The Duflo-Zuker mass model(s) and the three body issue

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Preliminaries (2011 version, updated)

"One mass formula stands above all others..."
"However, this does not mean that with Duflo-Zuker we have reached the end of history.." Quoted from
D. Lunney, J. M. Pearson and C. Thibault RMP **75** (2003) 1021; who refer to

J. Duflo and A.P. Zuker, Phys. Rev. C **52** (1995) R23; [DZ28 RMSD≈ 350 keV now 380 KeV]

Recently DZ has shown limitations and met WS competition (Phys. Rev. C **84**, 051303(R) (2011) Ning Wang and Min Liu).

However, once DZ rights and wrongs understood by studying DZ10 ∃ room to do better
(J. Duflo, 1996 unpublished, http://amdc.in2p3.fr/web/dz.html; RMSD≈ 550 keV now 580 keV)

J. Mendoza-Temis, J. G. Hirsch and A. P. Zuker Nuc. Phys. A **843** (2010) 14-36.

DZ10 is an invaluable summary of the DZ approach. It does not point to the end of history, but to a (Three Body) follow up of the story.

Grand Strategy 0

Guess form of Schrödinger many body solutions.

Which needs

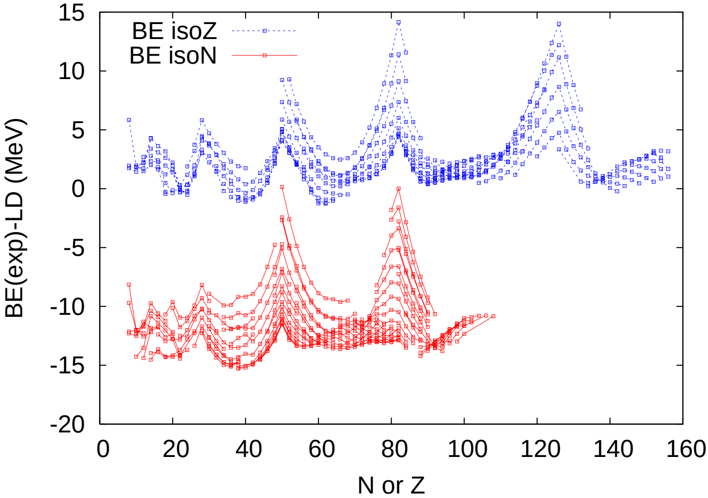
Clear idea of what the data say

Clear idea of what the NN Hamiltonian says

Clear idea(s) about the many body Shell Model

Some sort of idea of what the **FULL** Hamiltonian should look like

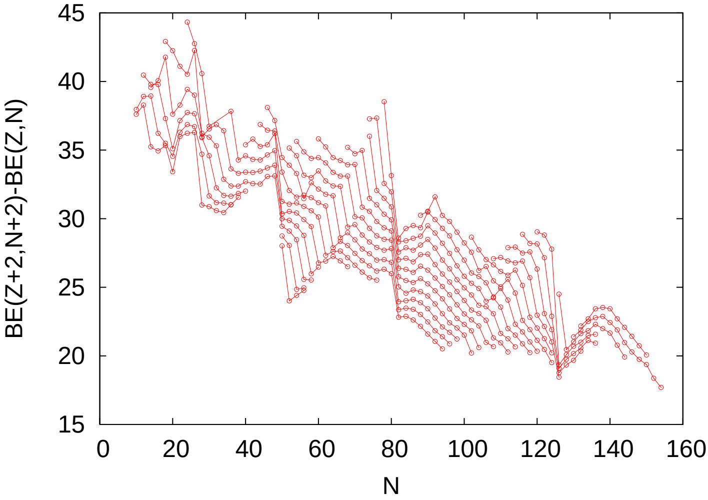
What has to be explained. BE: Shell effects + LD



$$\mathrm{LD} = 15.5A - 17.8A^{2/3} - 28.6\frac{4T(T+1)}{A} + 40.2\frac{4T(T+1)}{A^{4/3}} - \frac{.7Z(Z-1)}{A^{1/3}}.$$

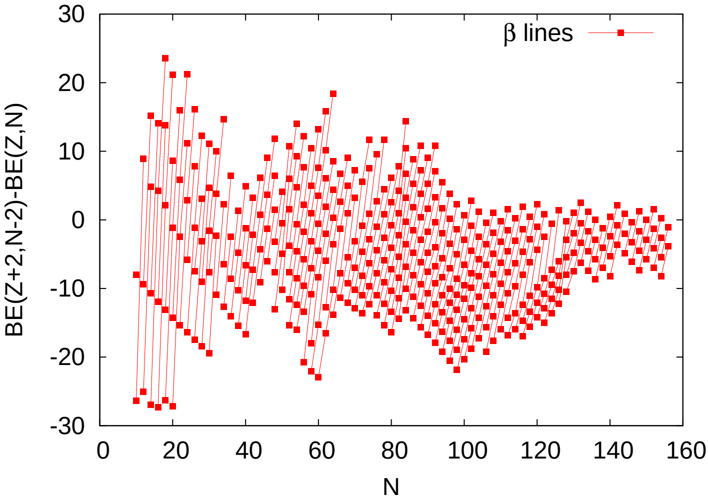
Alpha lines

Refine view of shell effects.
First at constant $t = N - Z$. Much stucture.



