LIMITS OF NUCLEAR STABILITY

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Dedicated to Adam Sobiczewski in honour of his 70th birthday

The modern version of the liquid-drop model (LSD) is compared with the macroscopic part of the binding energy evaluated within the Hartree–Fock–Bogoliubov procedure with the Gogny force and the relativistic mean field theory. The parameters of a liquid-drop like mass formula which approximate on the average the self-consistent results are compared with other models. The limits of nuclear stability predicted by these models are discussed.

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1. Introduction

The self-consistent calculations with effective nucleon-nucleon forces of the Gogny [1] or Skyrme [2] types as well as the relativistic mean field theory (RMFT) [3] are very successful in describing many features of nuclei. The theoretical estimates of the binding energy of nuclei which are not far from stability agree well with the measured data. Nevertheless, the progress made in experimental nuclear physics over the last years, like discovery of superheavy nuclei or isotopes close to the proton or neutron drip lines, demand for a more careful checking of the theoretical model predictions and probably some revision of their parameters.

It is also interesting to see how well other theories work that are simpler than the self-consistent ones in particular the Strutinsky's macroscopic–microscopic method [4] and if it is still possible to apply them in order to calculate successfully properties of nuclei close to the proton or neutron drip lines. The liquid-drop model, which was recently developed in the Lublin–Strasbourg collaboration ((LSD) Lublin–Strasbourg Drop) [5], describes very accurately the binding energies of presently known isotopes [6]

when the shell, pairing and congruence corrections estimated in Refs [7, 8] are added to the macroscopic energy. The root-mean-square deviation of the experimental binding energies *versus* those predicted by the LSD model is even smaller than the ones given by other more elaborated theories like the finite-range droplet [8], the Thomas–Fermi model of Ref. [7] or the self-consistent Hartree–Fock calculation with the Skyrme forces [2].

Is it possible to extract the shell effects from the self-consistent energy and obtain an estimate of the macroscopic energy hidden in these models? This is done successfully, we belive in the present work, for the Skyrme and Gogny forces and for the relativistic mean field theory (RMFT).

The aim of the present paper is to compare the parameters of the liquid-drop models like the historical one of Myers and Świątecki [9] or the of the LSD [5] parametrization either with the liquid-drop parameters which approximate on the average the binding energies evaluated in the Hartree–Fock (HF) self-consistent calculations with the Gogny force [10] or within the RMFT [11]. We are also going to find the average (macroscopic) positions of the proton and neutron drip lines as well as the fission limit (vanishing macroscopic fission barrier) predicted by these macroscopic models.

In Sec. 2 an overview of the Gogny–HFB model and the RMFT is given and the way in which we remove the shell effects from the self-consistent energies is described. The liquid-drop formulae for the macroscopic part of the binding energy are recalled. In Sec. 3 the Gogny and RMFT liquid-drop parameters are compared with those of other phenomenological models. The average positions of the β-stability valley and the proton and neutron drip lines predicted by these models are evaluated. The zero-hight limit of the LD fission barrier is determined. At the end of the paper conclusions are gathered and perspectives for further investigation proposed.

2. Theory

2.1. Gogny force

The Gogny density-dependent effective nucleon–nucleon force is of the following form [1]

$$\begin{aligned} V_{12} \;=\; & \sum_{i=1}^{2} \left(W_i + B_i\hat{P}_\sigma - H_i\hat{P}_\tau - M_i\hat{P}_\sigma\hat{P}_\tau\right) e^{-\frac{(\vec{r}_1-\vec{r}_2)^2}{\mu_i^2}} \\ & + i\; W_{\mathrm{LS}}\; (\overleftarrow{\nabla_1 - \nabla_2}) \times \delta(\vec{r}_1-\vec{r}_2)(\overrightarrow{\nabla_1 - \nabla_2}) \cdot (\vec{\sigma}_1 + \vec{\sigma}_2) \qquad (1) \\ & + t_0\; (1 + x_0\hat{P}_\sigma)\, \delta(\vec{r}_1-\vec{r}_2) \left[\rho(\frac{\vec{r}_1+\vec{r}_2}{2})\right]^\gamma + V_{\mathrm{Coul}}\,, \end{aligned}$$

