Liquid Drop Model with Different Neutron versus Proton Deformations

A. Dobrowolski\textsuperscript{1}, K. Pomorski\textsuperscript{1,2}, J. Bartel\textsuperscript{2}

\textsuperscript{1}Katedra Fizyki Teoretycznej, Uniwersytet M.C. Skłodowskiej, Lublin, Poland
\textsuperscript{2}IReS – IN\textsubscript{2}P\textsubscript{3} – CNRS and Université Louis Pasteur, Strasbourg, France

October 29, 2018

Abstract

The nuclear binding energies for 28 nuclei including several isotopic chains with masses ranging from $A = 64$ to $A = 226$ were evaluated using the Skyrme effective nucleon-nucleon interaction and the Extended Thomas-Fermi approximation. The neutron and proton density distributions are assumed in the form of Fermi functions the parameters of which are determined so as to minimize the total binding energy of any given nucleus. The present study is restricted to quadrupole shapes, but the neutron and proton density distributions are free to have different deformations. A simple expression for the variation of the nuclear energy with the neutron–proton deformation difference is derived.

PACS number: 21.60.Jz, 21.10.Dr, 21.10.-k, 21.10.Pc

1 Introduction

The analysis of the experimental data on electron and $\alpha$–particle scattering, pionic atoms, and annihilation of antiprotons show that, in most nuclei, neutrons and protons have slightly different r.m.s. radii \cite{1}. The main reasons for this difference are the Coulomb repulsion between protons and unequal numbers of neutrons and protons.

Fully microscopic approaches of the Hartree-Fock (HF) type using the effective nucleon-nucleon interactions of the Skyrme or Gogny type \cite{2,3}, as well as the relativistic mean field theory \cite{4} reproduce in a rather satisfactory way the experimental proton and neutron r.m.s. radii and their isotopic shifts \cite{4,5,6}.

In deformed nuclei, neutron and proton density distributions are expected to have not only different radii, but also exhibit different shapes, i.e. different quadrupole and higher multipole deformations. An analysis of theoretical densities based on a surface multipole moment expansion shows that significant differences between neutron and proton deformations often occur

\textsuperscript{*}The work was partially sponsored by the Polish Committee of Scientific Research KBN No. 2P 03B 115 19, POLONIUM No. 017 04 UG (2001)
both in the ground state \[5\] as well as along the whole path to fission \[7\]. The Hartree-Fock-Bogolubov (HFB) calculation performed with the Gogny effective force in Ref. \[7\] for \(^{232}\)Th, \(^{236}\)U, \(^{238}\)U and \(^{240}\)Pu have shown that the multipole deformations of the proton and neutron density distributions of fissioning nuclei are far from being equal. The relative difference between them exceeds often 10 % and undergoes large variations which means that the thickness of the neutron skin does not remain constant as the fissioning nucleus elongates. The effect on the nuclear binding energy of these deformation differences was found to reach approximately 1.5 MeV, with fluctuations of the order of 1 MeV \[7\]. These variations are clearly not negligible compared to typical fission barrier heights.

Until now a large majority of macroscopic-microscopic type calculations of potential energy surfaces of fissioning nuclei assume equal deformations of proton and neutron distributions for both densities and single-particle potentials (see e.g. \[8, 9, 10\]). In view of the results obtained in Ref.\[7\], one can expect that such calculations predict fission barriers that are systematically about 1 MeV too high. In a sense things are even worth in the case of macroscopic-microscopic calculations as compared to the selfconsistent Hartree-Fock approach where deformation energy surfaces are usually generated through calculations with a constraint on some multipole moments of the mass distribution, which leaves protons and neutrons free to deform differently within this constraint, even though it of course turns out that these deformations are quite close to one another. One must note, however, that only the fluctuating part of the correction for the proton and neutron deformation difference can actually influence barrier heights calculated with the macroscopic-microscopic approach, since the average value of this difference can be taken into account in the fitting procedure of the parameters of the macroscopic (e.g. liquid drop) model. Neglecting the neutron-proton deformation differences in both the macroscopic and microscopic parts of the potential energy could then lead to an overestimation of spontaneous fission lifetimes by a few orders of magnitude in heavy and superheavy nuclei and could also have a non negligible effect on the binding energy difference between neighboring nuclei what will be reflected in predicted lifetimes for the \(\alpha\) or electron-capture decays.