Beta lines

Now at constant A. No structure.



Grand Strategy I

DZ10 contains 10 terms:
6 "macro", 3 "correlation", 1 "deformation"

"Macro" is LD, except for "Leading" term which goes $\asymp A$ **and** produces shell effects.

"Leading" is "Master" (from NN) plus corrections to have the right shell effects.

Two calculations are done : Macro+correlation and Macro+deformation. Lowest is kept.

Concentrate on Master

Grand Strategy II

Separate monopole H_m from multipole H_M.

$$H = H_m + H_M \tag{1}$$

$$H_m = \text{all quadratic forms in } a_r^+ \cdot a_s \tag{2}$$

$$H_{md} = \sum_{rs} m_r(m_s - \delta_{rs})V_{rs} + T_r \cdot T_s \text{ terms} \tag{3}$$

H_m contains **LD+shell effects** (and Hartree Fock and more). It defines model spaces.
H_M is responsible for SM configuration mixing.

From α and β lines we decide that T terms play little role in shell effects. So we study the m terms.

The Master Term

$$\mathbf{Diagonalize} \implies \mathbf{H_{md}} = \sum_{\alpha} \mathbf{E}_{\alpha} \sum_{\mathbf{ks}} \mathbf{U}_{\alpha \mathbf{k}} \mathbf{m_k} \mathbf{U}_{\alpha \mathbf{s}} \mathbf{m_s}$$

One term overwhelms all others, Calling m_p the number of particles in the major HO shell of principal quantum number p of degeneracy $D_p = (p+1)(p+2)$, we find $\mathbf{U_{0k} m_k \approx U_{0p} m_p = m_p / \sqrt{D_p}}$

$$\mathbf{M}_A \propto \frac{\hbar\omega}{\hbar\omega_0} \left(\sum_p \frac{m_p}{\sqrt{D_p}} \right)^2 \propto \frac{A^{1/3}}{\langle r^2 \rangle} \left(\sum_p \frac{m_p}{\sqrt{D_p}} \right)^2 \propto \tag{4}$$

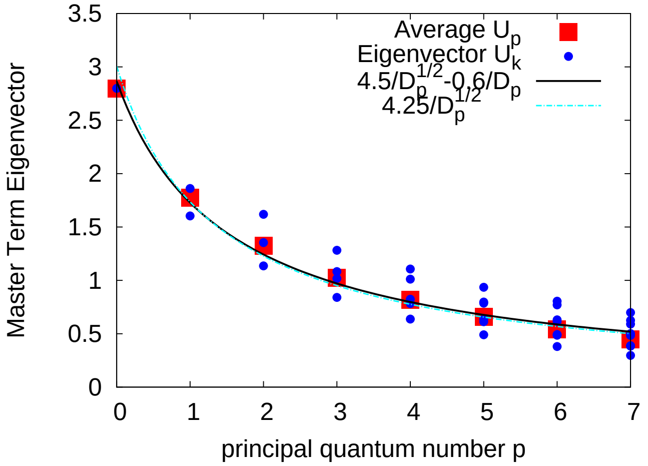
$$\frac{\mathbf{1}}{\mathbf{A^{1/3}}} \left(\sum_{\mathbf{p}} \frac{\mathbf{m_p}}{\sqrt{\mathbf{D_p}}} \right)^{\mathbf{2}} \asymp \frac{\mathbf{1}}{\mathbf{A^{1/3}}} (\mathbf{p_f + 2})^{\mathbf{4}} \approx (\mathbf{3/2})^{\mathbf{4/3}} \mathbf{A} \tag{5}$$

$$\text{Variant} \quad \frac{m_p}{\sqrt{D_p}} \longrightarrow \frac{m_p}{\sqrt{D_p}} \left(1 + \frac{\alpha}{\sqrt{D_p}}\right) \equiv \frac{m_p}{\sqrt{D_p}} u_p \tag{6}$$

Looks and origin of the Master Term

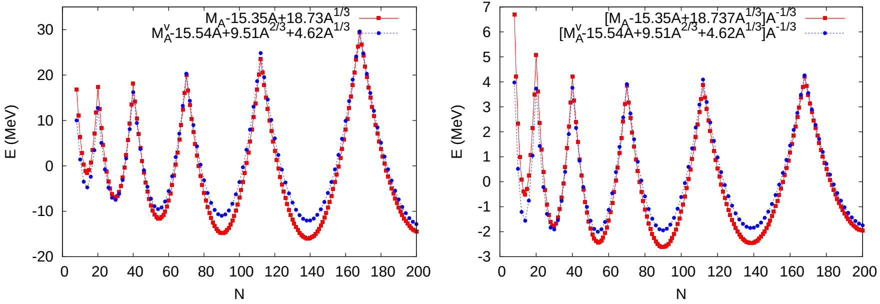
Just in case you wonder what we are up to:

Master Term contains bulk LD ; and some more...



