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Nuclear Mass Formula with a Neutron Skin Degree of Freedom and Finite-Range Model for the Surface Energy*

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We study the possibility of extending the model used by Möller and Nix in 1980 to calculate nuclear masses and fission barriers for nuclei throughout the periodic system, to include provision for the existence of a neutron skin.

The calculation [1] in 1980 yielded an r.m.s. deviation in the ground-state mass of 0.835 MeV and an r.m.s. in the fission barrier height of 1.331 MeV. This calculation used the approach where the energy as a function of shape is calculated as a sum of a macroscropic term and a microscopic term. The macroscopic term varies smoothly with particle number and deformation and changes by about 200 MeV during the fission of a heavy system. The microscopic term, which arises due to the non-uniform distribution of single-particle levels is a rapidly fluctuating term, where the magnitude of the fluctuations are typically a few MeV but may reach values of about 12 meV at doubly closed shells.

The values above, of the r.m.s. deviations, imply that the model of ref. [1] was very successful in describing ground state masses and fission barriers. In particular it was able to give correctly, for the first time, the fission barriers of medium heavy nuclei with A = 110 and A = 160. Also, in a survey of various mass models in ref. [2] the above model was the only one that yielded a smaller r.m.s. deviation, for a set of new masses determined in recent experiments, than was obtained in the original adjustment.

This model is fully discussed in refs. [1,3]. For orientation we give here its main features before we discuss our study of its generalization to include the description of compressibility effects and the neutron skin. The microscopic single-particle and pairing effects were determined from single-particle levels calculated for a Folded-Yukawa single-particle potetial. The macroscopic model used was similar to the standard liquid drop model [4] with the following important modifications:

1) In the surface energy expression the surface area was replaced by an expression that takes into account the reduction in surface energy due to the finite range of the nuclear force. This is important, for instance, for saddle point shapes with a well developed neck. The expression used was the Yukawa-plus-exponential model.
2) The Coulomb diffuseness correction was calculated exactly.
3) A charge asymmetry term and a proton form factor correction was added.
4) An A° term was included.

We have studied the possibility of generalizing the above model to describe compressibility effects and the effect of a neutron skin. These effects have been extensively studied earlier by Myers and Swiatecki [5] in the framework of the macroscopic "Droplet Model."

Arguments similar to those used to derive the "Droplet Model" may be used to generalize the model studied in ref. [1] to include neutron skin and compressibility effects. However, we found that the inclusion of a compressibility term with the standard choice of the compressibility coefficient K = 240 MeV, considerably increased the r.m.s. deviations.

We subsequently found that if we permitted the value of K to be determined by the masses themselves it was so large that its influence on nuclear properties became negligible. Consequently, we have chosen to limit our studies, for the moment, to the effects of including the neutron skin thickness as a degree of freedom in the model. No new parameters are introduced. The previously determined surface symmetry energy term is simply written in a slightly different form. This new form, taken from the Droplet Model theory, allows the generalization of the model of ref. [1] to give a fairly accurate description of isotopic trends in nuclear charge radii.

Below we give the expression for the nuclear potential energy, both the expression used by ref. [1] and the generalized expression we use here. Terms specific to the model of ref. [1] are written to the left, the modified terms specific to the generalized model studied here are written to the right, and terms common to both models are written across the page below.

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$$-a_1\,(1-K_v I^2)\,A + a_2\,(1-K_s I^2) A^{2/3} F_s \qquad\qquad +(-a_1 + J\bar{\delta}^2)A + (a_2 + kJ\bar{\delta}^2 B_s^2/F_s^2) A^{2/3} F_s$$

$$+ f(k_f r_p) \qquad\qquad + f_0(k_f r_p) - C_2 Z^2 A^{1/3} B_r - C_5 Z^2\,(B_w B_s / F_c)$$

$$+M_H Z + M_n N + a_0 A^0 + C_1 (Z^2/A^{1/3}) F_c - C_4 Z^{4/3}/A^{1/3} - C_a(N-Z) - a_{el} Z^{2.39} + \begin{cases} [\Delta/A^{1/2} - \frac{1}{2}\,\delta/A], & Z \text{ and } N \text{ odd} \\ \frac{1}{2}\,\delta, & Z \text{ or } N \text{ odd} \\ [\Delta/A^{1/2} - \frac{1}{2}\,\delta/A], & Z \text{ and } N \text{ even} \end{cases}$$

$$+W\left[\,|I| + \begin{matrix} 1/A, & Z = N \text{ odd} \\ 0, & \text{otherwise} \end{matrix}\right] + E_{shell}\,(Z,N,\text{ Shape}) + E_{pair}\,(Z,N,\text{ Shape}) + E_{zp}\,(\quad,N,\text{ Shape})$$