The aim of the present investigation is to develop a new term in the liquid drop type mass formula which will approximate the average variation of the binding energy when protons and neutrons deform in a different way. It seems to us that the most suitable approach to this goal is the Extended Thomas–Fermi (ETF) approximation \[11\] in connection with the Skyrme energy functional \[2\]. After a short outline of the model we present results of our calculations for a large sample of nuclei and derive a simple approximate expression which nicely reproduces the effect of the proton and neutron deformation difference in a deformed macroscopic model.

## 2 Description of the model

### 2.1 Skyrme density functional and the Thomas–Fermi approximation

In order to determine nuclear binding energies one often uses effective nucleon–nucleon interactions of the Skyrme type which describes quite accurately nuclear ground–state properties as well as the low-lying collective excitations \[12\]. For such an interaction the total energy density \(\mathcal{E}(\vec{r})\) is an algebraic function of the neutron and proton densities \(\rho_n\) and \(\rho_p\), of the kinetic energy densities \(\tau_n\) and \(\tau_p\) and the spin-orbit densities \(\vec{J}_n\) and \(\vec{J}_p\) \[2\].
\[
\mathcal{E}(\vec{r}) = \int \left\{ \frac{\hbar^2}{2m} [\tau_n + \tau_p] + \frac{1}{2} t_0 \left[ (1 + \frac{1}{2} x_0) \rho^2 - (x_0 + \frac{1}{2} \rho_n^2 + \rho_p^2) \right] \\
+ \frac{1}{4} (t_1 + t_2) \rho \tau + \frac{1}{8} (t_2 - t_1) (\rho_n \tau_n + \rho_p \tau_p) + \frac{1}{16} (t_2 - 3t_1) \rho \nabla^2 \rho \\
+ \frac{1}{32} (3t_1 + t_2) (\rho_n \nabla^2 \rho_n + \rho_p \nabla^2 \rho_p) + \frac{1}{4} t_3 \rho \rho_n \rho_p \\
- \frac{W_0}{2} \left[ \vec{J} \cdot \vec{\nabla} \rho + \vec{J}_n \cdot \vec{\nabla} \rho_n + \vec{J}_p \cdot \vec{\nabla} \rho_p \right] + \frac{1}{16} (t_1 - t_2) (\vec{J}_p^2 + \vec{J}_n^2) \right\} d^3 r ,
\]

where non-indexed quantities such as \( \rho \) stand for the sum of the corresponding quantities for neutrons and protons, as e.g.

\[
\rho = \rho_n + \rho_p \tag{2}
\]

and where \( t_0, t_1, t_2, t_3, x_0 \) and \( W_0 \) are force parameters which can be adjusted so as to reproduce nuclear ground-state properties (binding energies, radii, nuclear spectra, etc.).

In a first approximation the nuclear energy (without Coulomb term) could be calculated by using the Skyrme functional (1) and the Thomas-Fermi (TF) approximation where

\[
\tau_q = \frac{3}{5} (3\pi)^{2/3} \rho_q^{5/3} , \quad q = \{n, p\} .
\]

There is no contribution at this (TF) order of the semiclassical expansion to the spin-orbit density \( \vec{J}_q \) as the spin has no classical analogon. These terms are therefore omitted in the following calculations.