Master shell effects. $A^{1/3}$ scaling

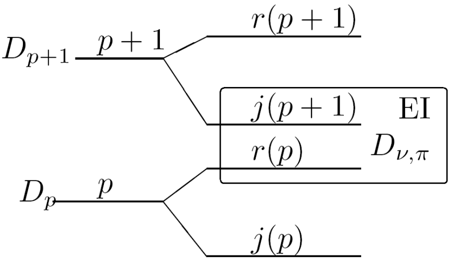
The two variants lead to different asymptotics
$M_A \asymp 17.05A - 20.87A^{1/3}$
$M_A^v \asymp 17.27A - 10.57A^{2/3} - 5.13A^{1/3}$



Master shell effects produced by M_A and M_A^v for $t = N - Z = 0$.
They are parabolic segments bounded by HO closures at $N = 8$, 20, 40, 70, 112 and 168, that scale asymptotically as $A^{1/3}$

The HO-EI transition

Big Problem: to transform HO closures into extruder-intruder (EI) ones at N,Z=28,50,82 and 126.The *NN* forces do not do it.



Restrict subshell structure to j_p and r_p. Relevant operators must be linear, quadratic and cubic forms involving

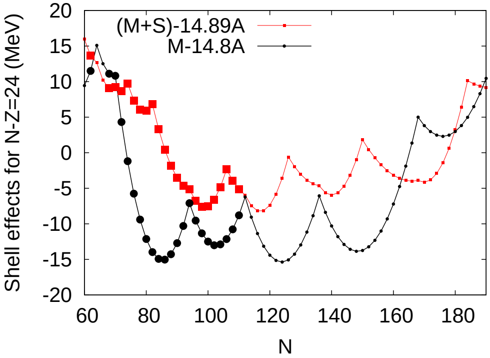
$m_p = m_{j(p)} + m_{r(p)}$ and

$s_p = \left[(pm_{j_p} - 2m_{r_p})/(p+2)\right] = \Gamma^{(1)}_{jr}$

The leading DZ10 term

By now it is clear that HO-EI transition must involve three body (3b) (Huge open problem. Originally ignored. See later)
DZ28 used some 12 2b terms. DZ10 uses a single leading one

$$M + S = M + \sum_p [u^{(1)} s_p + u^{(2)} m_p s_p / \sqrt{D_p}]$$



The HO-EI transition for $N - Z = 24$ even-even nuclei

DZ10 Stucture and evolution

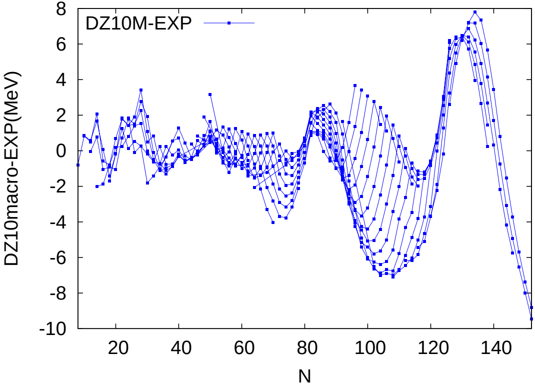
There are 10 terms:

1. Leading, contains basic shell effects. Goes asymptotically as A.
2. Surface, contains basic shell effects. Goes asymptotically as $A^{2/3}$.
3. Asymmetry, $T(T+1)/A$
4. Surface asymmetry, $T(T+1)/A^{4/3}$
5. Pairing, $mod(N,2) + mod(Z,2)$
6. Coulomb, $Z(Z-1)/A^{1/3}$
7. Cubic spherical "correlation"
8. Surface cubic spherical "correlation"
9. Quartic spherical correlation
10. Quartic deformation

Fits yield

- For the first six "macroscopic" terms, RMSD=2.88 MeV (LD RMSD=2.35 MeV) Looks bad, but
- For the first nine terms, RMSD=717 keV.
- For the ten terms, RMSD=567 keV

The DZI "macro" term and EI "correlations"



Notation, $\bar{m} = D - m \quad m^{(2)} = m(m-1) \quad \rho = A^{1/3}$

$$|\bar{0}\rangle = (1 + \sum_k \hat{A}_k)|0\rangle \Longrightarrow E = \langle 0|H_m|0\rangle + \langle 0|H_M \hat{A}_2|0\rangle \Longrightarrow$$

macro; $\dfrac{m_v \bar{m}_v}{D_v \rho}$; $\dfrac{m_v \bar{m}_v (m_v - \bar{m}_v)}{D_v^2 \rho}$; $\dfrac{m_v^{(2)} \bar{m}_v{}^{(2)}}{D_v^3 \rho}$ SO? GEMO

Digression: DZ rigths and wrongs

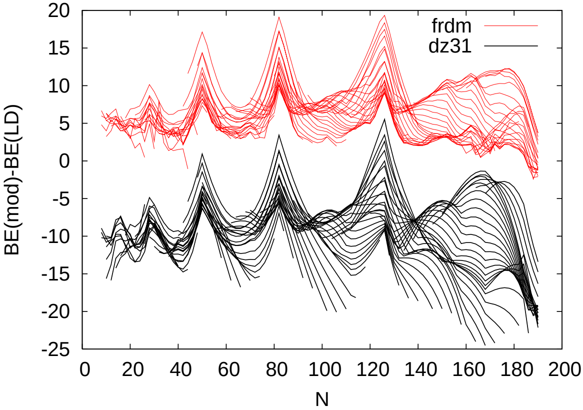
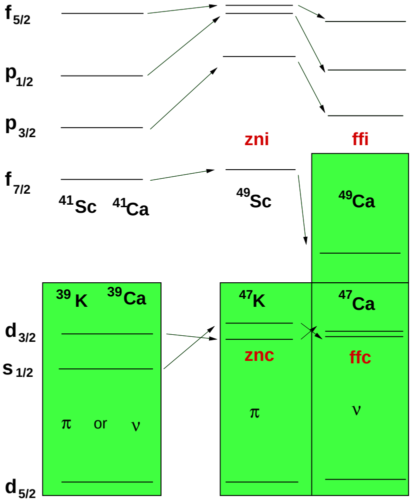


Figure: Binding energies related to LD for frdm and dz31 (arbitrary displacements).