which contains a central finite-range interaction, a zero-range spin-orbit term and a zero-range density dependent interaction, to which one has to add the Coulomb interaction in the case of protons. The central interaction is made up of two Gaussians one attractive, one repulsive with ranges μ_1 and μ_2 whose values are given below. $\hat{P}\sigma$ and $\hat{P}\tau$ denote the spin and isospin exchange operators respectively, and ρ represents the total density. We use the Gogny D1S [1] interaction, the parameters of which are given below

$$\begin{array}{llllll} W_1 &= -1720.30\,\text{MeV}, & W_2 &= 103.639\,\text{MeV}, \\ B_1 &= 1300.00\,\text{MeV}, & B_2 &= -163.483\,\text{MeV}, \\ H_1 &= -1813.53\,\text{MeV}, & H_2 &= 162.812\,\text{MeV}, \\ M_1 &= 1397.60\,\text{MeV}, & M_2 &= -223.934\,\text{MeV}, \\ \mu_1 &= 0.7\,\text{fm}, & \mu_2 &= 1.2\,\text{fm}, \\ t_0 &= 1390.6\,\text{MeV fm}^{3(1+\gamma)}, & x_0 &= 1, \\ \gamma &= 1/3, & W_{\text{LS}} &= 130\,\text{MeV fm}^5. \end{array} \tag{2}$$

When pairing correlations are neglected, the HFB approach reduces to the Hartree–Fock (HF) method which determines a self-consistent approximation of the nuclear mean-field. The corresponding ground state energy E_{HF} includes a contribution E_{shell} from shell effects which can be evaluated by applying the Strutinsky smearing procedure [4] to the HF single-particle level distribution. Subtracting E_{shell} from the self-consistent HF energy one obtains an energy which can be considered as a macroscopic, liquid-drop like contribution E_{macr}.

2.2. Relativistic mean field theory

The RMFT is based on the Lagrangian density

$$\begin{aligned} \mathcal{L} \;=\; & \bar{\psi}_i \left[\gamma^\mu \left(i\partial_\mu - g_\omega \omega_\mu - g_\rho \vec{\rho}_\mu \cdot \vec{\tau} - e\frac{1+\tau_3}{2} A_\mu \right) - M - g_\sigma \sigma \right] \psi_i \\ & + \frac{1}{2}(\partial\,\sigma)^2 - \left(\frac{1}{2} m_\sigma^2 \sigma^2 + \frac{1}{3} g_2 \sigma^3 + \frac{1}{4} g_3 \sigma^4 \right) \\ & - \frac{1}{4} \Omega_{\mu\nu} \Omega^{\mu\nu} + \frac{1}{2} m_\omega^2 \omega^2 - \frac{1}{4} \vec{R}_{\mu\nu} \vec{R}^{\mu\nu} \\ & + \frac{1}{2} m_\rho^2 \vec{\rho}^{\,2} - \frac{1}{4} F_{\mu\nu} F^{\mu\nu} \,. \end{aligned} \tag{3}$$

It consists of nucleon (barion) fields ψ and electromagnetic fields $\vec{A}$, the ω, $\vec{\rho}$ mesons fields with scalar (central), vector, and tensor term and the nonlinear σ meson potential, where

$$\Omega^{\mu\nu} = \partial^\mu \omega^\nu - \partial^\nu \omega^\mu \,,$$

$$\vec{R}^{\mu\nu} = \partial^{\mu}\vec{\rho}^{\nu} - \partial^{\nu}\vec{\rho}^{\mu} - g_{\rho}(\vec{\rho}^{\mu} \times \vec{\rho}^{\nu}),$$
$$F^{\mu\nu} = \partial^{\mu}A^{\nu} - \partial^{\nu}A^{\mu}. \tag{4}$$

