of the F_{s2} folding model term (using eq. (2)) produces a small reduction in $\Delta\rho/\rho_0$ that is negligible on the scale of this figure. The dashed line illustrates the much more dramatic effect which is produced by including the second term in eq. (13). The behavior of this complete expression corresponds very closely to that found in earlier Thomas-Fermi calculations. (See fig. 30 of ref. [17].) It also corresponds quite closely to the behavior we have noted recently in studies of Hartree-Fock calculations[12]. This is all the more remarkable when we recall that the coefficients of this new phenomenological term were determined solely from a least squares fit to masses and fission barriers. No considerations regarding density distributions governed their determination.



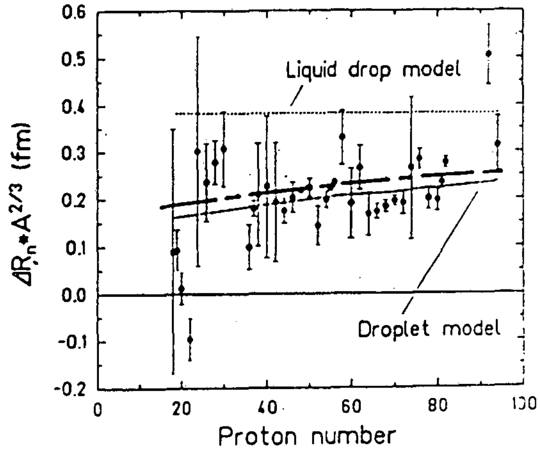


Fig. 3 Fractional deviation of the central density versus $A^{-1/3}$ predicted by the model for hypothetical uncharged nuclei with N = Z.

Fig. 4 The slope ΔR_n (times $A^{2/3}$) of the equivalent sharp change radius versus neutron number is plotted against the charge number Z of the isotopic sequence being considered.

Earlier DM fits to masses had suffered from a disturbing tendency of some of the parameters (notably K and L) to take on unphysical values unless they were constrained. The fit that resulted from fixing the values of such quantities[10]) gave values of J and Q that resulted in poor mass predictions for nuclei far from stability. Discussions of these discrepancies often centered around the asymptotic nature of the DM expansion, and this is just the point that is being addressed by eq. (4). Its inclusion (which must be regarded as empirical at this point) results in substantial improvement in the predictions, elimination of the problem of unphysical parameter values, and significant improvement for nuclei far from stability.

We find that the quantity L is approximately zero (and not well determined). This result also characterizes a number of Skryme forces whose nuclear asymmetry properties have been studied in detail[18]). We also find that the value of Q has increased substantially over earlier determinations. The increase in Q and reduction in L combine to leave nearly unchanged the predictions of the model for isotope shifts in nuclear charge radii. In fig. 4, from ref. [19]), the quantity plotted against the charge number Z is $A^{2/3}$ times the slope governing the increasing size of the charge distribution with increasing neutron number, δR_n. As can be seen in the figure, the Liquid Drop Model predicts that this quantity should be a constant, $(r_0/3)$, which is about twice as large as the measured values for nuclei throughout the periodic table. The Droplet Model of ref. [10]) is represented by the dashed line in the figure, and the predictions of the FRDM described here are given by the dot dashed line.

It is interesting to note that the further developments of the Droplet Model that are described here are bringing the values of the coefficients more in line with those associated with the Skyrme force Hartree-Fock calculations discussed by F. Tondeur in these proceedings.