Try LD-free H_m from cs ± 1 spectra: DZII GEMO



Evolution of $(cs \pm 1\ )$ spectra from ^{40}Ca to ^{48}Ca

Some examples of cs ± 1 spectra

12	Ca	**20 19**	33	Ca	**20 21**	2	K	**19 28**	33	Ca	**20 27**
2	1.9	2.40	13	1.9	2.00	12	0.2	0.36	12	2.6	2.58
22	6.2	6.00	3	3.8	4.00	22	5.7	5.70	2	3.2	2.60
1	13.7		23	5.9	6.00	1	14.2		22	8.6	8.00
			44	7.5				znc			ffc
13	Ca	**20 29**	33	Sc	**21 28**	13	Ni	**28 29**	24	Zr	**40 51**
3	1.9	2.00	13	4.0	4.00	23	1.0	0.77	4	1.2	1.20
23	3.9	4.00	3	5.5	5.50	3	1.4	1.11	14	2.1	2.00
44	4.9		23	5.0	4.70	44	3.3	3.50	34	3.0	2.70
24	8.3	ffi	44	8.2	zni	24	7.1		55	3.6	
44	In	**49 82**	14	Sn	**50 81**	35	Sn	**50 83**	34	Sb	**51 82**
3	0.1	0.35	4	0.3	0.33	45	1.2	(1.56)	24	1.3	0.96
13	1.2		55	0.9	0.24	15	1.3	(0.85)	55	2.7	2.79
23	3.8		24	1.6	1.52	5	2.3	(2.00)	14	2.9	2.71
33	7.8		34	2.4	2.43	66	2.3		4	2.9	
4	Tl	**81 126**	5	Pb	**82 125**	46	Pb	**82 127**	45	Bi	**83 126**
14	0.5	0.35	25	0.5	0.57	56	0.9	0.78	35	1.2	0.90
55	1.2	1.35	15	0.7	0.90	26	1.2	1.57	66	2.2	1.60
24	1.9	1.68	66	1.6	1.63	77	1.9	1.42	25	2.6	2.83
34	4.4	4.60	35	2.1	2.34	6	2.0	2.03	15	2.9	3.12
44	7.9		45	3.0	3.41	36	2.3	2.49	5	3.6	3.60
			55	8.2		16	2.6	2.54	46	7.0	

Excitation energies. Orbits labeled by $j-1/2$ p, so 12 and 2, say, stand for $j=3/2$ and $j=1/2$ in the $p=2$ shell, (i.e. $0d_{3/2}$ and $1s_{1/2}$).

cs ± 1 gaps. NOT included in fit

	C	**6 6**	O	**8 8**	O	**8 14**	Si	**14 14**
ΔN	7.9	13.78	6.5	11.52	4.0	4.11	7.1	8.71
ΔZ	7.9	14.01	6.5	11.53	6.5	9.99	7.1	8.84
	Ca	**20 20**	Ca	**20 28**	Ni	**28 28**	Ni	**28 40**
ΔN	5.2	7.28	4.8	4.80	7.4	6.39	2.8	2.85
ΔZ	5.2	7.24	4.9	6.18	7.4	6.47	6.4	5.91
	Ni	**28 50**	Zr	**40 50**	Sn	**50 82**	Pb	**82 126**
ΔN	5.7		4.7	4.77	4.3	4.89	3.0	3.43
ΔZ	6.5		1.8	2.00	5.5	6.07	3.5	4.20

ΔN= 2BE(Z N)-BE(Z N+1)-BE(Z N-1)

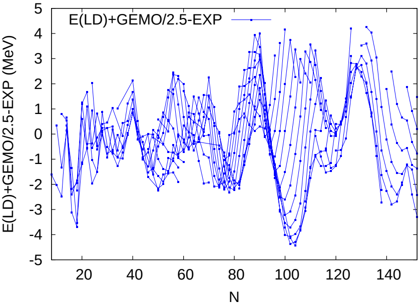
ΔZ= 2BE(Z N)-BE(Z+1 N)-BE(Z-1 N).

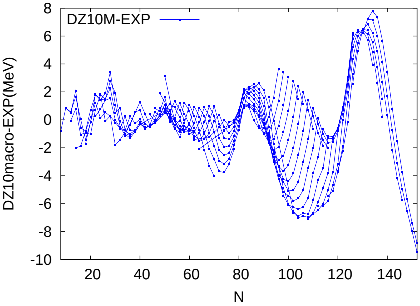
Calculated first, experimental next.

GEMO masses

How does DZ10 monopole relate to “true” GEMO H_m ?

Calculate GEMO masses subject to a 2.5 contraction and add LD.