In the above expression F_s, F_c, f and f_0 are given by:

$$F_s = -\frac{A^{-2/3}}{8\pi^2 r_0^2 a^3} \iint_V \left(\frac{|\bar{r}-\bar{r}'|}{a} - 2\right) \frac{e^{-|\bar{r}-\bar{r}'|/a}}{|\bar{r}-\bar{r}'|}\, d^3r\, d^3r' \quad ,$$

$$F_c = \frac{15}{32\pi^2} \cdot \frac{1}{(r_0 A^{1/3})^5} \iint_V \frac{d^3r\, d^3r'}{|\bar{r}-\bar{r}'|} \left\{ 1 - \left[1 + \frac{1}{2}\,\frac{|\bar{r}-\bar{r}'|}{a_{den}} \right] e^{-\frac{|\bar{r}-\bar{r}'|}{a_{den}}} \right\} ,$$

$$f(k_f r_p) = -\frac{1}{8}\,\frac{r_p^2 e^2}{r_0^3} \left[\frac{145}{48} - \frac{327}{2880}\,(k_f r_p)^2 + \frac{1527}{1209600}\,(k_f r_p)^4 \;\frac{Z^2}{A} \right] ,$$

and f_0 simply keeps the first term in this expression.

The quantity $k_f = [(9/4)\pi Z/A]^{1/3}/r_0$ is the Fermi wave number. The quantities F_s, F_c and f are discussed in refs. [1,2]. We have in this work chosen the constants that multiply the integrals in the expressions for F_s and F_c such that F_s and F_c are 1 for a sphere in the limit the diffuseness constant goes to zero. The quantity f accounts for the effect of the finite size of the proton.

In this study we have truncated the expression f and keep only the first term. In the mass formula we investigate here (right column in the expression above for the potential energy) there enters the quantity $\bar{\delta}$. The quantity $\bar{\delta}$ represents the bulk nuclear asymmetry, it is defined by $\bar{\delta} = [(\rho_n - \rho_z)/\rho_{bulk}]$, and it is related to the overall asymmetry $I = (N-Z)/A$ by the "geometrical" relationship, $\bar{\delta} = I - \frac{3}{2}(t/R)$, where t is the neutron skin thickness and R the nuclear radius. When the energy of the nucleus is minimized with respect to the skin thickness the following expression for $\bar{\delta}$ is obtained:

$$\bar{\delta} = \left[I + \frac{3}{16} \cdot \frac{C_1}{Q} \cdot Z A^{-2/3}\,(B_v B_s/F_s)\right] \Big/ \left[1 + \frac{9}{4} \cdot \frac{J}{Q} \cdot A^{-1/3}\,(B_s^2/F_s)\right].$$

This expression should be considered as auxiliary to the mass equation itself since it must be used to calculate $\bar{\delta}$ for subsequent substitution.

The quantities B_s, B_v, B_r and B_w are the Droplet Model surface, neutron skin, volume redistribution and surface redistribution energies respectively [5]. Furthermore we have

$$C_1 = \frac{3}{5}\,\frac{e^2}{r_0}\,, \quad C_2 = \frac{C_1}{336J}\,, \quad C_4 = \frac{5}{4}\,\frac{3^{-2/3}}{2\pi}\,C_1, \quad C_5 = \frac{1}{64}\,\frac{C_1^2}{Q}, \quad \text{and } k = \frac{9}{4}\,\frac{J}{Q}\,.$$

$$F = a \left[\sum_{i=1}^{N_m} (m_i^{calc} - m_i^{exp})^2 \right] / N_m + \frac{(1-a)}{2} \left[\sum_{i=1}^{N_b} (b_i^{calc} - b_i^{exp})^2 \right] / N_b$$

Here m stands for ground-state mass and b for the fission-barrier height. Thus F is a weighted sum of the r.m.s. deviation for the ground-state masses and for the fission-barrier heights. Because of the strong coupling between the volume and surface energy term it was not possible to determine a few parameters from an adjustment to fission-barrier heights alone, as was done in ref.[1] where the surface energy coefficient a_s and the surface symmetry coefficient κ_s could be determined from an adjustment to fission barriers alone. In our investigation here we take from ref.[3] the values of the following parameters:

M_H	= 7.289034 MeV	hydrogen-atom mass excess	δ	= 20 MeV	pairing-asymmetry constant
M_n	= 8.071431 MeV	neutron mass excess	r_p	= 0.80 fm	proton room-mean-square radius
e^2	= 1.4299764 MeV fm	square of electronic	r_0	= 1.16 fm	nuclear-radius constant
a_{den}	= $0.99/2^{1/2}$fm	range of Yukawa function in Coulomb energy calculation	a	= 0.68 fm	range of Yukawa-plus exponential potential
a_{el}	= 1.433×10^{-5}MeV	electronic-binding constant	c_a	= 0.212 MeV	charge-asymmetry constant
Δ	= 12 MeV	pairing-energy constant			