5. Final Remarks

The development of nuclear mass formulae since the thirties has been characterized by a dramatic improvement in the treatment of shell effects in the sixties and by a more gradual improvement in the smooth part of the equations. Very roughly speaking, the standard Liquid Drop formula considered energy terms of order A and $A^{2/3}$, the Droplet Model extended the expansion to order $A^{1/3}$, and ref. [11]) brought out a significant improvement in the fits associated with an A^0 term (a constant). In the past few years the folding model has also begun to focus attention on the existence of an exponential, non-analytic term in $A^{-1/3}$, inaccessible to a Droplet Model type of expansion in this parameter (see also Grammaticos[20])). The development described in the present paper, based on including an adjustable exponential term of this type, demonstrates the practical utility of such a term and its relation to the problem of surface-tension squeezing of light nuclei. It seems to us that the limit of a useful Droplet Model type of power expansion in $A^{-1/3}$ is probably reached around A^0, and that future efforts should concentrate on a better understanding of the "exponential," non-analytic term. This term focuses attention on a specific feature of a light system, for which the range of the interaction begins to be comparable with its size. This is the opposite extreme from the limit underlying the standard (leptodermous) treatment of saturating systems. Such non-analytic terms might be described as dealing with "desaturating" effects, which begin to dominate for small (holodermous) systems. A general discussion of such terms and their incorporation in mass formulae is an outstanding problem for the future.

The authors wish to acknowledge stimulating discussions with J. R. Nix concerning a number of important features of this work and the continued critical interest of J. M. Pearson and F. Tondeur in the Droplet Model and its limitations.

This work was supported by the Director, Office of Energy Research, Division of Nuclear Physics of the Office of High Energy and Nuclear Physics of the U.S. Department of Energy under Contract DE-AC03-76SF00098.

References

1) C. F. von Weizsäcker, Z. Physik 96 (1935) 431

2) H. A. Bethe and R. F. Bacher, Rev. Mod. Phys. 8 (1936) 82-229

3) W. J. Swiatecki, in W. H. Johnson, Jr., editor, Proc. Second Int. Conf. on Nucleidic Masses (Springer-Verlag, Vienna, 1964) p. 58-66

4) M. Brack, J. Damgaard, A. S. Jensen, H. C. Pauli, V. M. Strutinsky, and C. Y. Wong, Rev. Mod. Phys. 44 (1976) 320-406

5) W. H. Johnson, Jr., editor, Proc. Second Int. Conf. on Nucleidic Masses (Springer-Verlag, Vienna, 1964)

6) R. C. Barber, editors, Proc. Third Int. Conf. on Atomic Masses (Univ. of Manitoba Press, Winnipeg, 1967)

7) J. H. Sanders and A. H. Wapstra, editors, "Atomic Masses and Fundamental Constants 4" (Plenum, London, 1972)

8) J. H. Sanders and A. H. Wapstra, editors, "Atomic Masses and Fundamental Constants 5" (Plenum, New York, 1975)

9) J. A. Nolen, Jr. and W. Benenson, editors, Atomic Masses and Fundamental Constants 6 (Plenum Press, New York, 1979)

10) W. D. Myers
Droplet Model of Atomic Nuclei, IFI/Plenum Data Co., New York, N.Y. (1977)

11) P. Moller and J. R. Nix, Nucl. Phys. A361 (1981) 117-146

12) J. Treiner, W. D. Myers, W. J. Swiatecki, and M. Weiss, manuscript in preparation

13) W. D. Myers and W. J. Swiatecki, Ann. Phys. (N.Y.) 84 (1974) 186-210

14) G. A. Leander, R. K. Sheline, P. Möller, P. Olanders, I. Ragnarsson, and A. J. Sierk, Nucl. Phys. A388 (1982) 452

15) A. H. Wapstra and K. Bos, At. Data Nucl. Data Tables 19 No. 3 (1977)

16) A. H. Wapstra, 1981 Mass Evaluation, private communication

17) W. D. Myers and W. J. Swiatecki, Ann. Phys. (N.Y.) 55 (1969) 395-505

18) M. Farine, J. M. Pearson, and B. Rouben, Nucl. Phys. A304 (1978) 317-26

19) W. D. Myers and K-H Schmidt, Nucl. Phys. A410 (1983) 61-73

20) B. Grammaticos, Ann. Phys. (N.Y.) 139 (1982) 1-13

TECHNICAL INFORMATION DEPARTMENT
LAWRENCE BERKELEY LABORATORY
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720