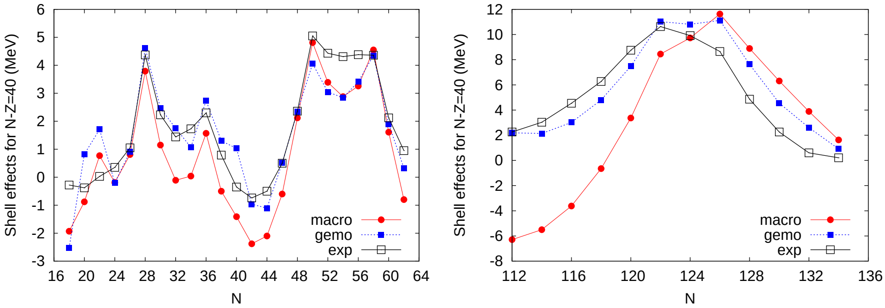


Beware of y-axis scales. Comment on RMSD

Comment on majestic cubics.

Predicted monopole shell effects for t=8,40

corrected asymptotics, 2.5 compression



- If a closure exists, it is there, but;
- If it is there, it does not necessarily exist.

$N = 22$, $Z = 14$ erased closure. $N = 28$, $Z = 20$ and $N = 36$, $Z = 28$ good closures. $N = 40, Z = 32$ erased closure. $N = 50$, $Z = 42$ and $N = 58$, $Z = 50$ good closures.

Speculate on 3b Master

$$A = \sum_p m_p = \sum_{p=0}^{p_f} 2(p+1)(p+2) \Longrightarrow \frac{2(p_f+3)^{(3)}}{3}. \tag{7}$$

$$\mathcal{K}^d = \frac{\hbar\omega}{2} \sum_p m_p(p+3/2) \Longrightarrow \frac{\hbar\omega}{4}(p_f+3)^{(3)}(p_f+2) \tag{8}$$

$$\mathcal{V}^d \approx \hbar\omega\mathcal{V}_0 \left(\sum_p \frac{m_p}{\sqrt{D_p}} + \hat{\Omega} \right)^2 \Longrightarrow \hbar\omega\mathcal{V}_0[p_f(p_f+4)]^2, \tag{9}$$

$$\tag{10}$$

As $\mathcal{K}^d$ and $\mathcal{V}^d$ go as $\hbar\omega$ no way to saturate. Try to add

$$\mathcal{V}^{d_3} \approx (\hbar\omega)^2\beta\mathcal{V}_0 \left(\sum_p \frac{m_p}{D_p} + \hat{\Omega}_1 \right) \left(\sum_p \frac{m_p}{\sqrt{D_p}} + \hat{\Omega}_2 \right)^2$$

$$\Longrightarrow (\hbar\omega)^2\beta\mathcal{V}_0 p_f^3(p_f+4)^2. \tag{11}$$

ETC...

The correct HO-EI transition mechanism I
Monopole technology: Invariant decomposition

Use $D^{(2)} = D(D-1)$, $m^{(2)} = m(m-1)$, $\bar{m} = D - m$. Define

$$\Gamma^{(1)}_{st} = \left(\frac{m_s}{D_s} - \frac{m_t}{D_t}\right)\frac{D_s D_t}{D_s + D_t} = -\left(\frac{\bar{m}_s}{D_s} - \frac{\bar{m}_t}{D_t}\right)\frac{D_s D_t}{D_s + D_t} = -\bar{\Gamma}^{(1)}_{st} \quad (12)$$

$$\Gamma^{(2)}_{st} = \left(\frac{m^{(2)}_s}{D^{(2)}_s} + \frac{m^{(2)}_t}{D^{(2)}_t} - \frac{2 m_s m_t}{D_s D_t}\right)\frac{D^{(2)}_s D^{(2)}_t}{(D_s + D_t)^{(2)}} = \bar{\Gamma}^{(2)}_{st} \equiv \Gamma^{(2)}_{st}(\bar{m}_s, \bar{m}_t) \quad (13)$$

and replace "cartesian" linear and quadratic forms by invariant ones

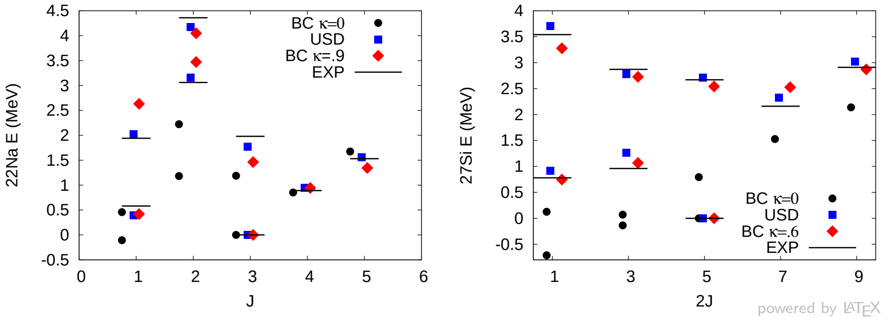
$$m_s \equiv m_p + \Gamma^{(1)}_{s1} \quad (14)$$

$$\frac{m_s(m_t - \delta_{rs})}{1 + \delta_{rs}} \equiv \frac{1}{2} m_p(m_p - 1) + (m_p - 1)\Gamma^{(1)}_{st} + \Gamma^{(2)}_{st}, \quad (15)$$