### 2.2 The model with sharp-surface distribution

If only ellipsoidal deformations are considered, one can describe the surfaces of nuclei by a very simple parameterization, using a single deformation parameter \( \sigma \). The lengths of the axis of the axially symmetric ellipsoids are then given by [3]:

\[
\begin{align*}
a &= b = R_0_q \exp \left[ -\frac{1}{2} \sigma_q \right] , \\
c &= R_0_q \exp \left[ \sigma_q \right] ,
\end{align*}
\]

where \( R_0^{(n)} \) and \( R_0^{(p)} \) are the radii of the neutron and proton distributions respectively. Obviously \( \sigma > 0 \) correspond to prolate and \( \sigma < 0 \) to oblate deformations. Introducing the isospin parameter

\[
I = \frac{N - Z}{A} \tag{5}
\]

the following dependence on \( A \) and \( I \) was obtained in the RMF calculation of Ref. [3]

\[
R_0_p = 1.237 \left( 1 - 0.157 I - \frac{0.646}{A} \right) A^{1/3} \text{ fm} , \tag{6}
\]

\[
R_0_n = 1.176 \left( 1 + 0.250 I + \frac{2.806}{A} \right) A^{1/3} \text{ fm} . \tag{7}
\]

For ellipsoidal deformations it can be shown that the nuclear surface is given by

\[
R_q(\theta) = \frac{ac}{\sqrt{a^2 \cos^2(\theta) + c^2 \sin^2(\theta)}} . \tag{8}
\]
It is obvious that in the case of different deformations and sharp distributions of protons and neutrons there will appear regions in which there exist only protons or neutrons and other regions where both types of particles coexist. In order to evaluate the nuclear energy in such a case, the Skyrme functional depending on the nucleon densities, can be separated in three terms depending only on the proton density, only on the neutron density and an interaction term depending on the densities of both type of particles:

\[
V_q = \frac{1}{4} t_0 (1 - x_0) \rho_q^2 + \frac{1}{8} (t_1 + 3t_2) \rho_q \tau_q + \frac{3}{32} (t_2 - t_1) \rho_q \nabla^2 \rho_q ,
\]

(9)

where \( q = \{ n, p \} \),

\[
V_{pn} = t_0 (1 + x_0) \rho_p \rho_n + \frac{1}{4} (t_1 + t_2) (\rho_p \tau_n + \rho_n \tau_p)
- \frac{1}{16} (3t_1 - t_2) (\rho_p \nabla^2 \rho_n + \rho_n \nabla^2 \rho_p) + \frac{1}{4} t_3 (\rho_n^2 \rho_p + \rho_p^2 \rho_n) .
\]

(10)

Finally, \( E \) can be written as

\[
E = \frac{\hbar^2}{2m} (\tau_n + \tau_p) + V_p + V_n + V_{pn} .
\]

(11)

The total nuclear energy \( E_{\text{nuc}}(N, Z) \) is then given as the volume integral of \( E(\vec{r}) \).

\[
E_{\text{nuc}}(N, Z) = \int E(\vec{r}) \, d^3 r .
\]

(12)

In the case of a sharp surface distribution the changes of the nuclear part of the energy as a function of deformation can be just expressed as the product of the volume \( \Omega_{pn} \) where protons and neutrons coexist and the term of the energy density connected with the interaction of these two types of particles:

\[
\Delta E_{\text{nuc}}(\Delta \sigma) = V_{pn} \Omega_{pn} ,
\]

(13)

where

\[
\Omega_{pn} = \frac{4}{3} \pi (R_{0n})^3 \left\{ \left[ 1 - \left( \frac{R_{pn}}{R_{0n}} \right)^2 \exp(\Delta \sigma) - 1 \right] \exp(3\Delta \sigma) - 1 \right\}^{3/2}
- \frac{4}{3} \pi (R_{0p})^3 \left\{ \left[ 1 - \left( \frac{R_{pn}}{R_{0p}} \right)^2 - 1 \right] \exp(-3\Delta \sigma) - 1 \right\}^{3/2}.
\]

(14)

with \( \Delta \sigma = \sigma_n - \sigma_p \).