The masses of nucleons M and mesons m_{ω}, m_{ρ}, m_{σ} and the coupling constants $g_{\omega}, g_{\rho}, g_{\sigma}, g_2, g_3$ are the free parameters of the RMFT. The NL3 [3] set of parameters is chosen in our calculations

$$\begin{aligned} M &= 939 \text{ MeV}, & g_{\sigma} &= 10.217, \\ m_{\sigma} &= 508.194 \text{ MeV}, & g_{\omega} &= 12.868, \\ m_{\omega} &= 782.501 \text{ MeV}, & g_{\rho} &= 4.474, \\ m_{\rho} &= 763.000 \text{ MeV}, & g_2 &= -10.431/\text{fm}, \\ & & g_3 &= -28.885. \end{aligned} \tag{5}$$

2.3. Strutinsky renormalization

The single-particle level scheme obtained within the self-consistent calculation (SCC) is used together with the Strutinsky shell-correction method to evaluate the shell correction E_{shell} to the binding energy.

$$E_{\text{shell}} = \sum_{\text{occ}} 2e_{\nu} - \tilde{E}, \tag{6}$$

where the sum runs over all occupied levels. The single particle levels up to a cut-off energy of $\lambda + 15$ MeV, are used to obtain the smoothed energy from the Strutinsky integral

$$\tilde{E} = 2 \int_{-\infty}^{\lambda} e\bar{\rho}(e)\, de. \tag{7}$$

The average level density $\bar{\rho}(e)$ was obtained by smoothing of the single-particle level density $\rho(e) = \sum_{\nu} \delta(e - e_{\nu})$ with the Gauss function multiplied by the 6th order correction polynomial f

$$\bar{\rho}(e) = \frac{1}{\gamma\sqrt{\pi}} \int_{-\infty}^{+\infty} \rho(e')\, e^{-\left(\frac{e-e'}{\gamma}\right)^2} f\left(\frac{e-e'}{\gamma}\right) de'. \tag{8}$$

The width parameter of the Gauss function $\gamma = 1.2\,\hbar\omega$ with $\hbar\omega = 40\, A^{-1/3}$ MeV corresponds to the average position of the Strutinsky plateau condition of shell corrections for the chosen 150 spherical even–even nuclei.

The macroscopic part of the binding energy is equal to the difference between the self-consistently calculated energy without pairing interaction and the total (neutron plus proton) shell correction

$$E_{\rm macr} = E_{\rm HF} - E^n_{\rm shell} - E^p_{\rm shell}\,. \tag{9}$$

These values evaluated for several mass numbers A and isospins $I = (N-Z)/A$ are approximated by the Myers–Świątecki type formula [9]

$$E_{\rm macr} = E_{\rm vol} + E_{\rm surf} + E_{\rm cur} + E_{\rm Coul}\,, \tag{10}$$

$$E_{\rm macr}(Z,A) = -b_{\rm vol}\left(1-\kappa_{\rm vol}\,I^2\right)A + b_{\rm surf}\left(1-\kappa_{\rm surf}\,I^2\right)A^{2/3} + b_{\rm cur}\left(1-\kappa_{\rm cur}\,I^2\right)A^{1/3} + b_{\rm Coul}\frac{Z^2}{A^{1/3}} - C_4\frac{Z^2}{A}\,, \tag{11}$$

where $b_{\rm Coul}$ is connected with the charge-radius parameter $r_0^{\rm ch}$ by

$$b_{\rm Coul} = \frac{3}{5}\frac{e^2}{r_0^{\rm ch}}\,. \tag{12}$$

3. Results

The Gogny–HFB with the D1S force and the RMFT calculations with the NL3 set of parameters were performed in Refs [10,11] for those 150 even–even nuclei between the proton and neutron drip lines which have according to Ref. [8] a quadrupole moment almost equal to zero. These are: $^{38-50}$Ca, $^{82-90}$Sr, $^{96-140}$Sn, $^{80-84}$Sm, $^{162-220}$Pb isotopes, $N = 50$ with $A = 86$–92, $N = 82$ with $A = 122$–164, and $N = 126$ with $A = 174$–224 isotones and 30 other spherical nuclei along the β stability line.