The correct HO-EI transition mechanism II

To bring about correct EI transition, modify realistic interaction by adding

$$(a_2 + b_2 m_p)\Gamma^{(2)}_{j(p)r(p)} \equiv \kappa(m)\Gamma^{(2)}_{j(p)r(p)}$$

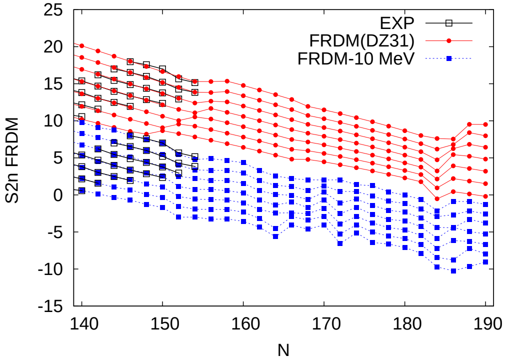


Bibliographical Notes

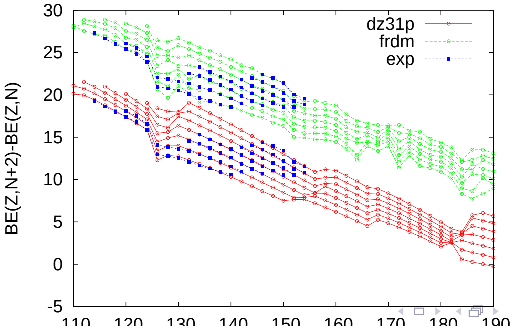
- AMDC. http://amdc.in2p3.fr; http://amdc.in2p3.fr/web/dz.html
- EP:76. E. Pasquini, Ph.D thesis (ULP Strasbourg) Report CRN/76-14
- EPAPZ:78. E. Pasquini and A. P. Zuker, *Proceedings of the Topical conference on Physics of Medium Light Nuclei* Florence 1978, edited by P. Blasi and R. A. Ricci (Editrice Compositori, Bologna)
- Zuker:94. On the microscopic derivation of a mass formula. A.P. Zuker, Nucl. Phys. **A576** (1994) 65.
- Dufour,Zuker:96. The realistic collective Hamiltonian. M. Dufour and A.P. Zuker, Phys. Rev. C **54** (1996) 1641.
- Duflo,Zuker:1995. Microscopic mass formulas. J. Duflo and A.P. Zuker , Phys. Rev. C **52** (1995) R23
- Duflo,Zuker:1999. The Nuclear Monopole Hamiltonian, J. Duflo and A. P. Zuker, Phys. Rev. C **59**, 2347R (1999).
- Duflo,Zuker:2002 Mirror displacement energies and neutron skins. J. Duflo and A. P. Zuker, Phys. Rev. C **66**, 051304R (2002).
- LPT:2003. Recent trends in the determination of nuclear masses D. Lunney, J. M. Pearson and C. Thibault RMP **75**, pags. 1021-1082 (2003).

- Caurier *et al.*:2005. The Shell Model as a Unified View of Nuclear Structure: E. Caurier, G. Martínez-Pinedo, F. Nowacki, A. Poves, A. P. Zuker, nucl-th/0402046. RMP.**77**, pags. 427-488 (2005).
- Zuker:2003. Three body monopole corrections to the realistic interactions, A. P. Zuker PRL **90** 042502.
- Schwenk,Zuker:2006. Shell-model phenomenology of low-momentum interactions Achim Schwenk and Andrés P. Zuker, Phys. Rev. C 74, 061302(R) (2006).
- MHZ:09. Mendoza-Temis, J. G. Hirsch and A. P. Zuker, The anatomy of the simplest Duflo-Zuker mass formula, nucl-th 09 120882.

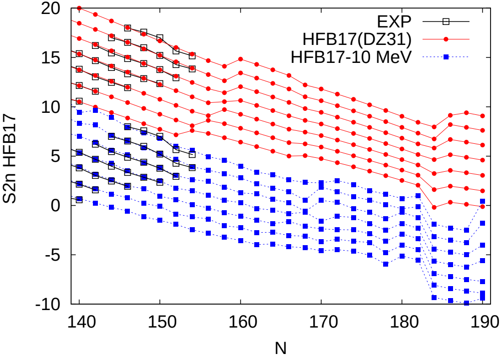
MODEL	AME03	DZ10	DZ31	FRDM	FRDM(DZ10)	FRDM(DZ31)
AME03	0.000	0.551	0.363	0.655	0.618	0.578
DZ10	0.551	0.000	0.427	0.721	0.282	0.543
DZ31	0.363	0.427	0.000	0.662	0.495	0.457
FRDM	0.655	0.721	0.662	0.000	0.663	0.491
FRDM(DZ10)	0.618	0.282	0.495	0.663	0.000	0.464
FRDM(DZ31)	0.578	0.543	0.457	0.491	0.464	0.000
HFB17	0.581	0.770	0.603	0.735	0.764	0.655
HFB17(DZ10)	0.590	0.219	0.470	0.689	0.202	0.497
HFB17(DZ31)	0.471	0.567	0.339	0.657	0.556	0.466

