Nuclear masses, shell effects and deformations

Jorge G. Hirsch G.

Instituto de Ciencias Nucleares, UNAM, México

hirsch@nucleares.unam.mx

C. Barbero, A. Mariano, UNLP, Argentina
J. Mendoza-Temis, GSI, Germany
A. Zuker, IN2P3, France

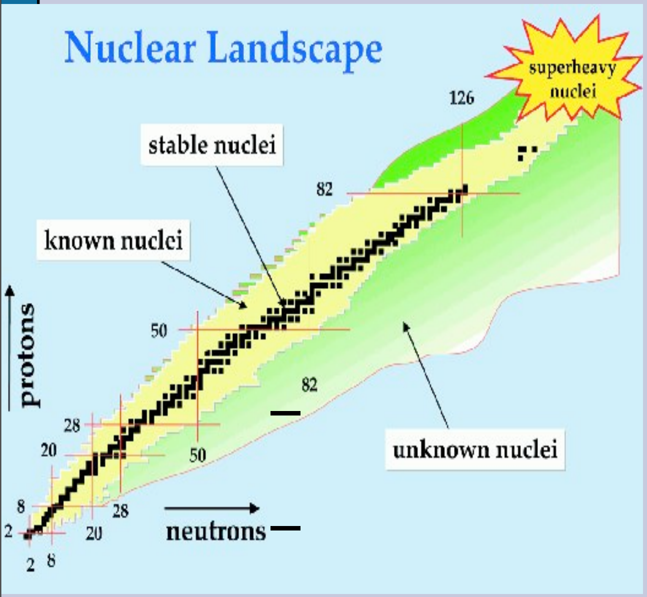
Beauty in Physics, Cocoyoc, May 14-18, 2012.

Challenging a common belief

"The liquid-drop energy of a *spherical nucleus* is described by a Bethe-Weizsäcker mass formula."

"It is common practice to describe nuclear masses and radii of *spherical closed-shell nuclei* in terms of a mean field and add deformation and other shell effects as corrections."

Nuclear Mass is the most fundamental property of nuclei



Some methods to predict nuclear masses:

- The liquid drop model (LDM).
- Algebraic extensions of the LDM.
- The Duflo-Zuker microscopic mass formula.
- The finite range droplet model (FRDM).
- HFB methods.
- Density functional theory.
- The Garvey-Kelson relations and their integration.

The models

- The Liquid Drop Model (LDM)
- The Duflo-Zuker model (DZ)
- The Modified DZ model

The reference set

Atomic Mass Evaluation 2003 (AME03)

G. Audi, A.H. Wapstra y C. Thibault,
Nucl. Phys. A 729, 337 (2003)

2149 nuclei with $N \geq 8, Z \geq 8$

The figure of merit

$$RMS = \left\{ \frac{\sum (BE_{exp}(N,Z) - BE_{th}(N,Z))^2}{N} \right\}^{1/2},$$

Liquid Drop Model 1

A.E.L. Dieperink and P. Van Isacker, Eur. Phys. J. A42 269279 (2009).

$$E_{LDM1}(N,Z) = -a_v A + a_s A^{2/3} + S_v \frac{6}{4T(T+1)} A(1 + yA^{-1/3}) + a_c \frac{Z(Z-1)}{(1-\Lambda)A^{1/3}} - a_p \frac{\Delta(N,Z)}{A^{1/3}}$$

$$\Lambda \equiv \frac{N-Z}{6Z(1+y^{-1}A^{1/3})}, \quad \Delta \equiv 2 \text{ (e-e)}, 1 \text{ (odd A)}, 0 \text{ (o-o)}$$

6 parameters

Bulk and surface effects are treated consistently

Liquid Drop Model 2

N. Wang, M. Liu and X. Wu, Phys. Rev. C81 044322 (2010)

$$
\begin{aligned}
E_{LDM2}(N,Z) \quad &= -a_v A + a_s A^{2/3} + a_c \frac{Z(Z-1)}{A^{1/3}}(1 - Z^{-2/3}) \\
&+ a_{sym}(N-Z)^2/A + a_{pair}\frac{\delta_{np}}{A^{1/3}}
\end{aligned}
$$

$$
\delta_{np} \equiv \quad 2- \mid \mathrm{I} \mid (\text{e-e}), 1(\text{odd A}), \mid \mathrm{I} \mid (\text{o-o})
$$

$$
a_{sym} \equiv \quad c_{sym}\left[1 - \kappa/A^{1/3} + \frac{(N-Z)/A}{2+|N-Z|}\right]
$$

6 parameters

Isospin dependence of the symmetry term and pairing

Liquid Drop Model 3

G. Royer, M. Guilbaud and A. Onillon, Nucl. Phys. A847 (2010) 24.

$$
\begin{aligned}
E_{LDM3}(N,Z) \quad &= -a_v(1-k_v I^2)A + a_s(1-k_s I^2)A^{2/3} \\
&+\frac{3}{5}\frac{e^2 Z(Z-1)}{r_0 A^{1/3}} - f_p Z^2/A - a_{c,exc} Z^{4/3}/A^{1/3} \\
&+a_k(1-k_k I^2)A^{1/3} + E_{pair} + E_{Wigner}
\end{aligned}
$$

$$
\mid \mathrm{I} \mid \equiv \quad (N-Z)/A
$$

11 parameters

Cuadratic isospin corrections,

proton form factor f_p + charge exchange $a_{c,exc}$,

curvature terms (a_k, k_k)

9 fits were performed employing the 3 LDM formulas.

1st fit: global of all the nuclei in AME03 with $N \geq 8$, $Z \geq 8$.

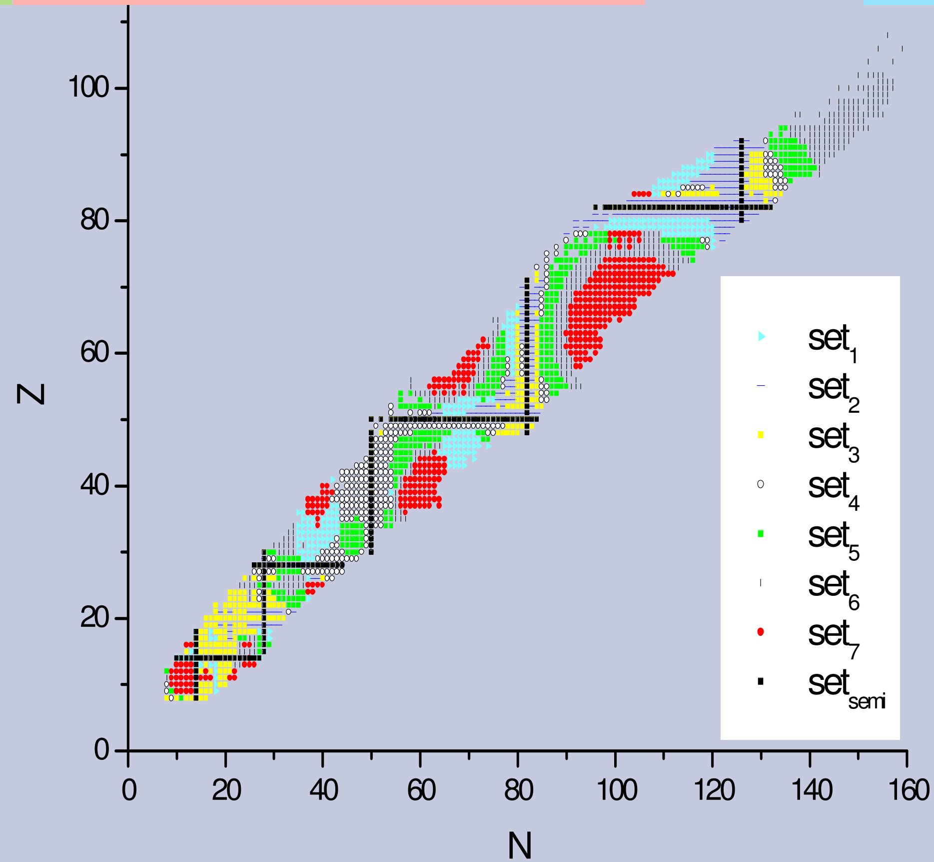
2nd-8th fit: 7 regions with different quadrupole deformations, taken from FRDM, (P. Möller, J.R. Nix, W.D. Myers, W.J. Swiatecki, At. Data Nucl. Data Tables 59 (1995) 185.)