One should notice that for this type of nucleon densities, the terms of \( E(\vec{r}) \) with \( \Delta \rho \) vanish, so that the nuclear energy doesn’t change during the deformation process as long as the proton and neutron distribution don’t cross each other, since the volumes between the sharp surfaces is kept constant. After the surfaces intersect the energy rapidly decrease because there the region in which protons and neutrons coexist \( \Omega_{pn} \) changes its volume as a function of the deformation. This fact leads to the changes of the term \( V_{pn} \), while terms \( V_p \) and \( V_n \) are constant. A typical behavior of the binding energy with growing proton–neutron deformation difference is presented in Fig. 1. The model with the uniform density distribution is, of course, too rough to make a realistic estimates but nevertheless it should give some idea about the main effect.
2.3 The model with the Fermi-type distribution.

More accurate estimates of the change of the binding energy when the protons and neutrons deform differently can be made with diffuse density profiles. In the following we have chosen for our analysis the density distributions in the form of Fermi functions

$$
\rho_q(r, \theta) = \frac{\rho_{0q}}{1 + \exp\left(\frac{r - R_q(\theta)}{a_q(\theta)}\right)},
$$

where $$\rho_{0q}$$ are the saturation density parameters obtained from the normalization conditions:

$$
\int \rho_p(r)d^3r = Z, \quad \int \rho_n(r)d^3r = N
$$

and where $$R_q(\theta)$$ is given by Eq. (8). The surface width parameters $$a_q$$, are $$\theta$$ dependent and equal to

$$
a_q(\theta) = \sqrt{\sin^4(\theta) + \cos^4(\theta) + \sin^2(\theta)\cos^2(\theta)[\exp(3\sigma_q) + \exp(-3\sigma_q)]} a_0
$$

a definition which guarantees that the surface diffuseness is constant along the direction perpendicular to the surfaces of the ellipsoids. The parameters $$\{R_{0n}, a_{0n}, R_{0p}, a_{0p}\}$$ characterizing the spherical density distribution of neutrons and protons are obtained by a minimization procedure of the energy functional [1] within the second order ETF approximation [11] and using the Skyrme SIII force [14].

3 Results of the fits

The calculation were performed for 28 even-even nuclei involving several isotopic chains from Ni to Th. We suppose that the deformation of these nuclei can be characterized by a single global deformation parameter $$\alpha$$ plus a quadrupole type deformation parameter $$\Delta \tilde{\beta} = \tilde{\beta}_n - \tilde{\beta}_p$$ measuring the difference in the proton versus neutron deformation. The global deformation of the nucleon distribution can be e.g. defined through the parameter $$\alpha$$ introduced by Myers and Świątecki [13]

$$
\alpha^2 = 2\pi \int_0^{\pi} d\theta \left[ \frac{R(\theta) - R_{00}}{R_{00}} \right]^2,
$$

where $$R(\theta)$$ is the half-density radius of the nucleon distribution of the deformed nucleus and $$R_{00}$$ the radius of the corresponding spherical distribution. For an ellipsoidal deformation as characterized by Eq. (4) $$\alpha$$ can be easily expressed in terms of the parameter $$\sigma$$ and one obtains

$$
\alpha^2 = \sigma^2[1 - \frac{1}{7}\sigma + \mathcal{O}(\sigma^2)]
$$

In order to be able to express the total energy as a function of the difference $$\Delta \tilde{\beta}$$ between the proton versus neutron deformation we need to find a way to express this difference in a way which is independent of the specific choice of the deformation parameters like e.g. in Eq. (3). We have chosen to define parameters $$\tilde{\beta}_q$$ as:

$$
\tilde{\beta}_q = \frac{Q_{20}^{(q)}}{Q_{00}^{(q)}},
$$
where the $Q^{(q)}_{00}$ are the monopole and $Q^{(q)}_{20}$ the quadrupole moments of the proton and neutron distribution with:

$$Q^{(q)}_{\lambda 0} = \int \rho_q(\vec{r}) r^2 P_\lambda d^3r ,$$ \hfill (21)

and where

$$Q^{\text{tot}}_{00} = Q^{(n)}_{00} + Q^{(p)}_{00} ,$$

$$\tilde{Q}^{(p)}_{00} = Q^{\text{tot}}_{00} \frac{Z}{A} ,$$

$$\tilde{Q}^{(n)}_{00} = Q^{\text{tot}}_{00} \frac{N}{A} .$$ \hfill (22)

are the so-called average monopole moments for protons and neutrons respectively.