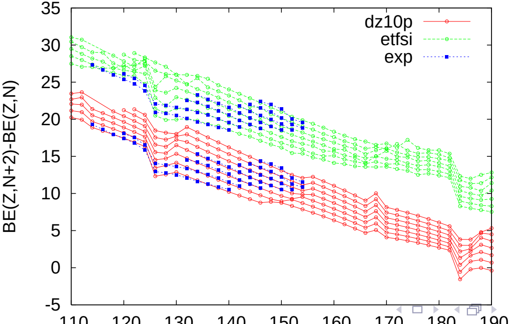


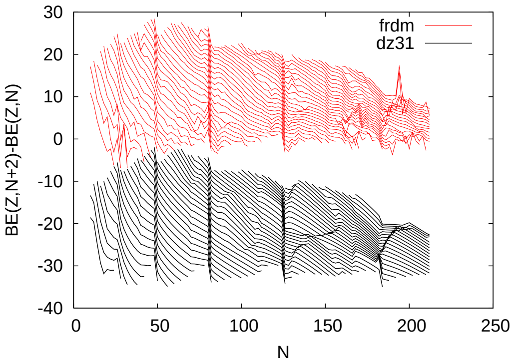
EXP
FRDM(DZ31)
FRDM-10 MeV
S2n FRDM
N
25
20
15
10
5
0
-5
-10
-15
140
150
160
170
180
190

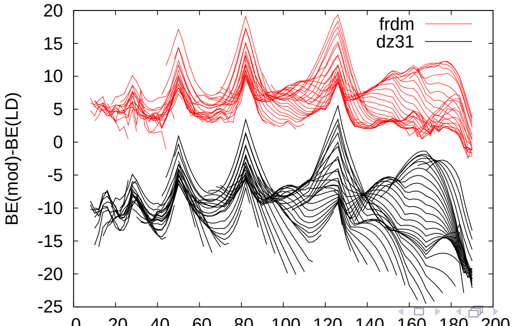


dz31p
frdm
exp
BE(Z,N+2)-BE(Z,N)
30
25
20
15
10
5
0
-5
110
120
130
140
150
160
170
180
190

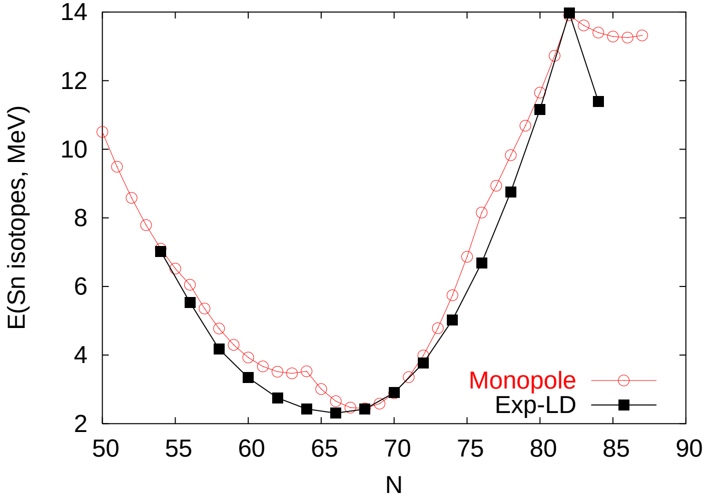

EXP
HFB17(DZ31)
HFB17-10 MeV
S2n HFB17
N
20
15
10
5
0
-5
-10
140
150
160
170
180
190


dz10p
etfsi
exp
BE(Z,N+2)-BE(Z,N)
35
30
25
20
15
10
5
0
-5
110
120
130
140
150
160
170
180
190


frdm
dz31
BE(Z,N+2)-BE(Z,N)
N
30
20
10
0
-10
-20
-30
-40
0
50
100
150
200
250

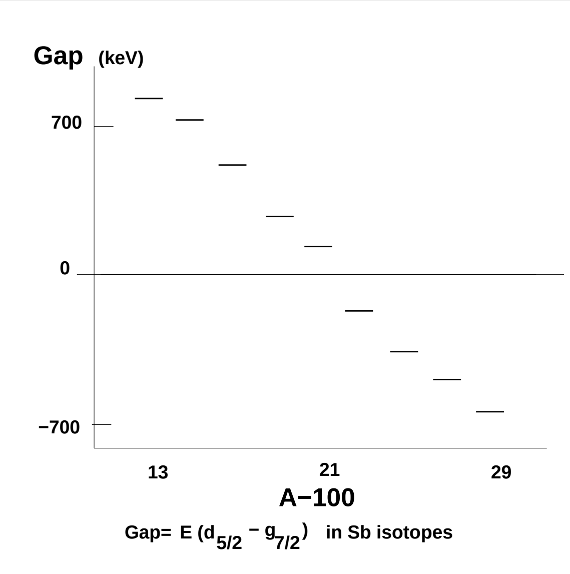

frdm
dz31
BE(mod)-BE(LD)
20
15
10
5
0
-5
-10
-15
-20
-25
0
20
40
60
80
100
120
140
160
180
200

More of the same for Sn



Comment on contraction factor

Example of monopole drift in Sb



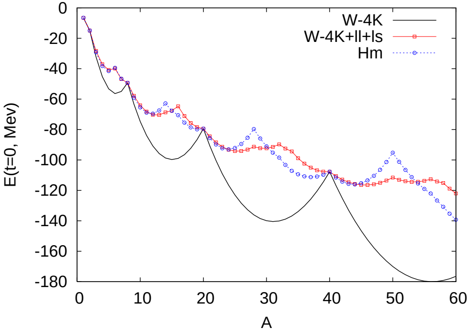
How filling $0h_{11/2}$ changes things; E=0 for $1d_{5/2}$.

DZII on cs $\pm$ 1: Trick to separate bulk

(Duflo.Zuker:1999)

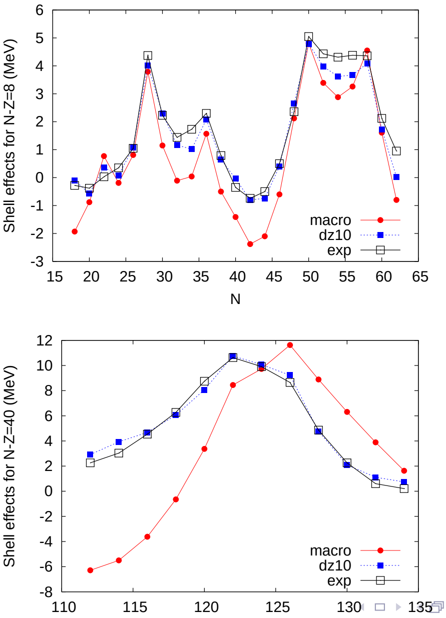
$$M_A - 4K = \left(\sum_p \frac{m_p}{\sqrt{D_p}}\right)^2 - 2\sum_p m_p(p+3/2)$$

$$H_m^s = M_A - 4K + l\cdot s + l\cdot l + \text{2b drift terms} \quad (16)$$

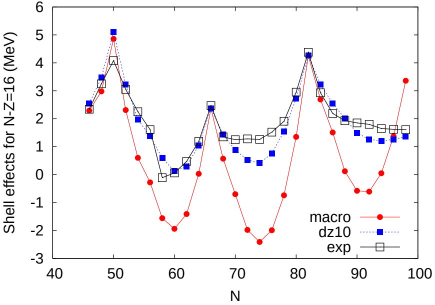


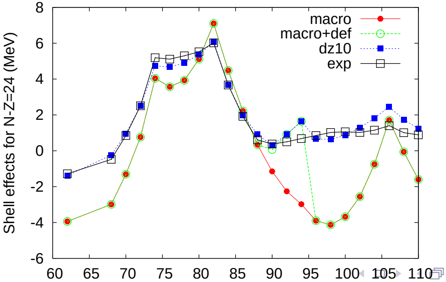
Six-parameter fit to 90 known $cs \pm 1$ spectra $\Longrightarrow$ rmsd=220 keV

How DZ10 correlation works t=8,40

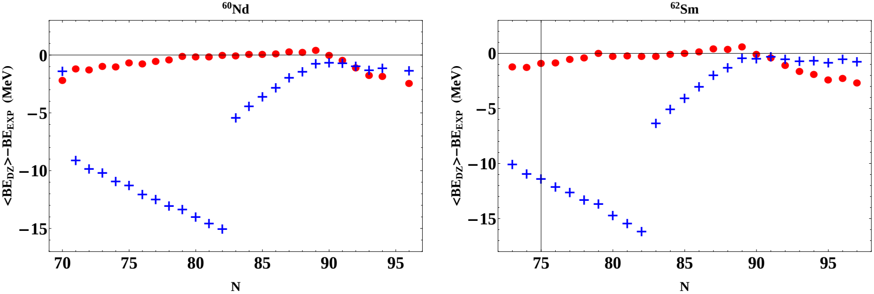


How DZ10 correlation works t=16,24



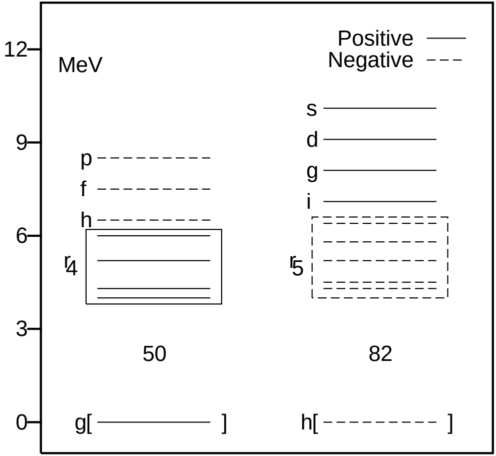


Deformation in DZ10



Deformation

Schematic single particle spectrum above ^{132}Sn. r_p is the set of orbits in shell p excluding the largest. For the upper shells the label l is used for $j = l + 1/2$



$B(E2)\uparrow$ in e^2b^2 compared with experiment

$$Q_0 = 56e_\pi + (76+4n)e_\nu, \qquad (17)$$

$B(E2)\uparrow = 10^{-5}\mathrm{A}^{2/3}Q_0^2$

N	Nd	Sm	Gd	Dy
92	4.47	4.51	4.55	4.58
	2.6(7)	4.36(5)	4.64(5)	4.66(5)
94	4.68	4.72	4.76	4.80
			5.02(5)	5.06(4)
96	4.90	4.95	4.99	5.03
			5.25(6)	5.28(15)
98	5.13	5.18	5.22	5.26
				5.60(5)