9th fit: Only semi-magic nuclei.

The 9 regions

global	1	2	3	4	5	6	7	semi
ϵ_2^{ini} ϵ_2^{fin}	-0.65 -0.11	-0.11 0.00	0.00 0.04	0.04 0.12	0.12 0.18	0.18 0.23	0.23 0.65	
2149	258	252	332	272	307	364	364	185

oblate | spherical | prolate



The rms (in keV) in each region

C. Barbero, J. G. Hirsch, A. Mariano, Nucl. Phys. A84 (2012) 81-97.

	global	1	2	3	4	5	6	7	semi magic
LDM1	2387	1313	1676	2063	1746	1053	870	746	2113
LDM2	2374	1254	1675	2069	1762	1021	838	656	2056
LDM3	2422	1183	1597	2151	1517	986	819	629	1967

oblate spherical prolate

The three Liquid Drop Models give very similar results:

- spherical nuclei have an rms close to 2000 keV

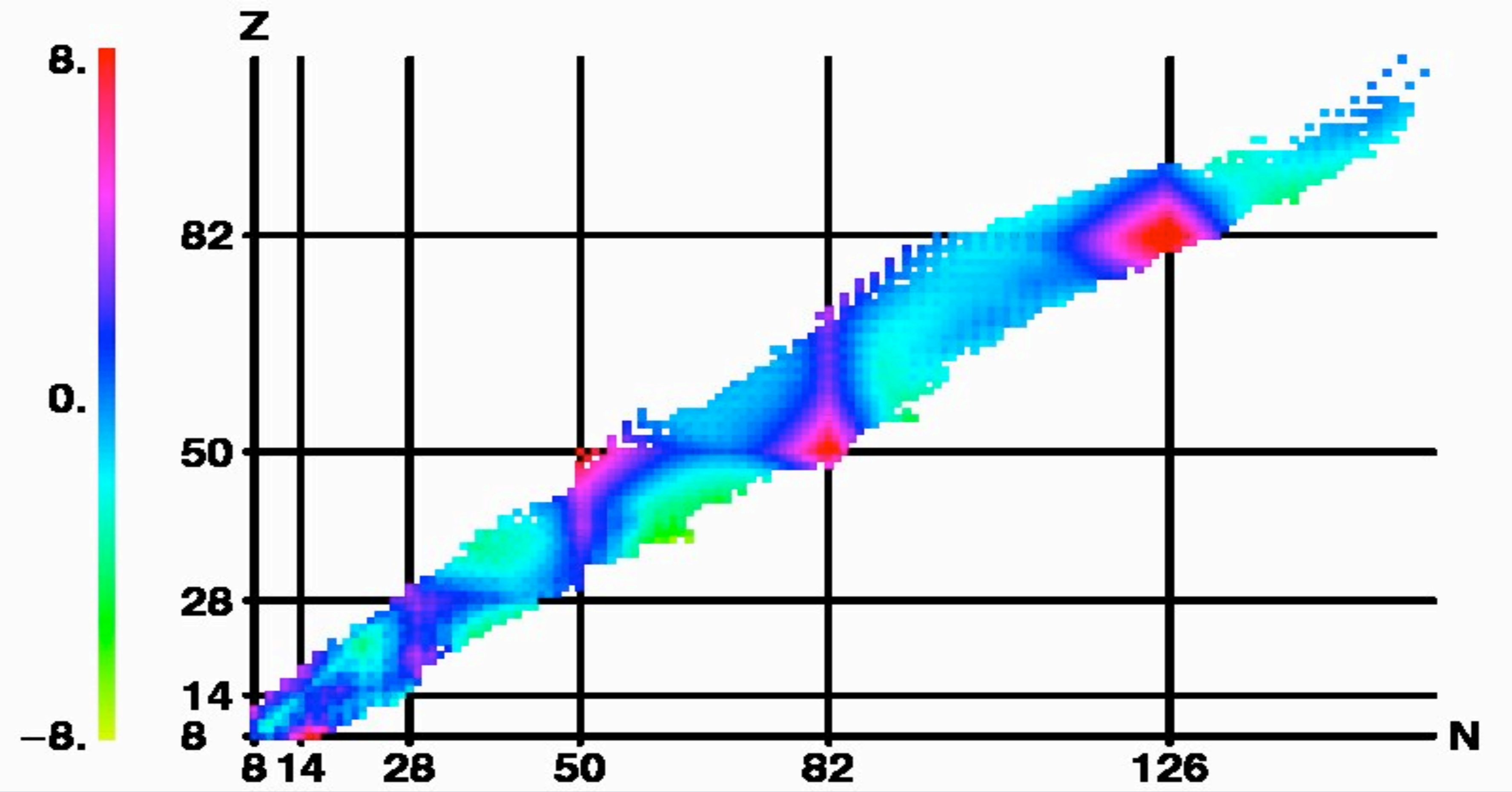
- deformed prolate nuclei have an rms around 600-900 keV.

- The same effect is observed when pairing effects are removed.

The more prolate the nuclei, the best the LDM fits them.

LDM, global fit

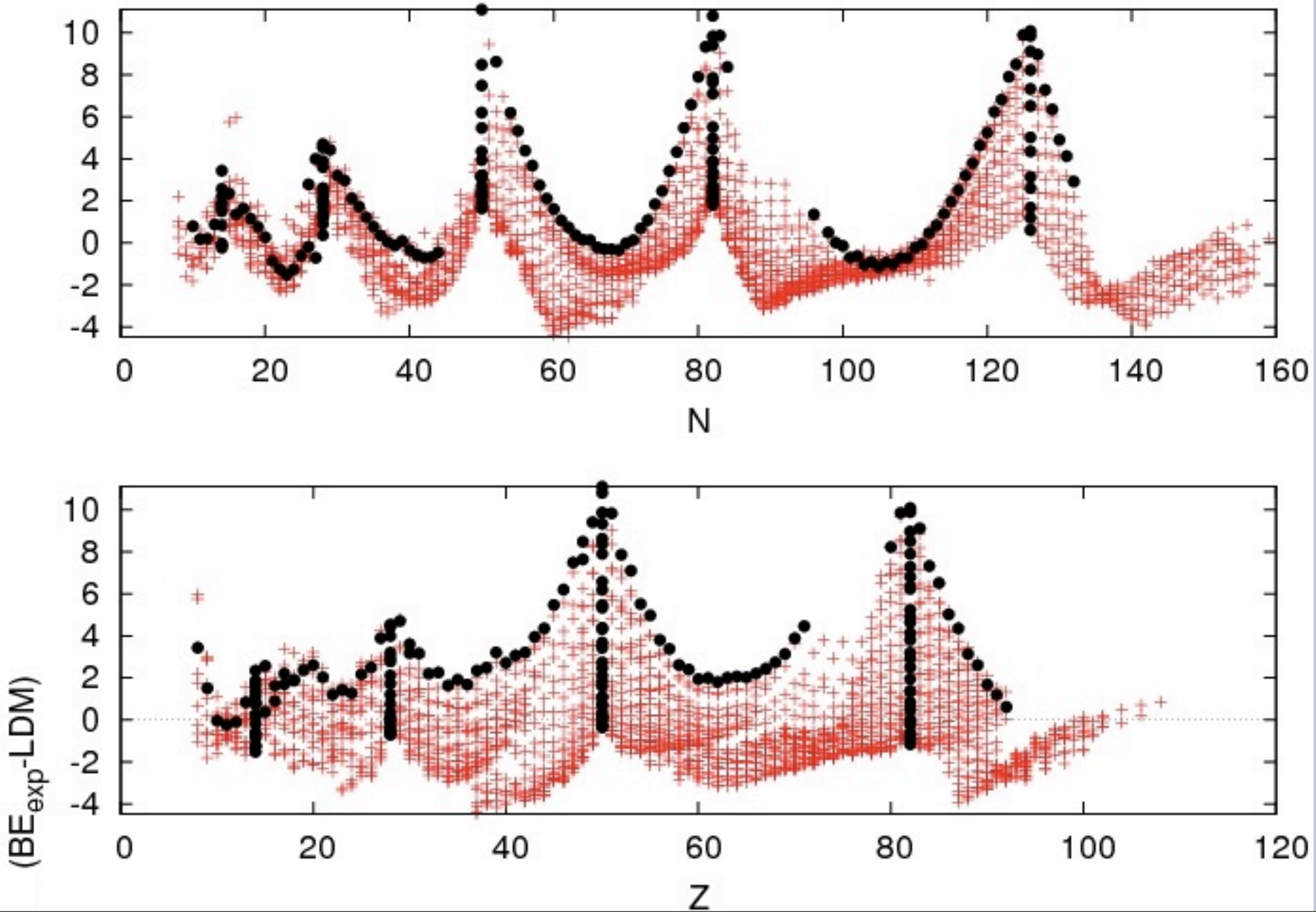
$$\text{RMS} = 2.40\ \text{MeV}, \quad \text{N,Z} \geq 8$$
$$\text{RMS} = 2.42\ \text{MeV}, \quad \text{N,Z} \geq 28$$



Differences between experimental and fitted masses

The major challenge in the construction of an algebraic microscopic mass formula is the proper description of the shell effects.

The shell effects



ELSEVIER

Nuclear Physics A576 (1994) 65–108

NUCLEAR PHYSICS A

On the microscopic derivation of a mass formula

Andrés P. Zuker

Physique Théorique, Centre de Recherches Nucléaires, IN2P3-CNRS / Université Louis Pasteur, BP 20, F-67037 Strasbourg Cedex 2, France

10.1. Implementing the minimal-mass formula

$$E_{\mathrm{LD}} = V_{AA}A + v_{AA}A^{2/3} + \frac{v_{AT}T}{A^{1/3}} + \frac{V_{TT}T^2}{A} + \frac{v_{TT}T^2}{A^{4/3}} + \frac{\delta_{\mathrm{p}}}{A^{1/2}} + \frac{V_c Z^2}{A^{1/3}},$$

$$E(N, Z) = E_{\mathrm{LD}} + \max\left[\bar{\omega}\sum_R\left(\frac{n\bar{n}}{D_\nu} + \frac{z\bar{z}}{D_\pi}\right), \kappa + \sigma\sum_R \frac{z}{D_\pi}\right],$$

PHYSICAL REVIEW C VOLUME 52, NUMBER 1 JULY 1995

RAPID COMMUNICATIONS

Microscopic mass formulas

J. Duflo[1] and A.P. Zuker[2]

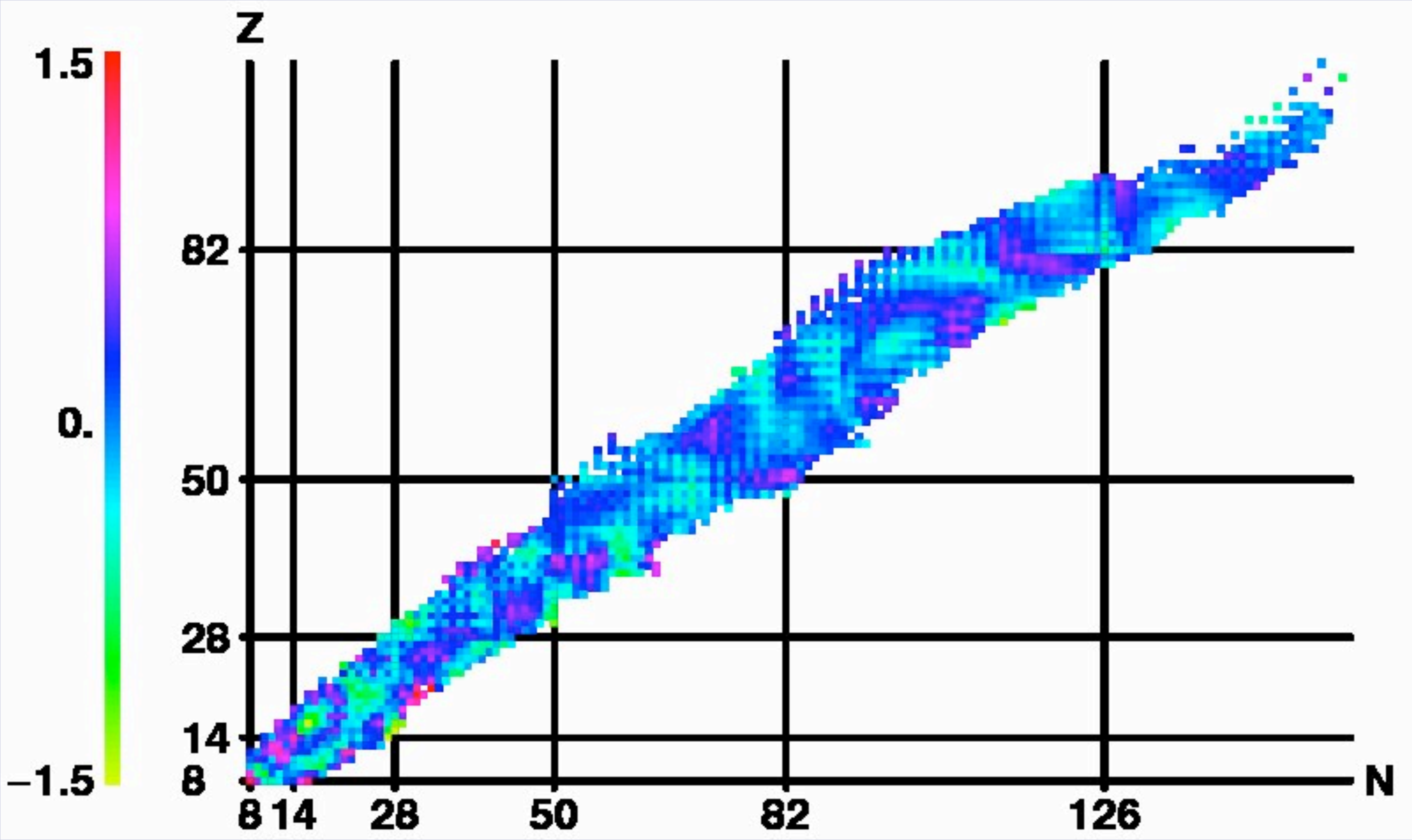
A functional of the occupation numbers, includes explicitly deformation effects.
Inspired in the shell model.
Has 33 parameters.

H_m $\alpha=1/2$ $R_c=A^{1/3}(1-(T/A)^2)$

$FMA=(\Sigma MA_{\pi})^2$ $FSA=(\Sigma SA_{\pi})^2$ $FCA=\Sigma MA_{\pi}D_{\pi}^{-1/2}\Sigma SA_{\pi}D_{\pi}^{-1/2}$

DZ, global fit

$$\mathrm{RMS} = 0.35\ \mathrm{MeV}, \quad \mathrm{N,Z} \geq 8$$
$$\mathrm{RMS} = 0.31\ \mathrm{MeV}, \quad \mathrm{N,Z} \geq 28$$



Differences between experimental and fitted masses

How does DZ work?

J. Mendoza Temis, J.G. Hirsch and A. Zuker,
Nucl. Phys. A 843 (2010) 14

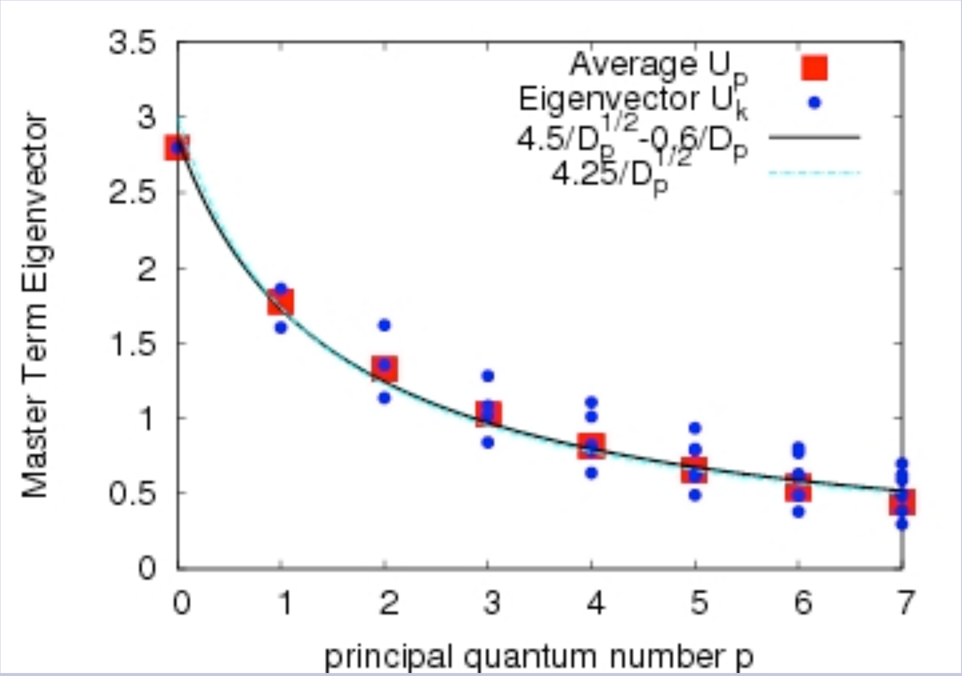
- The monopole part (J=0) of the many-body Hamiltonian can be factorized

$$H_m = \sum_{\mu} E_{\mu} \left(\sum_{k} m_k U_{k_{\mu}} \sum_{\beta} m_{\beta} U_{\beta_{\mu}} \right), \quad m_k = a_k^{\dagger} a_k$$

U is a unitary transformation which diagonalize the monopole Hamiltonian, with eigenvalues *E.*

Numerical studies of realistic interactions (chiral N3LO) show that only one eigenvalues dominates.

$$E_1 \approx \hbar\omega \approx A^{-1/3}, \quad U_p \propto D_p^{-1/2}$$



$D_p = (p+1)(p+2)$ is the degeneracy of the major HO shell of principal quantum number *p*

The master term M

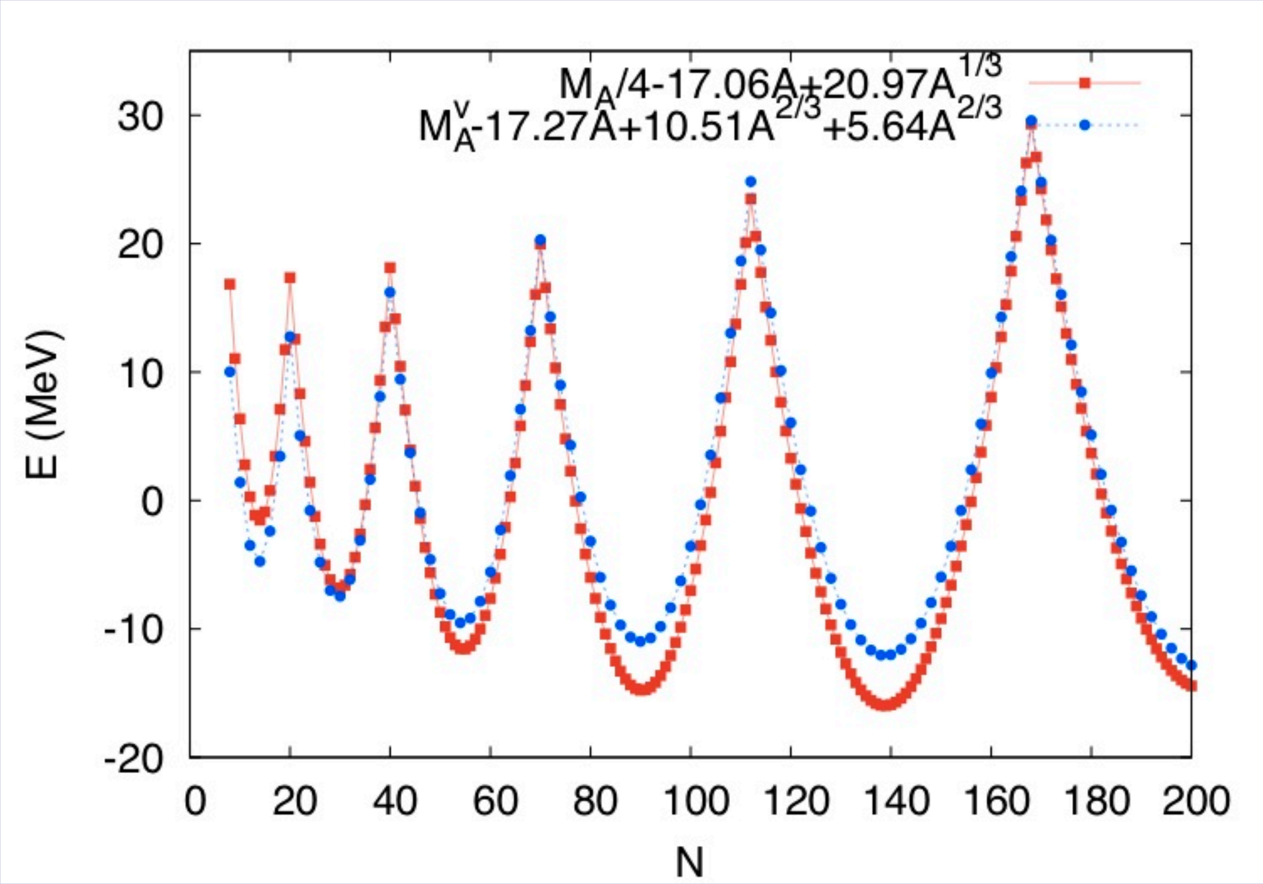
$$M = M_N + M_Z,$$

$$M_N \equiv \frac{1}{\rho}\left(\sum_p^{p_{f\nu}} \frac{n_p}{\sqrt{D_p}}\right)^2, \quad M_Z \equiv \frac{1}{\rho}\left(\sum_p^{p_{f\pi}} \frac{z_p}{\sqrt{D_p}}\right)^2$$

$$\rho = \langle r^2 \rangle / A^{1/3} = A^{1/3}\left[1 - 0.5\left(\frac{t}{A}\right)^2\right]^2.$$

- This is the basic building bock of the DZ model.
- Asymptotically, M scales with A, represents a proper volume term.

The master term minus its asymptotic behavior



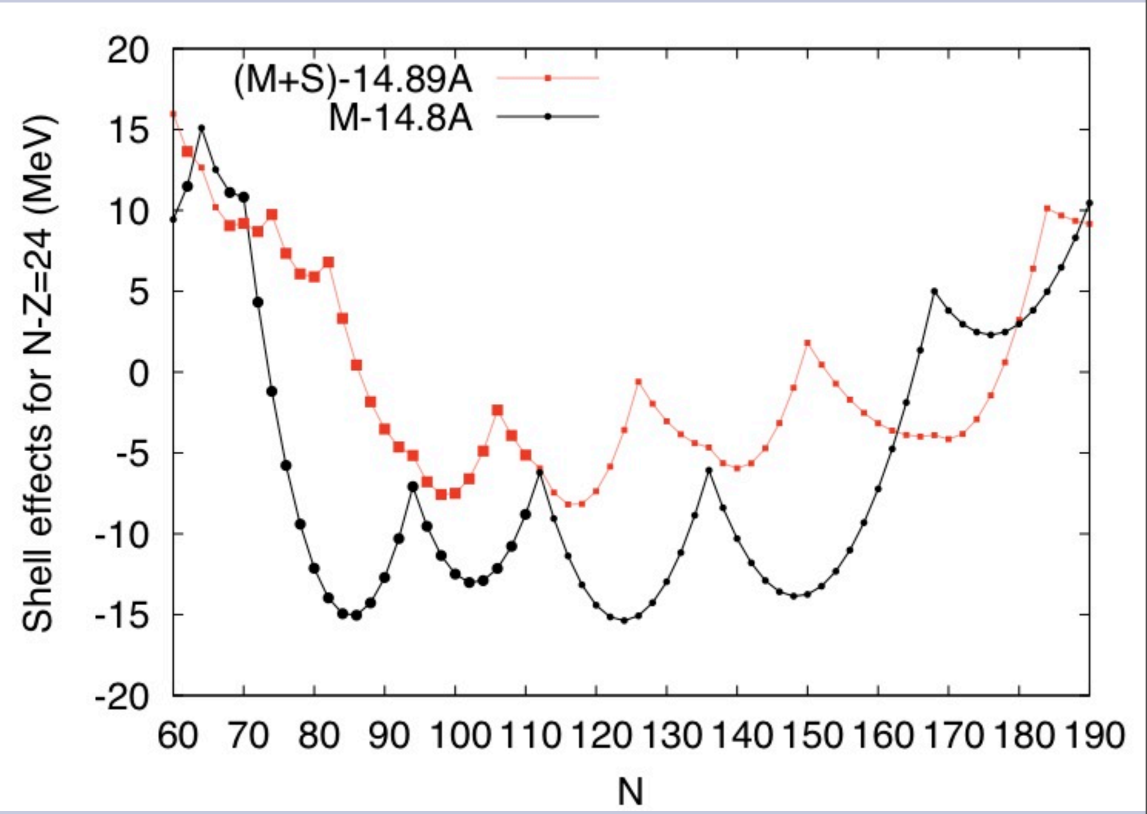
- HO shell closures, maximum scales with $A^{1/3}$

The HO-EI transition: Duflo's magic

$$S_\nu = \sum_p^{p_\nu} s_{\nu p} \frac{p^2+4p-5}{\sqrt{D_p}(p+2)} + \sum_p^{p_\nu} n_p s_{\nu p} \frac{p^2-4p+5}{D_p(p+2)}, \quad s_{\nu p} = \left[\frac{p n_{j_p} - 2 n_{r_p}}{2(p+1)}\right], \quad s_{\pi p} = \left[\frac{p z_{j_p} - 2 z_{r_p}}{2(p+1)}\right],$$

$$S_\pi = \sum_p^{p_\pi} s_{\pi p} \frac{p^2+4p-5}{\sqrt{D_p}(p+2)} + \sum_p^{p_\pi} z_p s_{\pi p} \frac{p^2-4p+5}{D_p(p+2)}, \quad S = (S_\nu + S_\pi)/\rho$$

- The evolution from HO (dots) to EI (squares) shell effects for N-Z=24 even-even nuclei.



The macroscopic DZ mass formula

$$\langle H_m \rangle = a_1 (M + S) - a_2 \frac{M}{\rho} - a_3 V_C - a_4 V_T + a_5 V_{TS} + a_6 V_P.$$

$$V_C = \frac{Z(Z-1)+0.76[Z(Z-1)^{2/3}]}{r_c};$$

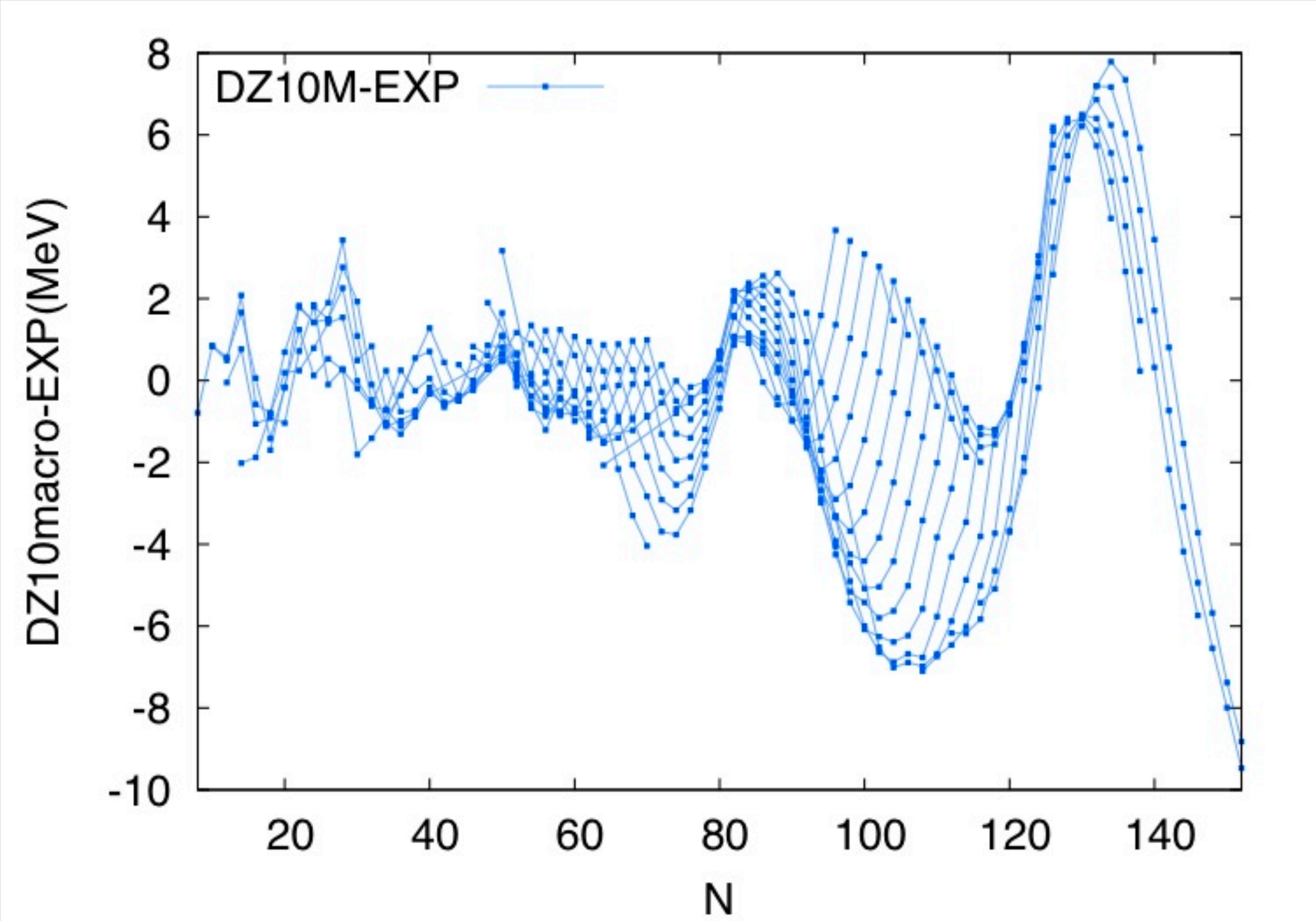
$$r_c = A^{1/3}\left[1 - \left(\frac{T}{A}\right)^2\right]$$

$$V_T = \frac{4T(T+1)}{A^{2/3}\rho},$$

$$V_{TS} \equiv \frac{4T(T+1)}{A^{2/3}\rho^2} - \frac{4T(T-\frac{1}{2})}{A\rho^4},$$

N	Z		V_P
even	even		$(2 - 2T/A)/\rho$
even	odd	$N > Z$	$(1 - 2T/A)/\rho$
odd	even	$N > Z$	$1/\rho$
even	odd	$N < Z$	$1/\rho$
odd	even	$N < Z$	$(1 - 2T/A)/\rho$
odd	odd		$2T/(A\rho)$

Differences between the binding energies predicted by DZ10 macro, and the experimental ones. Even-even nuclei (RMSD=2.86 MeV). Lines join points at constant t=N-Z.



Microscopic terms and deformation effects

$$s_3 = \frac{1}{\rho}\left[\frac{n_\nu \bar{n}_\nu (n_\nu - \bar{n}_\nu)}{D_\nu} + \frac{n_\pi \bar{n}_\pi (n_\pi - \bar{n}_\pi)}{D_\pi}\right], \quad s_4 = \frac{1}{\rho}\left[2^{(\sqrt{p_\pi}+\sqrt{p_\nu})} \cdot \left(\frac{n_\nu \bar{n}_\nu}{D_\nu}\right) \cdot \left(\frac{n_\pi \bar{n}_\pi}{D_\pi}\right)\right].$$

$$\langle H_s \rangle = a_7\, s_3 - a_8\, \frac{s_3}{\rho} + a_9\, s_4.$$

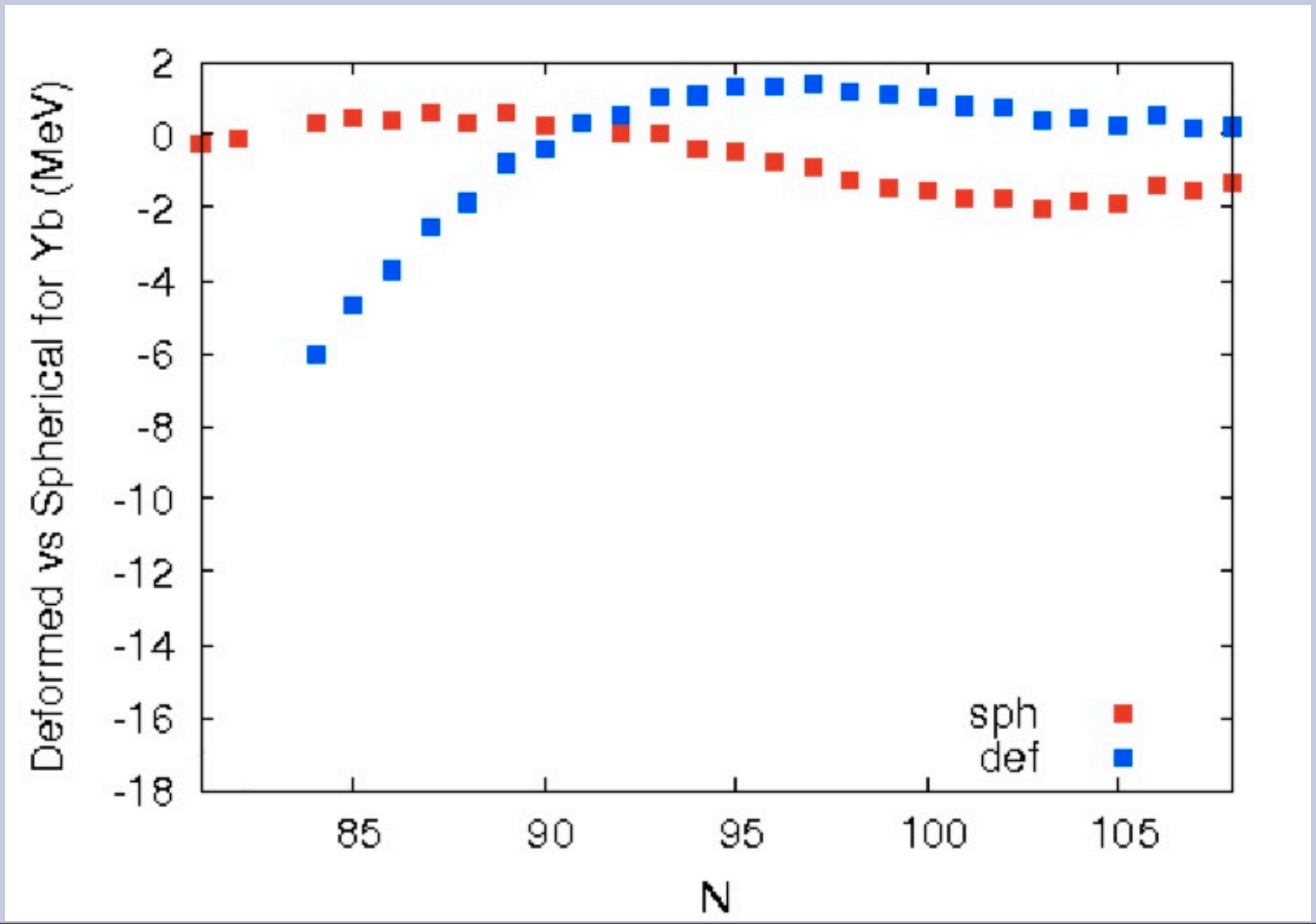
$$d_4 = \frac{1}{\rho}\left[\left(\frac{n'_\nu \bar{n'}_\nu}{D_\nu^{3/2}}\right) \cdot \left(\frac{n'_\pi \bar{n'}_\pi}{D_\pi^{3/2}}\right)\right], \quad n' = n - 4,\ \bar{n'} = \bar{n} + 4$$

$$\langle H_d \rangle = a_{10}\, d_4.$$

$$BE_{th} = \langle H_m \rangle + \langle H_s \rangle \qquad \text{if Z} < 50$$

$$BE_{th} = \langle H_m \rangle + max\left(\langle H_s \rangle, \langle H_d \rangle\right) \qquad \text{if Z} \geq 50$$

DZ10 deformed and spherical binding energies subtracted from the experimental ones for Yb isotopes.
The crossings signal the onset of deformation, which reproduces perfectly the N=90 transition region.



The master term revisited

J.G. Hirsch and J. Mendoza-Temis,
J. Phys. G: Nucl. Part. Phys. 37 064029

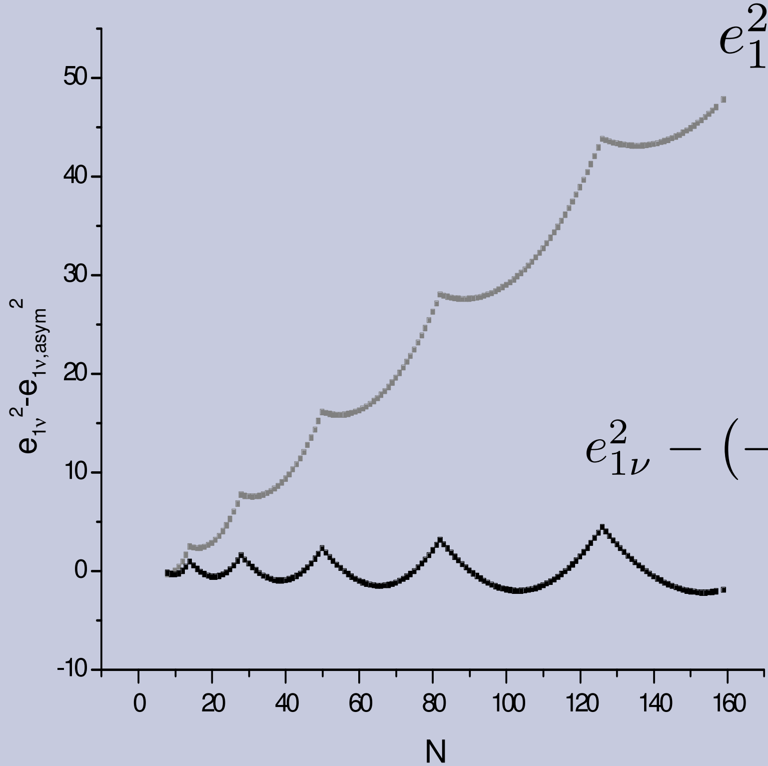
$$M_a = \frac{1}{\rho}\left(e_{1\nu}^2 + e_{1\pi}^2\right)$$

$$e_{1\nu} = \sum_{p_\nu} \frac{n_\nu}{\sqrt{D_{p_\nu}}}, \quad e_{1\pi} = \sum_{p_\pi} \frac{n_\pi}{\sqrt{D_{p_\pi}}},$$

$$D_{p_{\nu,\pi}} = (p_{\nu,\pi}+1)(p_{\nu,\pi}+2)+2$$

- The major shells are EI instead of HO
- It directly provides the observed shell closures

Difference between $e_{1\nu}^2$ and different approximations to describe its asymptotic behavior as a function of N



$$e_{1\nu}^2 - \left(\frac{(3N)^{2/3}}{2}\right)^2$$

$$e_{1\nu}^2 - \left(-0.90892 + 0.54259N^{1/3} + 0.98851N^{2/3} + 0.0018N\right)^2$$

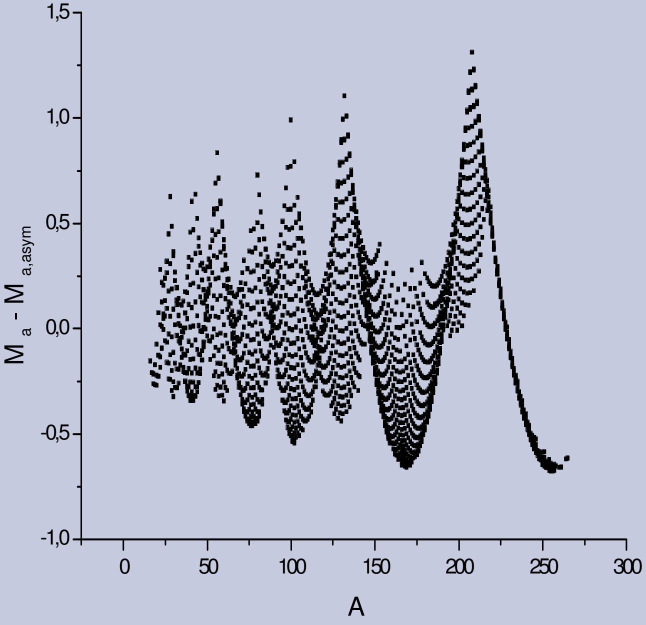
The rms (in keV) in each region employing the **macroscopic** sector of the two DZ models

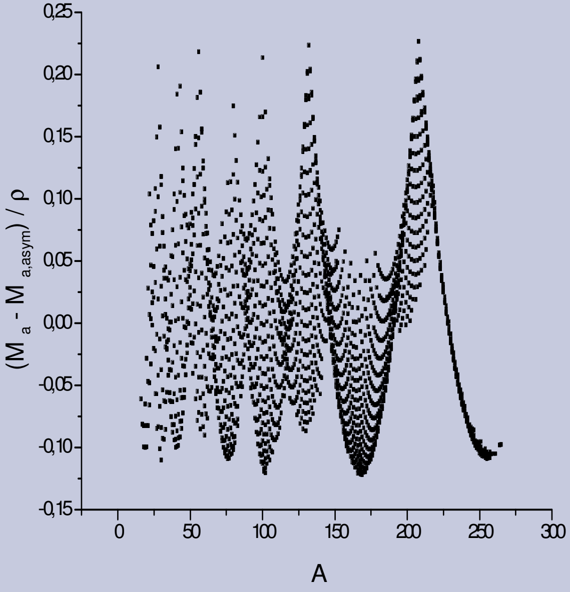
	global	1	2	3	4	5	6	7	semi magic
DZ1	2852	994	1969	1557	1392	2237	2562	1529	1392
DZ2	3443	1425	1544	2167	1717	1729	2047	2107	1973
		oblate	spherical	spherical	spherical		prolate	prolate	

- The ability of both models to describe masses of nuclei in spherical, prolate and semi-magic groups are now comparable.
- The global RMS are larger than those obtained with the LDM formulas.
- The RMS are in nearly all cases smaller using DZ1 (except in region 6).
- It is hard to find any correlation between the RMS and the regions with different deformations.

Combining LDM and DZ, val

$$E_{LDM1+DZ} = LDM1 + a_{vol}(M_a - M_{a,asym}) + a_{surf}(M_a - M_{a,asym})/\rho.$$





$$E_{LDM1+val} = LDM1 + b_1(n_v + z_v) + b_2(n_v + z_v)^2.$$

A.E.L. Dieperink and P. Van Isacker, Eur. Phys. J. A42 269279 (2009).

J. Mendoza-Temis, et al, Nucl. Phys. A799 , 84 (2008).

Combining LDM and DZ, val

	global	1	2	3	4	5	6	7	semi magic
LDM1+ DZ	1407	668	907	1026	755	784	791	647	952
LDM1+ val	1075	796	981	1006	828	711	836	615	1037

oblate spherical prolate

- The inclusion of shell effects reduces the global RMS from 2387 keV to 1407 (1075) keV when the LDM1+DZ (LDM1+val) model is used.
- Still show a visible tendency to describe better the deformed than spherical nuclei,
- The results obtained with both formulas look very similar, with a smaller global RMS in the valence model and some advantage of the LDM1+DZ model to describe semi-magic nuclei.

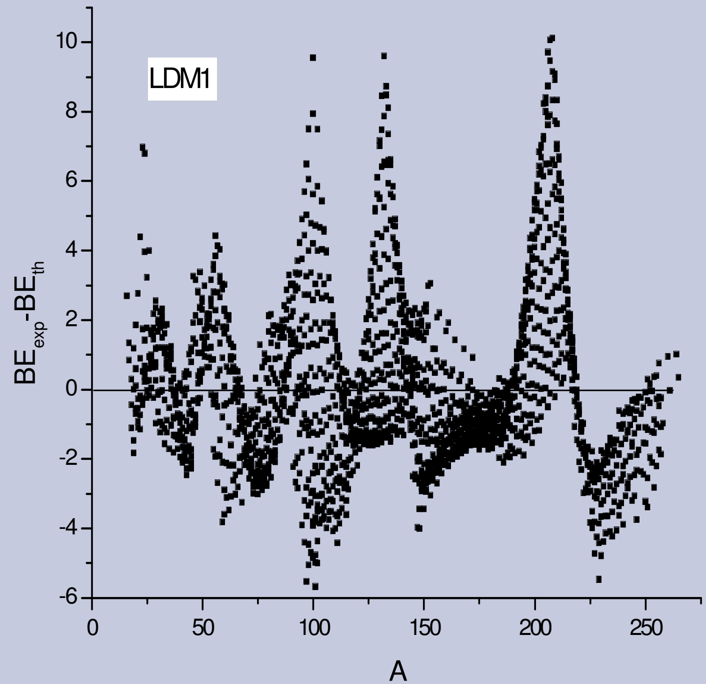
Combining LDM and DZ, val

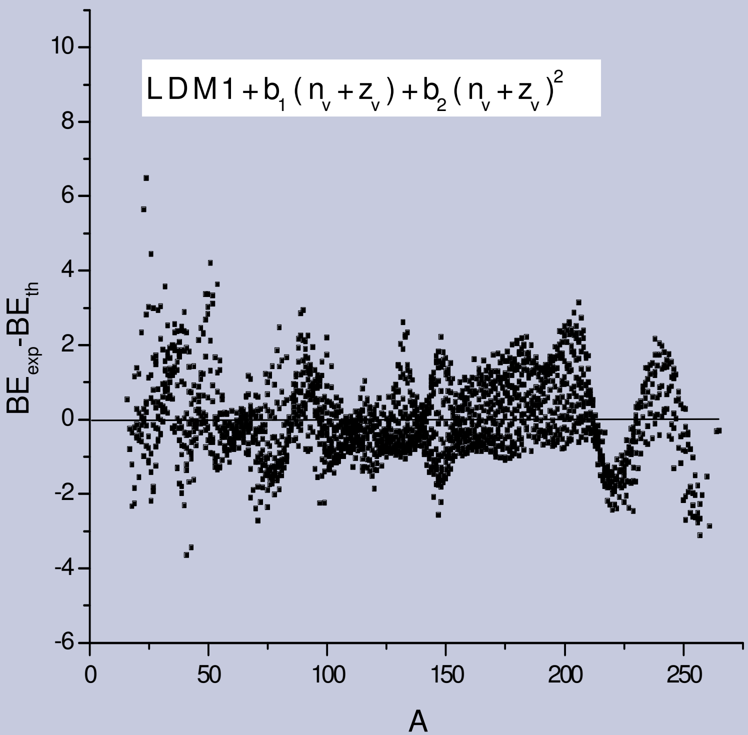
The relative stability of the parameters b_1 and b_2 in the LDM1+val model, is behind the comparatively small global RMS.

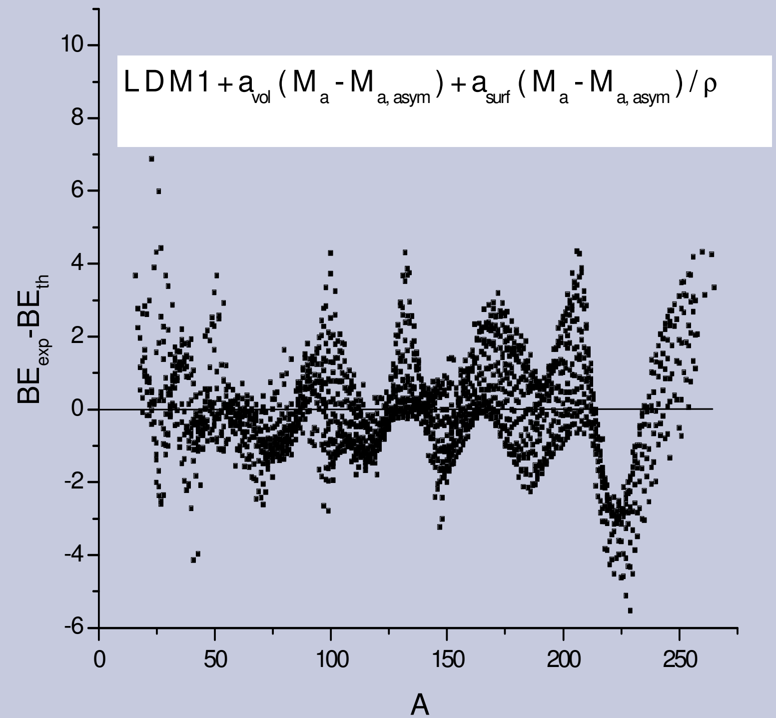
The shell surface and volume coefficients a_{surf} and a_{vol} of the LDM1+DZ model vary both in magnitude and in sign from one deformation region to another.

Being a limitation for a good global t, it offers at the same time the opportunity to relate these parameters with the deformation, a challenge which is left for future work.

Differences between experimental binding energies (Bexp) and theoretical results (Bth) for the thee models







Conclusions

- Liquid Drop Models fits deformed nuclei far better than spherical ones.
- The DZ model is based in a microscopic description of shell effects.
- An alternative DZ inspired master term was introduced.
- Adding two microscopic terms reduces noticeably the RMS of the fits.
- Improved master terms are still required for a good description of shell effects.
- Accurate mass formulas remain a challenge.

The shell corrections must be removed.

The LDM cannot describe them.

- A simple parameterization of shell effects: linear and quadratic dependence in the number of valence nucleons (F-spin)

Modified LDM (LDMM)

J. Mendoza-Temis, J. Barea, A. Frank, J.G. Hirsch, J.C. López Vieyra, I. Morales, P. Van Isacker, V. Velázquez, Nucl. Phys. A799 , 84 (2008).

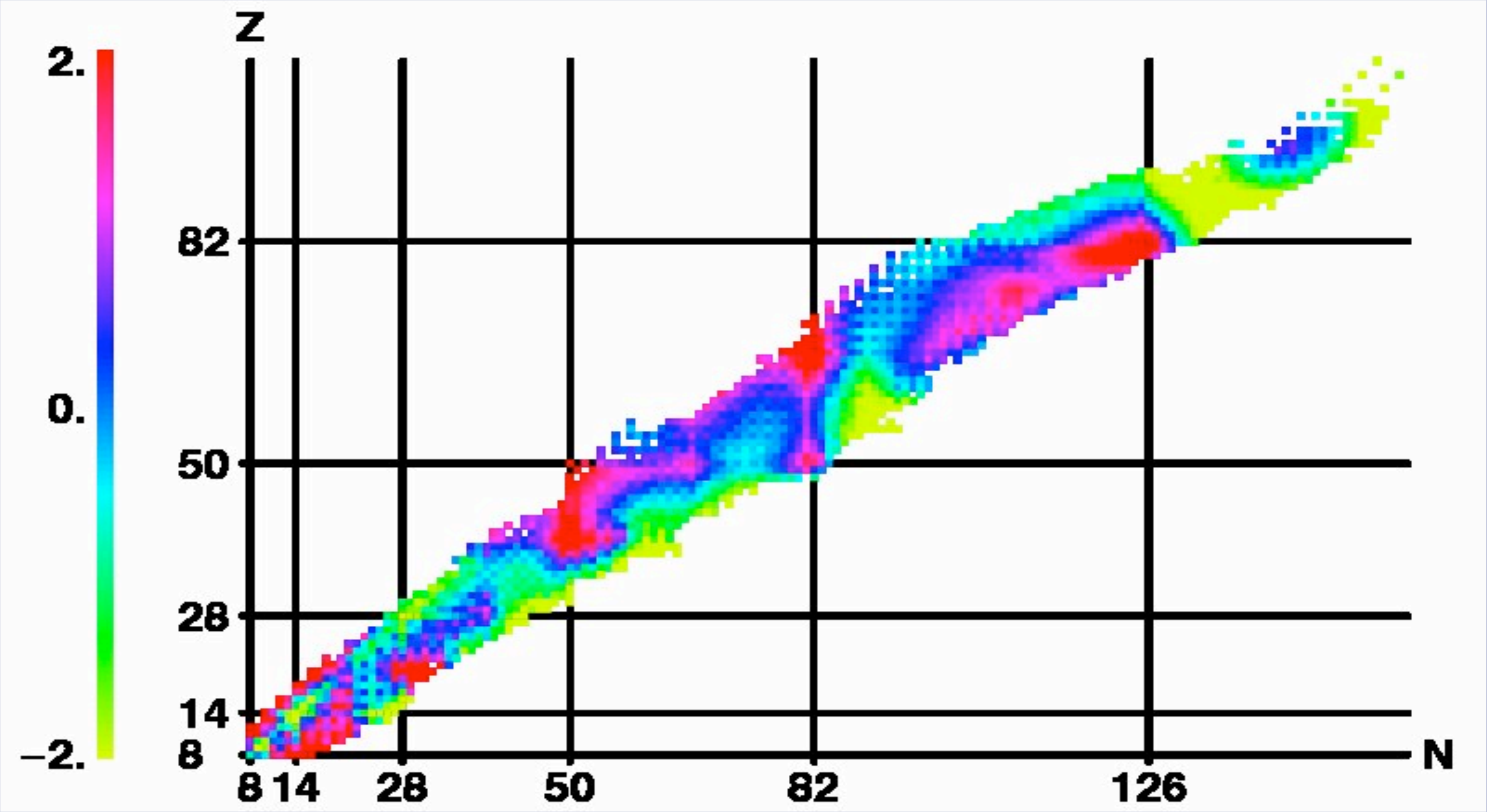
$$BE(N,Z) = a_v A - a_s A^{2/3} - a_c \frac{Z(Z-1)}{A^{1/3}} + a_p \frac{\delta(N,Z)}{A^{1/2}} - \frac{a_{vsym}}{1 + \frac{a_{vsym}}{a_{ssym}} A^{-1/3}} \frac{4T(T+r)}{A} - a_f F_{max} + a_{ff} F_{max}^2,$$

Includes two microscopic terms, linear and quadratic in the number of valence nucleons

$$F_{max} = n_\pi + n_\nu$$

LDMM, global fit

$$\text{RMS} = 1.33\ \text{MeV}, \quad \text{N,Z} \geq 8$$
$$\text{RMS} = 1.21\ \text{MeV}, \quad \text{N,Z} \geq 28$$



Differences between experimental and fitted masses

Modified Liquid Drop Model

A.E.L. Dieperink and P. Van Isacker, Eur. Phys. J. A42 269279 (2009).

$$
\begin{aligned}
E_{LDM1} &= -a_v A + a_s A^{2/3} + S_v \frac{4T(T+1)}{A(1+yA^{-1/3})} \\
&+ a_c \frac{Z(Z-1)}{(1-\Lambda)A^{1/3}} - a_p \frac{\Delta}{A^{1/3}}
\end{aligned}
$$

$$
E_{LDMM} = E_{LDM1} + b_1(n+z) + b_2(n+z)^2
$$

$$
E_{LDMM'} = E_{LDMM} + a_1 S_2 + a_2 (S_2)^2 + a_3 S_3 + a_{np} S_{np}
$$

where

$$
S_2 = \frac{n\bar{n}}{D_n} + \frac{z\bar{z}}{D_z}, \quad S_3 = \frac{n\bar{n}(n-\bar{n})}{D_n} + \frac{z\bar{z}(z-\bar{z})}{D_z},
$$

$$
S_{np} = \frac{n\bar{n}}{D_n}\frac{z\bar{z}}{D_z}, \quad \text{with} \quad \bar{n} \equiv D_n - n, \quad \bar{z} \equiv D_z - z,
$$

and D_n, D_z the degeneracy of the major valence shell.

The rms (in keV) in each region

	global	1	2	3	4	5	6	7	semi magic
LDM1	2387	1313	1676	2063	1746	1053	870	746	2113
LDM M	1075	796	961	1006	828	711	792	615	1037
LDM M’	887	627	740	902	634	561	619	574	817

oblate spherical prolate