We have found that contrary to the rapid change (Fig. 1) of the binding energy in case of the sharp-edge density distribution the nuclear part of energy varies almost parabolically with the proton and neutron deformation difference $\Delta \tilde{\beta}$ when the smooth density profile ([13]) is assumed for protons and neutrons.

The binding energy can then be parametrized in the following form

$$B(A, I, \alpha, \tilde{\beta}_n, \tilde{\beta}_p) = B_{\text{avr}}(A, I, \alpha) + a(A, I, \alpha) \cdot (\tilde{\beta}_n - \tilde{\beta}_p)^2 ,$$ \hfill (23)

where $B_{\text{avr}}$ is the part of the energy that is generated for equal deformations for protons and neutrons and which can be obtained e.g. form the standard liquid drop or droplet model. To determine the stiffness parameter $a$ of the parabolic form in $\Delta \tilde{\beta}$ we proceed in the following way:

For various nuclei with different values of the mass parameter $A$ and isospin parameter $I$ and for $\alpha \neq 0$ one finds that this parameter $a(A, I, \alpha)$ can be expressed in the form

$$a(A, I, \alpha) = a_0(A, I) [1 - c_2 \alpha(1 + c_3 I)] ,$$ \hfill (24)

where the deformation independent coefficient $a_0(A, I)$ can be parametrized as

$$a_0(A, I) = c_1 \left( \frac{A^{1/3}}{A} \right)^n .$$ \hfill (25)

The values found by our fitting procedure for the parameters $c_1$, $c_2$, $c_3$ and $n$ are the following

$$c_1 = 1.21 \text{ MeV} , \quad c_2 = 3.0 , \quad c_3 = 3.0 , \quad n = 4 .$$

The stiffness parameter $a(A, I, \alpha)$ evaluated for all considered isotopic chains is compared on the l.h.s. of Fig. 2 at $\alpha = 0$ deformation with the parameter $a_0(A, I)$, Eq. (25). The $\alpha$ deformation dependence of the parameter $a(A, I, \alpha)$ is illustrated on the r.h.s. of Fig. 2. We have also compared the above estimate of $a(A, I, \alpha)$ with the results obtained using two other Skyrme interactions. We have found that the estimates obtained with the Skyrme SII and SVII forces are identical to those of presented above for SIII within a 10%.

The quality of the fit of the binding energy as function of the deformation difference is demonstrated on Fig. 3 for three nuclei ($^{98}$Zr, $^{146}$Nd and $^{208}$Pb) and for three different values of the global deformation parameter $\alpha$ and compared with the corresponding ETF results.

In order to test the predictive power of equation (23) we have performed an additional calculation for three dysprosium isotopes (neutron deficient, $\beta$-stable and neutron rich) and compare in Fig. 4 their ETF energies (crosses) with the approximation given by (23) (solid
line) and this for three different deformation. As can be seen in Fig. 4 the agreement of both results is rather satisfactory in all cases, except for the very deformed neutron deficient $^{150}$Dy isotope.

When $\alpha \neq 0$ and $(\tilde{\beta}_n - \tilde{\beta}_p) = 0$, the energy is reproduced by the standard liquid drop model or any other macroscopic model.

4 Discussion and conclusions

We have found a very simple procedure to describe the influence on the total nuclear energy arising from the fact that neutron and protons might deform differently. The additional term in the nuclear mass formula which we obtain is proportional to the square of the deformation difference of both distributions and increases as $A^{4/3}$.