The adjustment procedure for determining the remaining parameters is fairly involved. As input we use shell and pairing corrections and zero-point energies calculated at the appropriate ground-state and saddle-point deformations. These are taken from the work of ref.[1]. We have also calculated the shape-dependent functions F_s, F_c, B_s, B_r, B_v and B_w at these same ground-state and saddle-point shapes. We then minimize the function F with respect to some set of parameters with prescribed initial values. We have checked that, although the function F is non-linear, the same result is obtained with very different sets of initial values. We consider the same set of experimental ground state masses and fission barriers as did ref. [1]. We have determined the remaining parameters of the model from adjustment to data by performing the minimization in the following steps. First we observe that the Wigner term was introduced to account for a V-shaped kink in the mass surface (see discussion in ref [7] for N = Z). Thus its magnitude is best determined by considering nuclei with N Z. We therefore determine the Wigner coefficient by considering only nuclei with $A \leq 70$. The resulting value of W is 22 MeV. In the following we therefore keep W fixed at 20 MeV. We now determine the parameters a_1, a_2, J, Q and a_0 by minimizing F with 1323 masses and 28 fission barriers taken into account. For the remaining parameters we find:

a_1	= 15.9837 MeV	volume energy constant	k	= 1.7029	surface symmetry factor
a_2	= 20.9406 MeV	surface energy constant	a_0	= 6.73 MeV	constant term
J	= 28.6275 MeV	symmetry energy			

and as discussed above, W = 20 MeV.

The resulting barrier r.m.s. deviation is 1.245 MeV and ground-state r.m.s. deviation is 0.843 MeV. We show, in fig. 1, plots of experimental and calculated ground-state shell corrections and their difference (which is identical to the difference between experimental and calculated masses). In fig. 2 we show experimental and calculated fission barriers and their difference. There seem to be no systematic increases in the deviations far from stability in these figures. We have, in addition, investigated the predictions of this model by calculating masses far from stability and comparing the calculated results to newly available data on masses that were not used in the determination of the model parameters. We find, for instance, that the model gives -51.26 MeV for the mass excess of ^{99}Rb (one of the most neutron-rich nuclei known) compared to an experimental value [8] of -50.60 MeV. Also other calculated results far from stability show very good agreement with new experimental data.

The effect of adding the neutron skin degree of freedom can be seen in fig. 3, from ref. [9]. 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 thefigure 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. [7] is represented by the dashed line in the figure, and the predictions of the combined model described here are given by the dot dashed line.

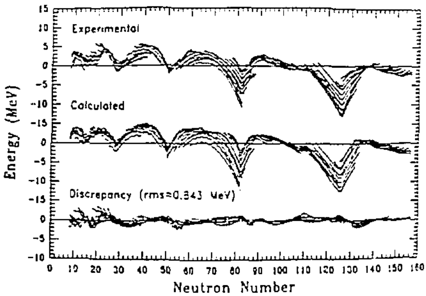

Figure 1.

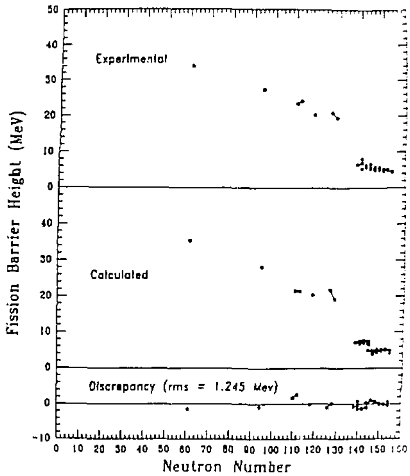

Figure 2.

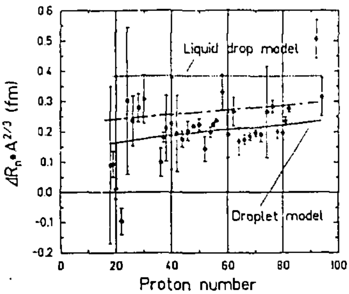

Figure 3.

By adding the neutron skin thickness degree of freedom from the Droplet Model we have been able to extend the results of ref.[1] to include a substantially improved prediction of the isotopic trends in charge radii. The excellent fit to masses and fission barriers is retained and no additional parameters are introduced. In addition, a number of important, and unresolved, issues are raised by this work. *For example, we find no indication of curvature or* compressibility effects even though there is substantial evidence in the literature that such effects should be present. At the moment we view the approach outlined here as an improvement over ref.[1] but phenomenological in nature because important physical effects have been suppressed to improve the fit to data.

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