3.1. Liquid-drop parameters

In Fig. 1 we can see the RMFT (solid lines) shell corrections evaluated in Ref. [11] in comparison with the results of Ref. [10] (dashed lines) obtained for the Gogny force. In the first panel of the multi-plot one can see the dependence on A of the neutron shell correction for six groups of Ca–Th isotopes, in the middle the proton shell corrections for three groups of $N = 50, 82, 126$ isotones and on the r.h.s. the neutron shell corrections for β stable isotopes. The proton shell corrections for the isotopes (left and right panel) and the neutron shell corrections for the isotones (middle panel) are practically constant as functions of A.

One notices that the shell corrections obtained in both theoretical models are, indeed, very similar. They show minima for the same magic numbers of one kind nuclei and differ from each other by not more than a few MeV.

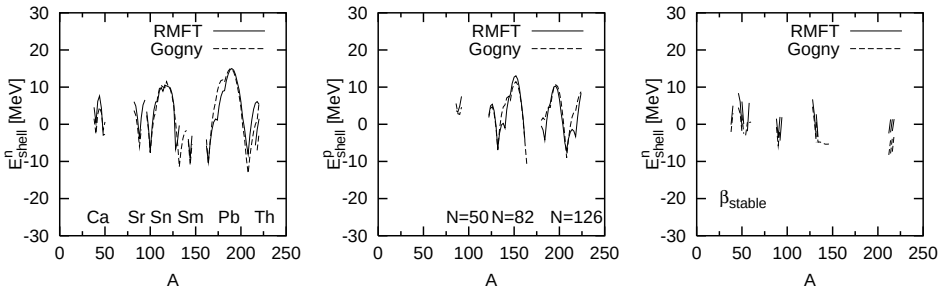

Fig. 1. Shell corrections obtained within the RMFT (solid lines) and with the Gogny force (dashed lines) as function of the mass number A. Neutron shell corrections (left) of Ca–Th isotopes, proton shell corrections for the $N = 50, 82, 126$ isotones (middle) and neutron shell corrections for the β stable nuclei (right).

The estimates of the macroscopic part of the HF–Gogny and RMFT binding energies obtained by subtracting the total shell correction from the self-consistent energy were used to find the parameters of the corresponding liquid-drop formula (11) by the least-square fit procedure. The resulting values of the parameters are compared in Table I with the traditional (MS-1966) Myers–Świątecki liquid-drop formula [9] and the modern phenomenological approach without (MS-2002) and with the curvature term (LSD) [5] fitted to presently available experimental masses [6] (using the microscopic (shell+pairing+deformation) energy corrections from Ref. [8]). During the last 35 years, as one can see in Table I, the liquid-drop parameters reproducing the experimental data did not change very much. The macroscopic part

TABLE I

The macroscopic energy parameters [11].

parameter	unit	MS-1966	MS-2002	LSD	RMFT	Gogny
$b_{\rm vol}$	MeV	15.667	15.848	15.492	15.185	15.649
$\kappa_{\rm vol}$		1.790	1.848	1.860	1.657	1.916
$b_{\rm surf}$	MeV	18.560	19.386	16.971	16.811	18.928
$\kappa_{\rm surf}$		1.790	1.983	2.294	1.209	2.108
$b_{\rm cur}$	MeV	—	—	3.860	—	—
$\kappa_{\rm cur}$		—	—	−2.376	—	—
$r_0^{\rm ch}$	fm	1.205	1.190	1.217	1.264	1.188
C_4	MeV	1.211	1.200	0.918	1.299	2.015

of the binding energies obtained with the Gogny force [10] is described by the set of LD parameters which is close to the newest fit (MS-2002) of the LD parameters to the experimental masses. The results obtained within the RMFT correspond to smaller values of the volume and the surface energies, while the Coulomb energy radius constant equal to 1.264 fm is substantially larger than its present phenomenological value (1.191 fm). On the contrary, the RMFT estimate of the Coulomb charge diffuseness parameter C_4 is much closer to its 'experimental' value as compared to the Gogny's value. The isospin dependence of the volume and the surface energies is weaker in the RMFT than the experimental one, while the Gogny force gives a slightly stronger dependence of both energies than the phenomenological (MS-2002) one.

It is rather difficult to discuss directly the parameters of the LSD approach because contrary to the other models it contains a curvature term, which slightly modifies volume and surface energy. Some features of the LSD model could be considered only after performing calculations for some series of isotopes, isotones as well as along the β-stability line. We are comparing the considered models in Fig. 2, where the differences of the LSD binding energy [5] and the corresponding energies evaluated using the Thomas–Fermi approximation [7] (solid lines), the old liquid-drop model of Myers and Świątecki [9] (dashed lines), the macroscopic approximations of the RMFT [11] (long dashed lines), and the Gogny–HFB results [10] (dotted lines) are given. The Thomas–Fermi binding energy is almost (except for very neutron deficient isotones) equal to the LSD estimates. The RMFT gives on average the largest absolute value of binding energy and its difference with respect the LSD prediction reaches up to 40 MeV for the heaviest nuclei. The Gogny results are close to the ones obtained with the LSD when the light β-stable nuclei are considered but for nuclei far from stability the Gogny energy is as a rule larger than the LSD one. The old liquid-drop model slightly overestimates the binding energies of nuclei.

All considered liquid-drop models give almost the same position of the β-stability line. In Fig. 3 a few cross-sections of the binding energy surface corresponding to $A = \text{const}$ are plotted as functions of the number of neutrons (N). The curves corresponding to different A are shifted in such a way that the minimum of the LSD energy corresponds to zero. The stiffness of the parabola corresponding to the different models listed in Table I diminishes with growing mass number A. The stiffness evaluated with the Gogny model is the smallest.

It is very interesting how the limits of stability are predicted by the liquid-drop models discussed in this paper. The proton drip line corresponds to the zero separation energy of two protons, *i.e.*

$$S_{2\mathrm{p}}(Z,A) = E_{\mathrm{macr}}(Z+1,A+1) - E_{\mathrm{macr}}(Z-1,A-1) = 0\,, \qquad (13)$$

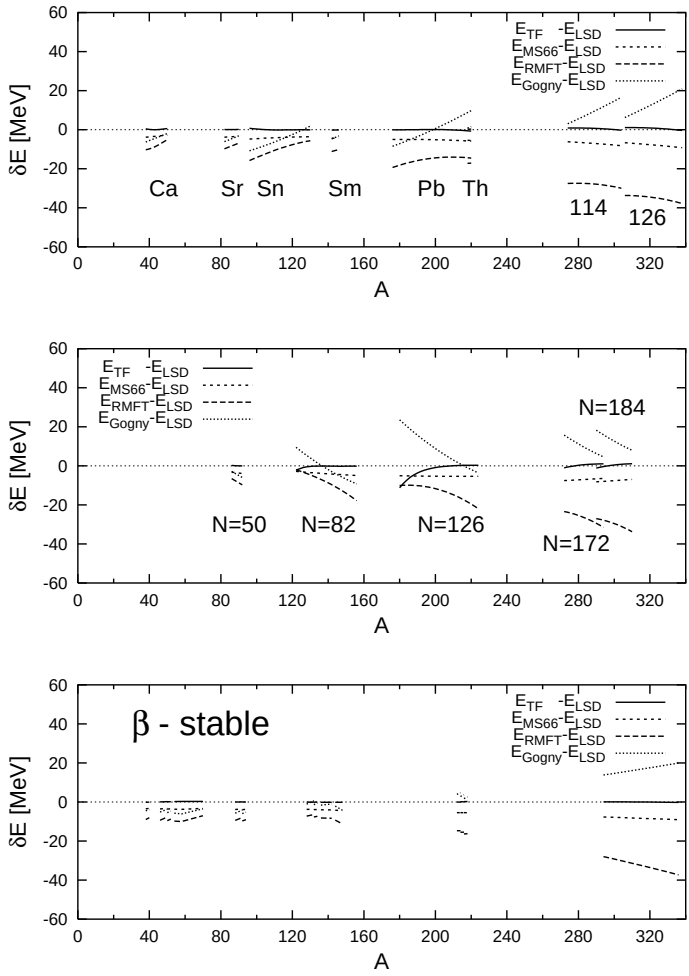

Fig. 2. Comparison of the macroscopic binding energies evaluated in the Thomas–Fermi model [7], extracted from the Gogny–HFB [10] and RMFT [11] self-consistent calculation and the traditional Myers–Świątecki [9] liquid-drop with the results obtained with the LSD [5].

while the neutron drip-line is connected with the zero separation energy of two neutrons, *i.e.*

$$S_{2\mathrm{n}}(Z,A) = E_{\mathrm{macr}}(Z,A+1) - E_{\mathrm{macr}}(Z,A-1) = 0\ . \tag{14}$$

The β-stability line corresponds to the minimum of the nuclear energy when the mass number is kept constant

$$\left(\frac{\partial E_{\mathrm{macr}}(Z,A)}{\partial N}\right)_{A=\mathrm{const}} = 0\,, \tag{15}$$

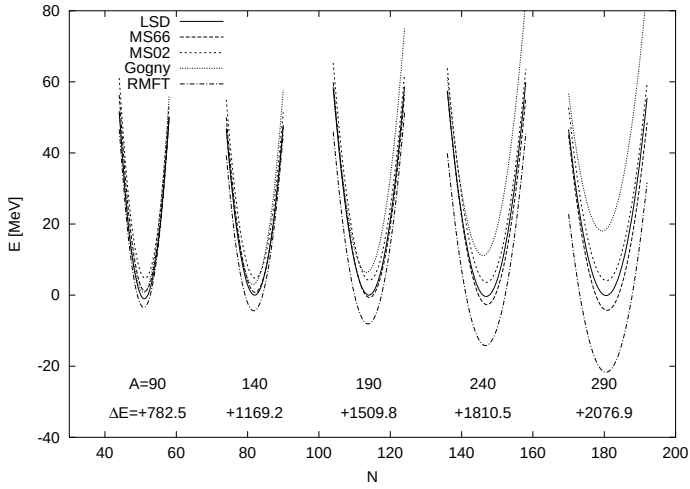

Fig. 3. A = const cross-sections of the macroscopic binding energies evaluated in the models listed in Table I as functions of the neutron number (N).

as shown on in Fig. 3. We have found that all estimates of the position of the β-stability line predicted by the models listed in Table I are close to each other and very well approximated by the Green formula

$$N - Z = \frac{0.4A^2}{200 + A}\,. \tag{16}$$

The other end of stability is connected with the vanishing of the fission barrier. The liquid-drop model gives the following estimates of this limit

$$x = \frac{E_{\rm Coul}}{2(E_{\rm surf} + E_{\rm cur})} = 1\,, \tag{17}$$

where x is the so-called fissility parameter.

All these parabolas corresponding to the LSD (solid lines), Gogny (dashed lines) and RMFT (dotted lines) macroscopic models are plotted in Fig. 4 on the (N, Z) plane. It is seen that all models give nearly the same estimates of the position of the proton drip-line while the neutron drip-lines are different. The RMFT predicts on average the existence of a larger excess of neutrons than the Gogny model, the LSD results are in between.

The fission barrier predicted by the LSD model vanishes already at proton number $Z = 114$ while in the macroscopic model extracted for the Gogny force the barrier goes to zero around $Z \approx 120$. The RMFT estimates are between these two limits.

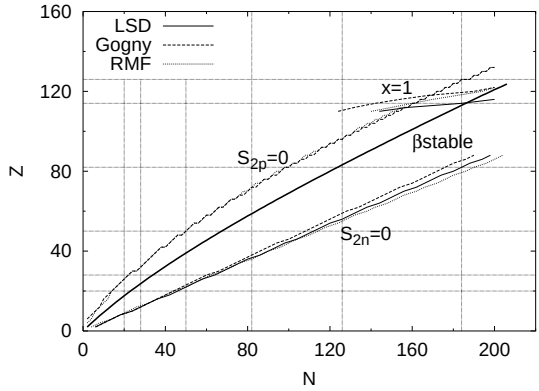

Fig. 4. β-stability line and the proton ($S_{2p} = 0$) and neutron ($S_{2n} = 0$) drip-lines as well as the LD fission limit ($x = 1$) estimated using the LSD, Gogny and RMF models (see Table I).

All above analysis is made within the macroscopic models and the true limits of stability can of course be different due to the importance of shell effects.

4. Conclusions

The following conclusions can be drawn from our investigation:

1. The shell corrections obtained in the RMFT with the NL3 set of parameters and within the Hartree–Fock mean-field calculation with the Gogny D1S force are similar.
2. The volume and surface part of the binding energy in the RMFT are smaller than the corresponding energies obtained with the Gogny model [10] as well as those fitted to the experimental masses [5, 7].
3. The isospin dependence of the volume and surface term obtained within the RMFT is too small in comparison with the experimental data.
4. The position of the β-stability and proton drip-lines are almost the same in all considered macroscopic models while the neutron drip-line predicted within the RMFT is shifted towards larger N as compared to the Gogny or LSD estimates.

Similar effects for deformed nuclei with the Gogny forces and various sets of RMFT parameters are under investigation.

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REFERENCES

[1] J.F. Berger, M. Girod, D. Gogny, *Comput. Phys. Commun.* **63**, 365 (1991).

[2] D. Vautherin, D.M. Brink, *Phys. Rev.* **C5**, 626 (1972).

[3] P. Ring, *Prog. Part. Nucl. Phys.* **37**, 193 (1996); G.A. Lalazissis, J. König, P. Ring, *Phys. Rev.* **C55**, 540 (1997).

[4] V.M. Strutinsky, *Nucl. Phys.* **A95**, 420 (1967).

[5] K. Pomorski, J. Dudek, submitted to *Phys. Rev.* **C**, (`nucl-th/0205011`).

[6] M. Antony, Nuclide Chart 2002, Impressions François, 103 Route de Marienthal, Haguenau, France; e-mail: `ela.myelin@ires.in2p3.fr.`

[7] W.D. Myers, W.J. Świątecki, *Nucl. Phys.* **A601**, 141 (1996).

[8] P. Möller, J.R. Nix, W.D. Myers, W.J. Świątecki, *At. Data Nucl. Data Tables* **59**, 185 (1995).

[9] W.D. Myers, W.J. Świątecki, *Nucl. Phys.* **81**, 1 (1966); *Ark. Phys.* **36**, 343 (1967).

[10] M. Kleban, B. Nerlo-Pomorska, J.F. Berger, J. Dechargé, M. Girod, S. Hilaire, *Phys. Rev.* **C65**, 024309 (2002).

[11] K. Mazurek, B. Nerlo-Pomorska, *Phys. Rev.* **C66**, 064305 (2002).