This suggest that it might be useful to generalize the currently used macroscopic-microscopic approaches in order to allow protons and neutrons to have different multipole deformations. One could start from a Strutinsky type prescription:

$$ E_{\text{Strut}}(\{\beta_\lambda^{(p)}\}, \{\beta_\lambda^{(n)}\}) = E_{\text{macr}}(\{\beta_\lambda^{(p)}\}, \{\beta_\lambda^{(n)}\}) + \delta E_{\text{micr}}^{(p)}(\{\beta_\lambda^{(p)}\}) + \delta E_{\text{micr}}^{(n)}(\{\beta_\lambda^{(n)}\}), \quad (26) $$

where both the macroscopic and and microscopic components depend on proton and neutron deformations. Then, performing a minimization with respect to e.g., the neutron multipole deformations while keeping proton deformations as independent variables (or the other way around), should give a more realistic description of potential energy surfaces. Details of such a method as, for instance, the way to generalize macroscopic models in order to include different deformations for protons and neutrons, are left for a future study.

It was already shown in Ref. [7] that taking into account the proton versus neutron deformation difference could shift the position of the ground state and saddle point in the potential energy surface by as much as 0.5 MeV. Such an effect could improve the predictions of nuclear masses as given by macroscopic–microscopic type of models [8] and change the predicted barrier heights. In consequence the effect discussed in the present paper could change the theoretical predictions of $\alpha$-decay and spontaneous-fission life times [8, 10].

Acknowledgements

Two of us (A.D. and K.P.) are very grateful for the nice hospitality extended to them by the Nuclear Theory Group of the IReS in Strasbourg.
References

[1] C.J. Batty, E. Friedman, H.J. Gils, and H. Rebel, Adv. Nucl. Phys. 19, 1 (1989).
[2] D. Vautherin, D.M. Brink, Phys. Rev. C5, 626 (1972).
[3] J. Dechargé and D. Gogny, Phys. Rev. C21, 1568 (1980).
[4] A. Baran, J. L. Egido, B. Nerlo-Pomorska, K. Pomorski, P. Ring, and L. M. Robledo, J. Phys. G21, 657 (1995).
[5] K. Pomorski, P. Ring, G. A. Lalazissis, A. Baran, Z. Lojewski, B. Nerlo-Pomorska, and M. Warda, Nucl. Phys. A624, 349 (1997).
[6] M. Warda, B. Nerlo-Pomorska, and K. Pomorski, Nucl. Phys. A635, 484 (1998).
[7] J.F. Berger and K. Pomorski, Phys. Rev. Lett. 85, 30 (2000).
[8] R. Smolańczuk, J. Skalski, and A. Sobiczewski, Phys. Rev. C52, 1871 (1995).
[9] P. Moeller, J.R. Nix, W.D. Myers, and W.J. Świątecki, Atomic Data Nucl. Data Tables 59, 185 (1995).
[10] Z. Lojewski and A. Staszczak, Nucl. Phys. A657, 134 (1999).
[11] M. Brack, C. Guet, H.-B. Håkansson, Phys. Rep. 123, 275 (1985).
[12] P. Quentin and H. Flocard, Ann. Rev. Nucl. Part. Sci. 28, 523, (1978).
[13] W.D. Myers, W.J. Świątecki, Nucl. Phys. 81, 1 (1966).
[14] M. Beiner, H. Flocard, Nguyen van Giai and P. Quentin, Nucl. Phys. A283, 29 (1975).
Figure captions

1. Typical behavior of the binding energy with growing neutron–proton deformation difference for the nucleus $^{208}$Pb and the sharp proton and neutron density distributions.

2. The mass number (l.h.s. figure) and the deformation (r.h.s. figure) dependence (crosses) of the stiffness parameter $a(A, I, \alpha)$ (Eq. 23) and its approximation by the formula (24) (solid lines).

3. The change of the binding energies due to different neutron–proton deformations as obtained in the ETF approach is compared with the approximate expression of Eq. (24).

4. The approximation (23) of the binding energy (solid line) made for three Dy isotopes and at three deformation points is compared with the ETF results (crosses) as function of the neutron-proton deformation difference.
Figure 1:
Figure 2:
Figure 3:
Figure 4: