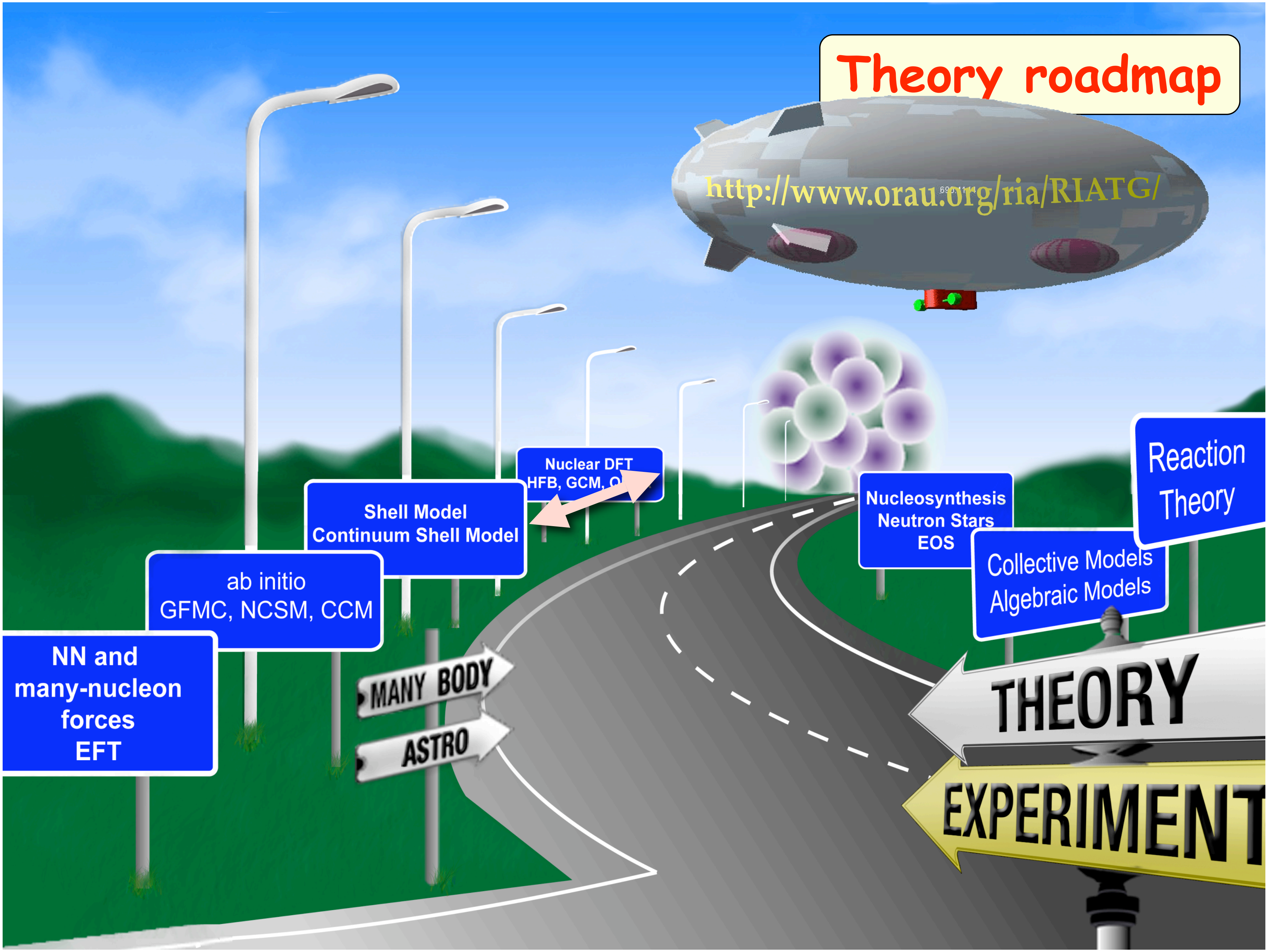
Fourteen billion years after the big bang.

Physics and the Real World, F.R. Ellis, Physics Today, July 2005

- **Intruder States in fp shell**
  - Shell Model - DFT
  - Time-odd terms
  - T=0 pairing?
- **Microscopic Leptodermous Expansion**
  - Robustness of LDM
  - What can we learn about LEDF?

Witold Nazarewicz (UT/ORNL)
DFT Workshop, INT 2005

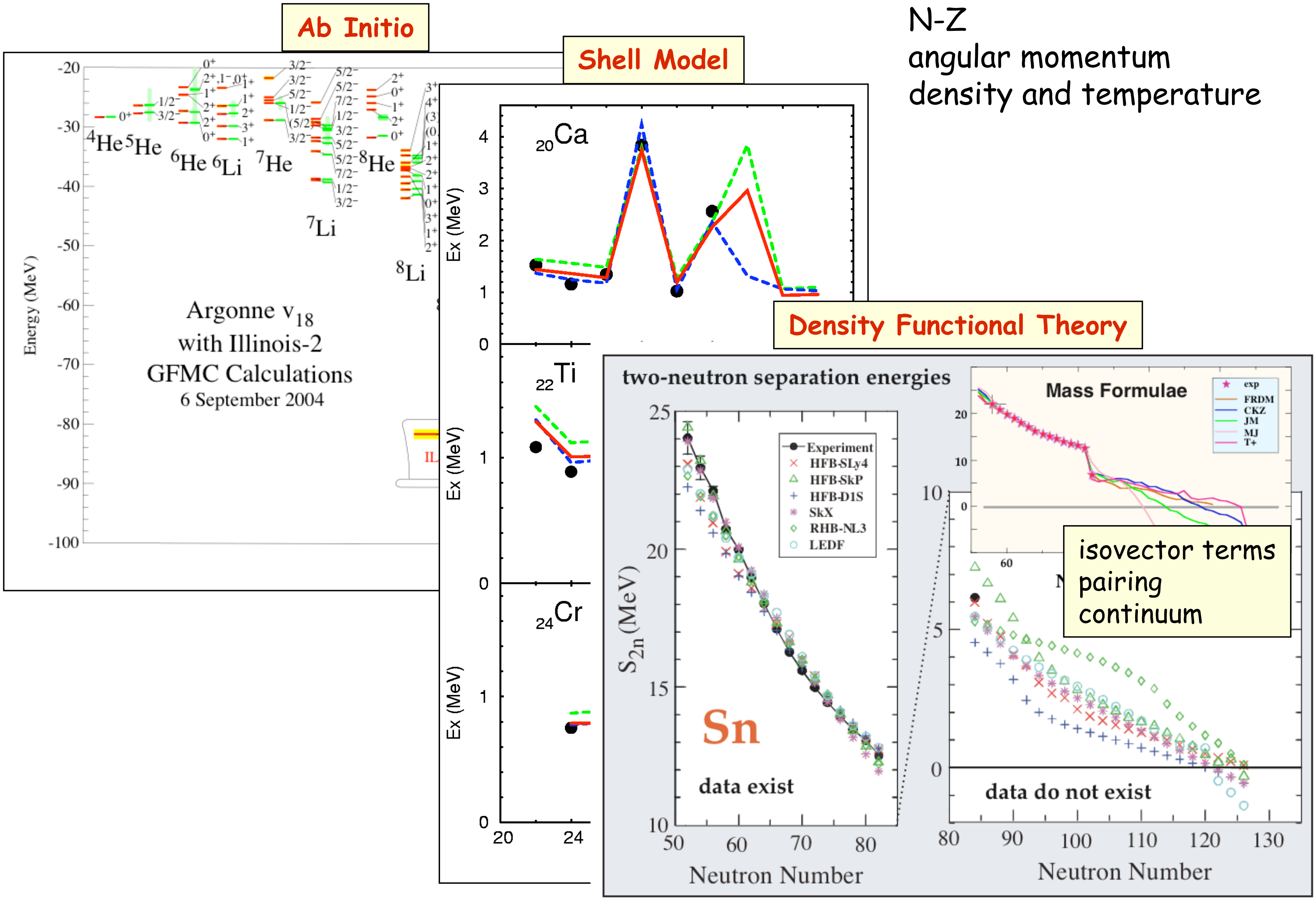
Selectivity and Amplification!!!



Theory roadmap
http://www.orau.org/ria/RIATG/
Reaction Theory
Nuclear DFT
HFB, GCM, Q
Shell Model
Continuum Shell Model
Nucleosynthesis
Neutron Stars
EOS
Collective Models
Algebraic Models
ab initio
GFMC, NCSM, CCM
NN and
many-nucleon
forces
EFT
MANY BODY
ASTRO
THEORY
EXPERIMENT

What are the missing pieces?

N-Z
angular momentum
density and temperature



Towards the Universal Nuclear Energy Density Functional

$\rho_0(\vec{r}) = \rho_0(\vec{r},\vec{r}) = \sum_{\sigma\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau)$ isoscalar (T=0) density $(\rho_0 = \rho_n + \rho_p)$

$\rho_1(\vec{r}) = \rho_1(\vec{r},\vec{r}) = \sum_{\sigma\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau)\tau$ isovector (T=1) density $(\rho_1 = \rho_n - \rho_p)$

$\vec{s}_0(\vec{r}) = \sum_{\sigma\sigma'\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma'\tau)\sigma_{\sigma'\sigma}$ isoscalar spin density

$\vec{s}_1(\vec{r}) = \sum_{\sigma\sigma'\tau} \rho(\vec{r}\sigma\tau;\vec{r}\sigma'\tau)\sigma_{\sigma'\sigma}\tau$ isovector spin density

$\vec{j}_T(\vec{r}) = \frac{i}{2}(\vec{\nabla}' - \vec{\nabla})\rho_T(\vec{r},\vec{r}')\big|_{\vec{r}'=\vec{r}}$ current density

$\vec{J}_T(\vec{r}) = \frac{i}{2}(\vec{\nabla}' - \vec{\nabla}) \otimes \vec{s}_T(\vec{r},\vec{r}')\big|_{\vec{r}'=\vec{r}}$ spin-current tensor density

$\tau_T(\vec{r}) = \vec{\nabla}\cdot\vec{\nabla}'\rho_T(\vec{r},\vec{r}')\big|_{\vec{r}'=\vec{r}}$ kinetic density

$\vec{\mathbf{T}}_T(\vec{r}) = \vec{\nabla}\cdot\vec{\nabla}'\ \vec{s}_T(\vec{r},\vec{r}')\big|_{\vec{r}'=\vec{r}}$ kinetic spin density

Local densities and currents + pairing...

Construction of the functional:
E. Perlinska et al.
Phys. Rev. C 69, 014316 (2004)

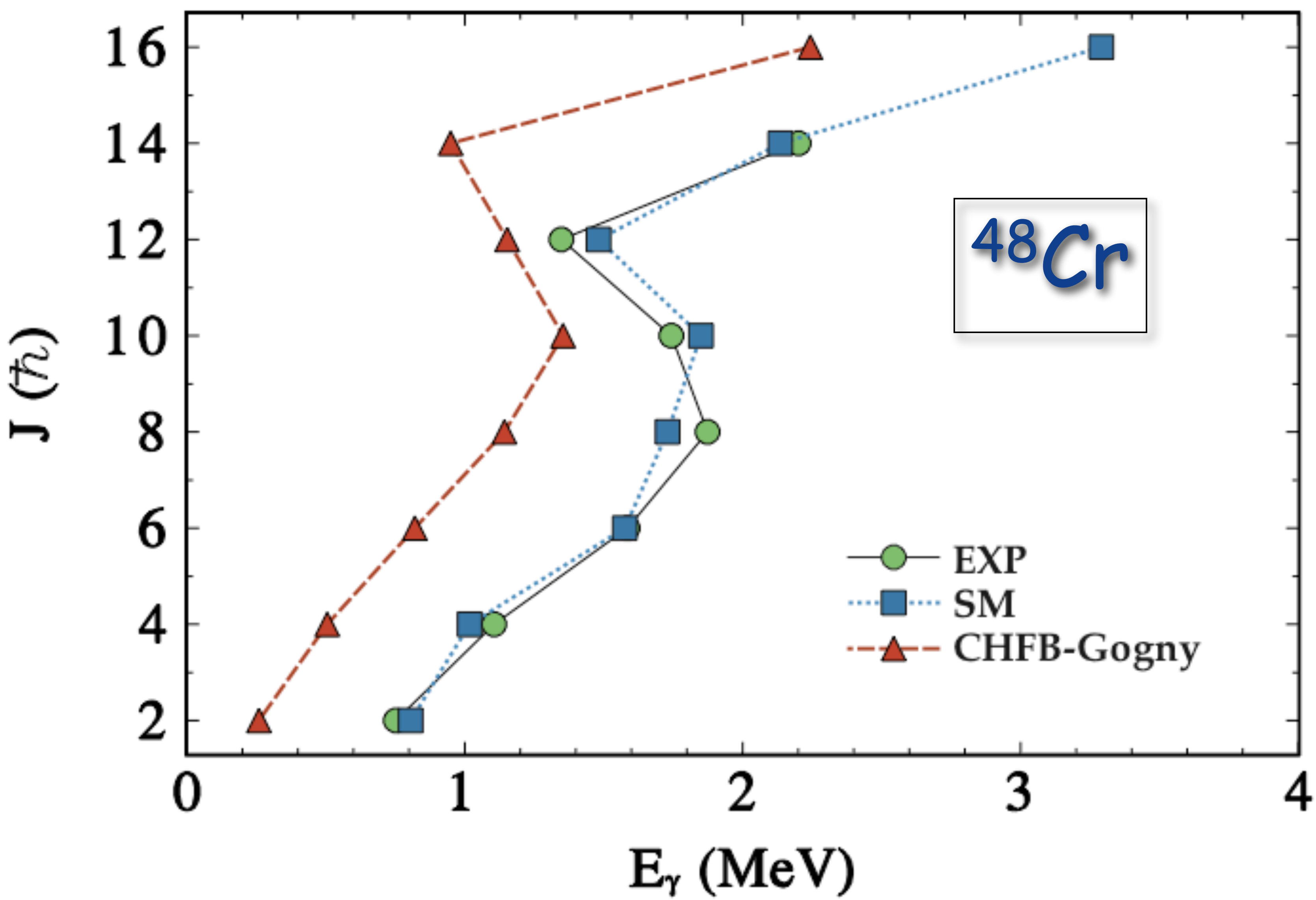
$$\mathcal{H}_T(\vec{r}) = C_T^{\rho}\rho_T^2 + C_T^{s}s_T^2 + C_T^{\Delta\rho}\rho_T\Delta\rho_T + C_T^{\Delta s}\vec{s}_T\Delta\vec{s}_T$$
$$+C_T^{\tau}\left(\rho_T\tau_T - j_T^2\right) + C_T^{T}\left(\vec{s}_T\cdot\vec{T}_T - \vec{J}_T^2\right) + C_T^{\nabla J}\left[\rho_T\vec{\nabla}\cdot\vec{J}_T + \vec{s}_T\cdot\left(\vec{\nabla}\times\vec{j}_T\right)\right]$$

Example: Skyrme Functional

Local is good!

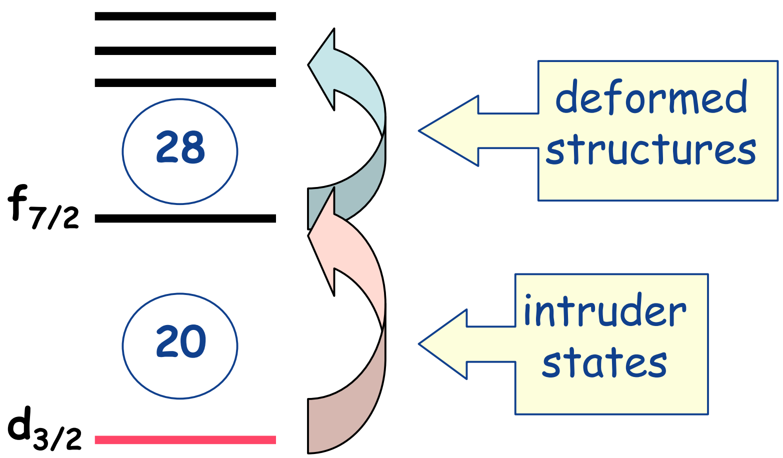
sdfp-shell nuclei: SM-DFT interface

E. Caurier et al., Phys. Rev. Lett. 75, 2466 (1995)

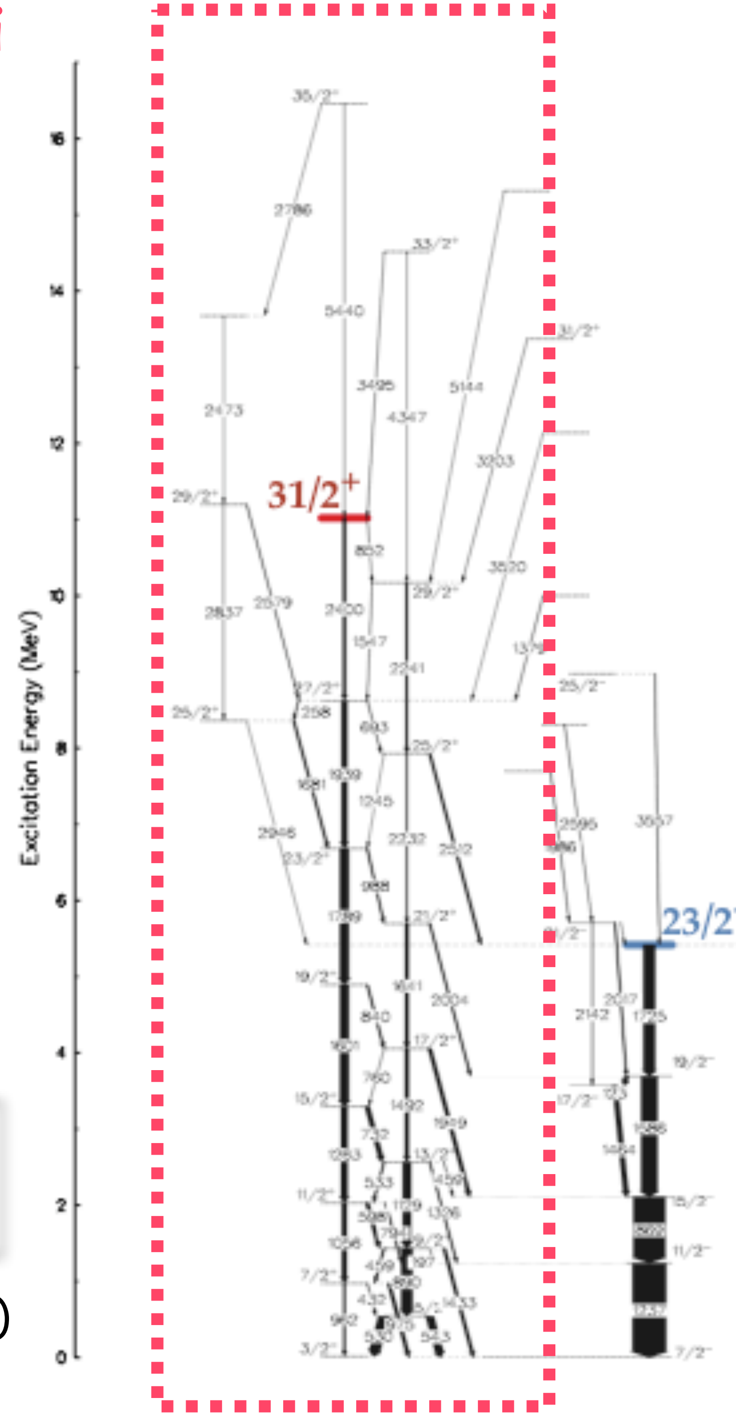


Intruder states in the sdpf nuclei

G. Stoitcheva, W. Satula, WN, D.J. Dean...

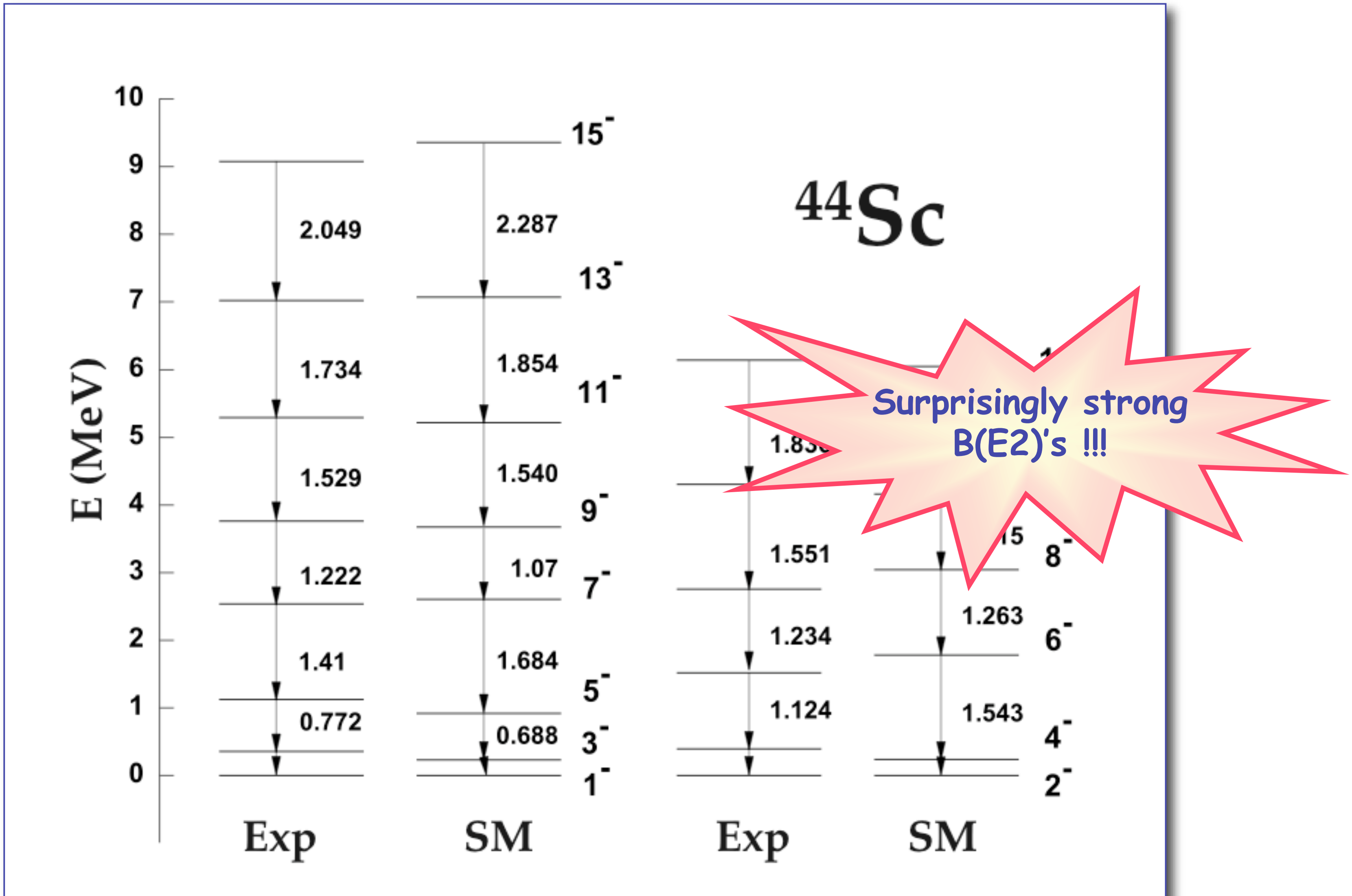


^{45}Sc



P. Bednarczyk et al., Acta Phys. Pol. B32, 747 (2001)

Competition between $\pi(d_{3/2}^{-1} f_{7/2}^{n+1})$ and $\nu(d_{3/2}^{-1} f_{7/2}^{n+1})$



M. Lach et al., E. Phys. J. A 25, 1 (2005)

Zdunczuk, Satula, Wyss, Phys.Rev. C71 (2005) 024305

$$\Delta E \equiv E(d^{-1}_{3/2} f^{n+1}_{7/2}) - E(f^{n}_{7/2})$$

	$f^n_{7/2}$:	$E[I_{max}]$	I_{max}	$d^{-1}_{3/2} f^{n+1}_{7/2}$:	$E[I_{max}]$	I_{max}	ΔE_{exp}
$^{42}_{20}Ca_{22}$		3.189	6^+		8.297	11^-	5.108
$^{44}_{20}Ca_{24}$		10.568	8^+		5.088	13^-	5.480
$^{44}_{21}Sc_{23}$		9.141	11^+		3.567	15^-	5.574
$^{45}_{21}Sc_{24}$		5.417	$23/2^-$		11.022	$31/2^+$	5.605
					15.701	$35/2^-$	10.284
$^{45}_{22}Ti_{23}$		7.143	$27/2^-$		13.028	$33/2^+$	5.885
$^{46}_{22}Ti_{24}$		10.034	14^+		15.549	17^-	5.515
$^{47}_{23}V_{24}$		10.004	$31/2^-$		15.259	$35/2^+$	5.255

- Excellent examples of single-particle configurations
- Weak configuration mixing
- Spin polarization!
- Experimental data available

J. Dobaczewski and J. Dudek, Phys. Rev. C52, 1827 (1995)
M. Bender et al., Phys. Rev. C65, 054322 (2002).

$$\mathcal{H}_t^{(TE)}(\boldsymbol{r}) = C_t^{\rho}\rho_t^2 + C_t^{\Delta\rho}\rho_t\Delta\rho_t + C_t^{\tau}\rho_t\tau_t + C_t^{J}\overleftrightarrow{J}_t^2 + C_t^{\nabla J}\rho_t\boldsymbol{\nabla}\cdot\boldsymbol{J}_t$$

$$\mathcal{H}_t^{(TO)}(\boldsymbol{r}) = C_t^{s}\boldsymbol{s}_t^2 + C_t^{\Delta s}\boldsymbol{s}_t\Delta\boldsymbol{s}_t + C_t^{T}\boldsymbol{s}_t\cdot\boldsymbol{T}_t + C_t^{j}\boldsymbol{j}_t^2 + C_t^{\nabla j}\boldsymbol{s}_t\cdot(\boldsymbol{\nabla}\times\boldsymbol{j}_t)$$

very poorly determined

Can be adjusted to the Landau parameters

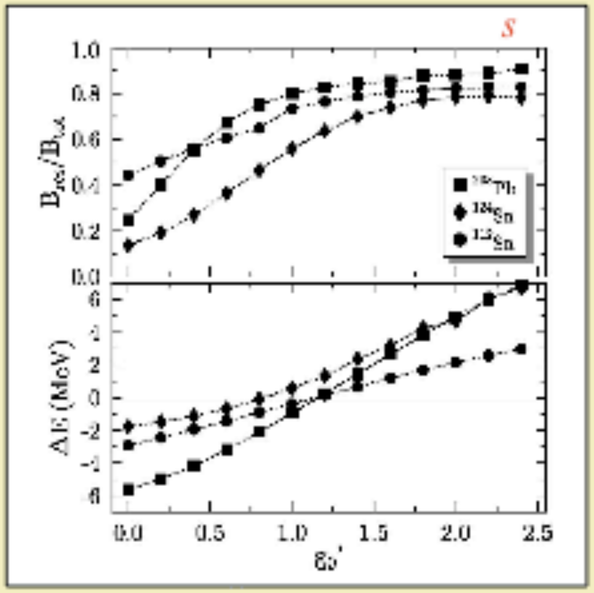
$$g_0 = 0.4, g_0' = 1.2, g_1 = -0.19, g_1' = 0.62$$

- Important for all I>0 states (including low-spin states in odd-A and odd-odd nuclei)
- Impact beta decay
- Influence mass filters (including odd-even mass difference)
- Limited experimental data available

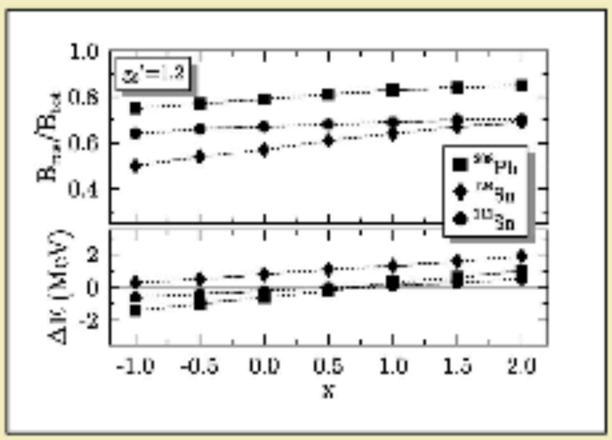
Cranked Skyrme Hartree-Fock

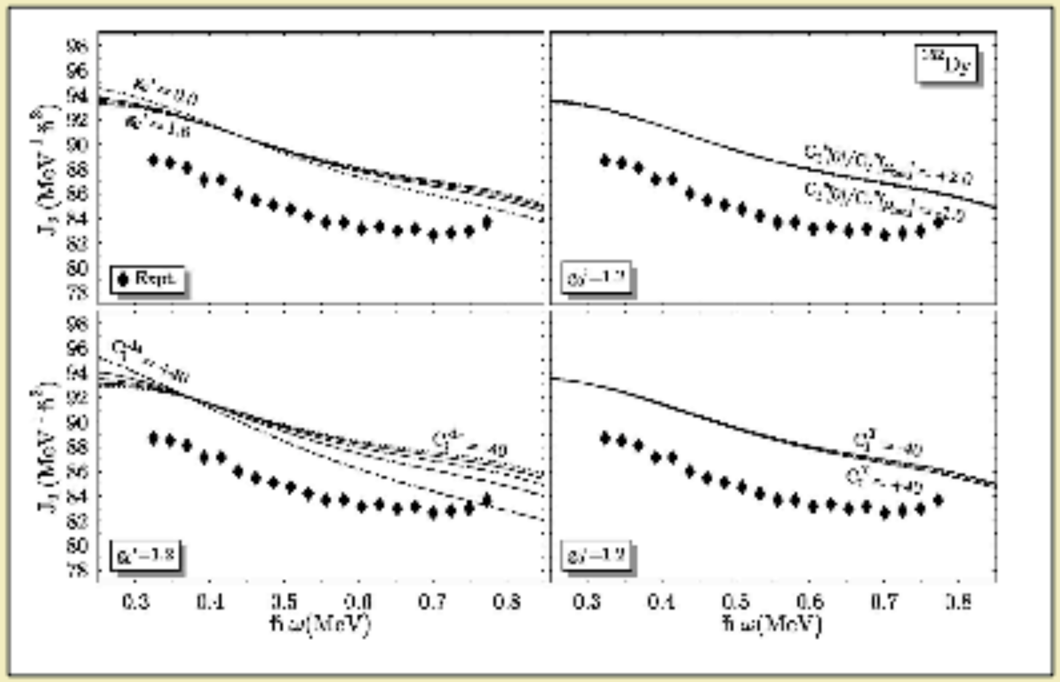
$$\mathcal{H} = \mathcal{H}^{\mathrm{even}} + \mathcal{H}^{\mathrm{odd}}$$

$$\mathcal{H}^{(TO)}_t(\boldsymbol{r}) = C^s_t \boldsymbol{s}^2_t + C^{\Delta s}_t \boldsymbol{s}_t \Delta \boldsymbol{s}_t + C^T_t \boldsymbol{s}_t \cdot \boldsymbol{T}_t + C^j_t \boldsymbol{j}^2_t + C^{\nabla j}_t \boldsymbol{s}_t \cdot (\boldsymbol{\nabla} \times \boldsymbol{j}_t)$$



M. Bender et al., Phys. Rev. C65, 054322 (2002)
adjustement to GT data and high spin states!



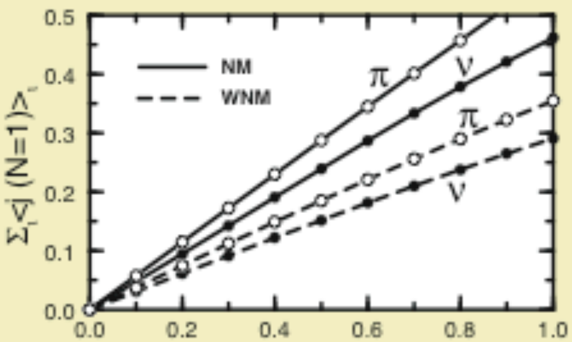


Cranked Dirac Equation

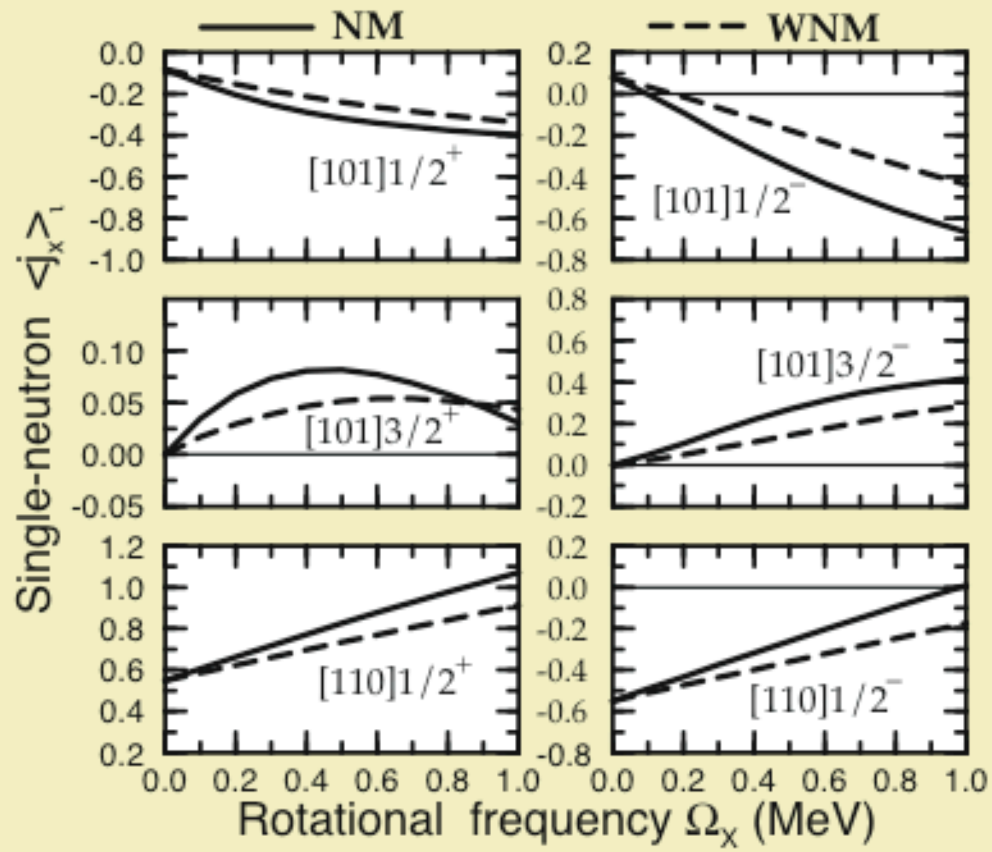
$$\left\{\vec{\alpha}\left[-i\vec{\nabla}-\vec{V}(\vec{r})\right]+V_0(\vec{r})+\beta\left[m+S(\vec{r})-\Omega_x J_x\right]\right\}\Psi_i=e_i\Psi_i$$

Magnetic Potential

$$V(\vec{r})=g_\omega\vec{\omega}(\vec{r})+g_\rho\tau_3\vec{\rho}(\vec{r})+e\frac{1-\tau_3}{2}\vec{A}(\vec{r})$$

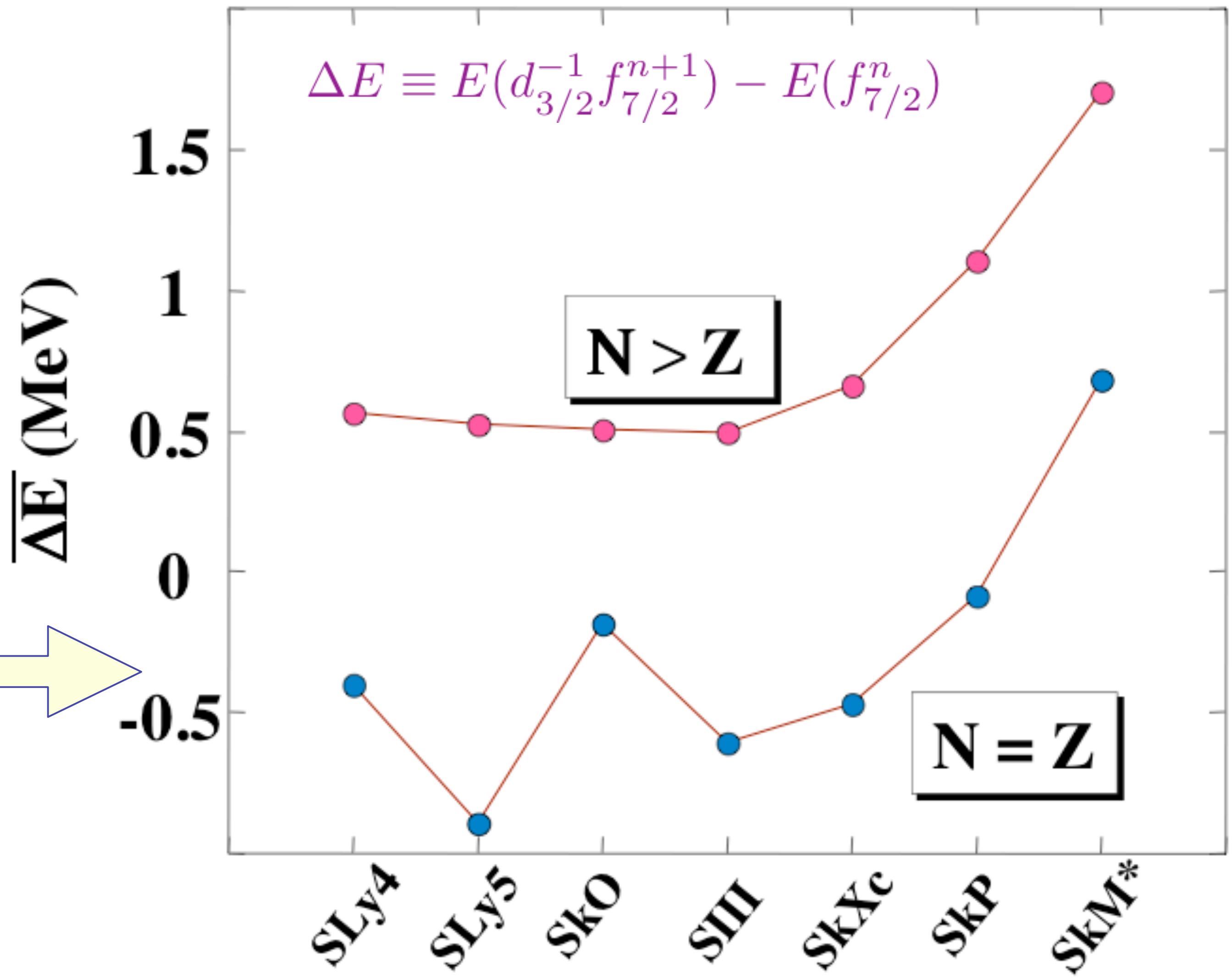


^{152}Dy



A.V. Afanasjev and P. Ring, Phys. Rev. C62, 031302 (2000)

Zdunczuk et al., Phys.Rev. C71 (2005) 024305



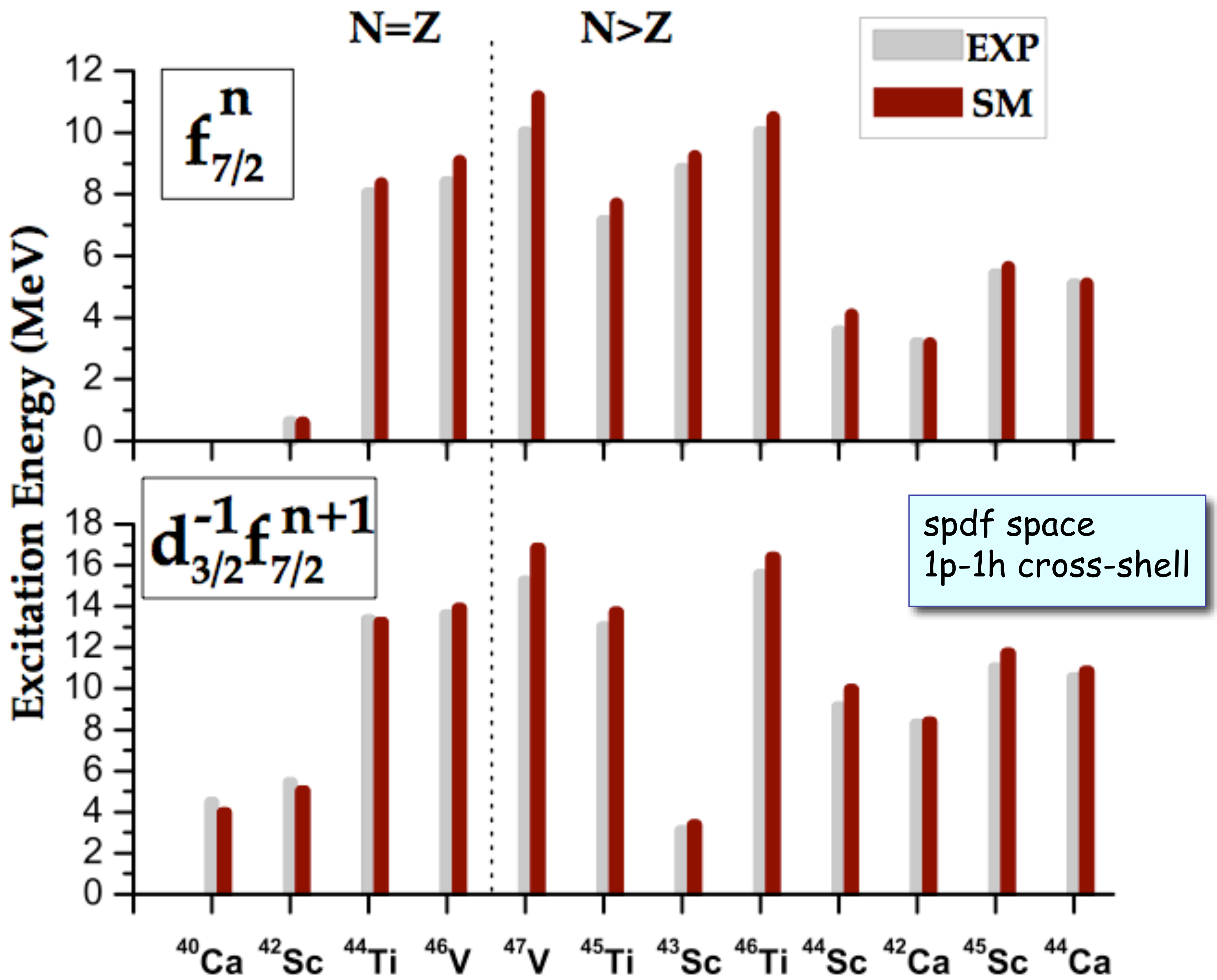
different behavior for N=Z and N>Z nuclei

$$V_{LS}(q,r) \approx \left\{ \frac{W_0}{r}\rho_0'(r) \pm \frac{W_1}{r}\rho_1'(r) \right\} \boldsymbol{\ell s}$$

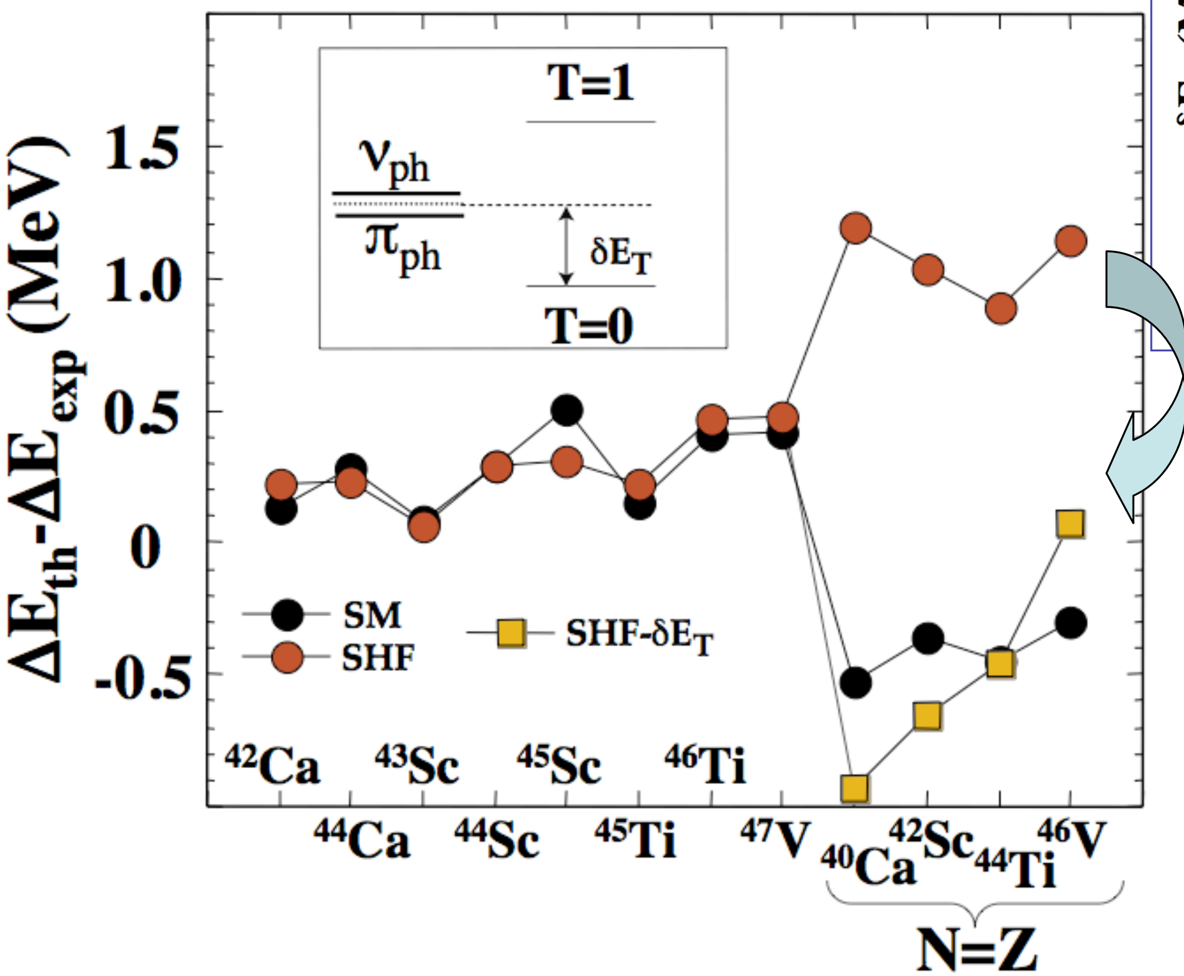
reduced by 5%

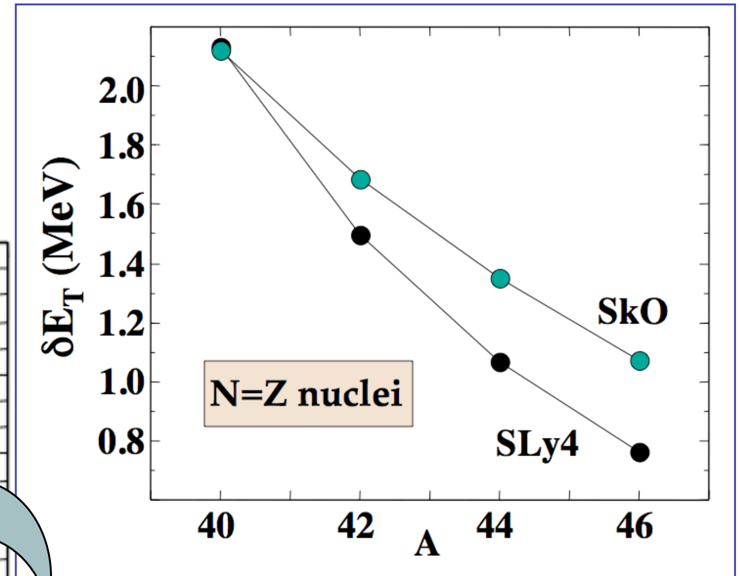
$W_1/W_0 = 1/3$ STD

$W_1/W_0 = -1$ "RMF"


N=Z
N>Z
EXP
SM
$f_{7/2}^{n}$
$d_{3/2}^{-1}f_{7/2}^{n+1}$
spdf space
1p-1h cross-shell
Excitation Energy (MeV)
0
2
4
6
8
10
12
14
16
18
^{40}Ca
^{42}Sc
^{44}Ti
^{46}V
^{47}V
^{45}Ti
^{43}Sc
^{46}Ti
^{44}Sc
^{42}Ca
^{45}Sc
^{44}Ca

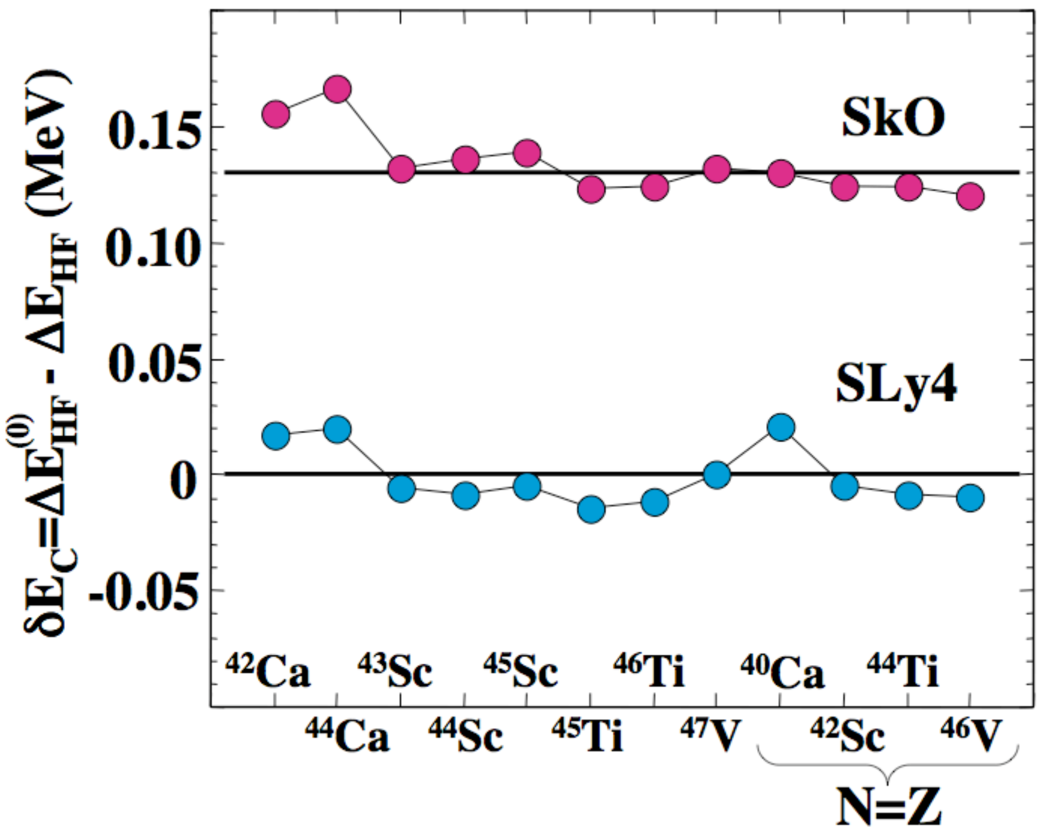
$$\delta E_T \equiv E([d_{3/2}^{-1} f_{7/2}^{n+1}]_{I_{max}}; T_z = \pm 1) - E([d_{3/2}^{-1} f_{7/2}^{n+1}]_{I_{max}}; T_z = 0)$$

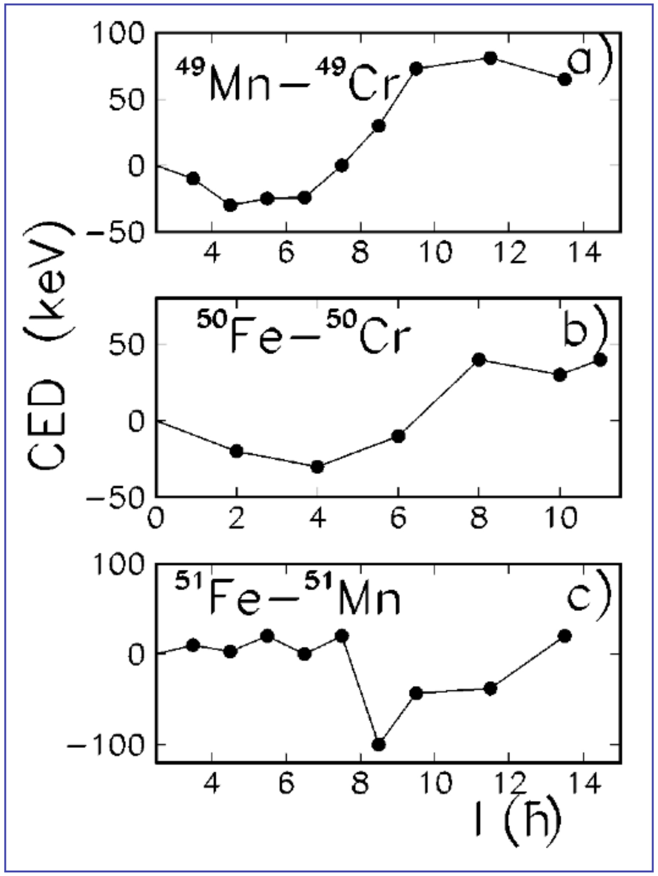




Coulomb correction: depends on Spin-Orbit term

Brandolini et al., PRC66, 021302 (2002)





- Consistency between SM and SHF
- Odd-T terms important
- Difference between N=Z and N≠Z

T=0 pairing?

From Finite Nuclei to the Nuclear Liquid Drop

Leptodermous Expansion Based on the Self-consistent Theory

P.G. Reinhard, M. Bender, W.N., T. Vertse

The parameters of the nuclear liquid drop model, such as the volume, surface, symmetry, and curvature constants, as well as bulk radii, are extracted from the non-relativistic and relativistic energy density functionals used in microscopic calculations for finite nuclei. The microscopic liquid drop energy, obtained self-consistently for a large sample of finite, spherical nuclei, has been expanded in terms of powers of $A^{-1/3}$ (or inverse nuclear radius) and the isospin excess (or neutron-to-proton asymmetry). In order to perform a reliable extrapolation in the inverse radius, **the calculations have been carried out for nuclei with huge numbers of nucleons**, of the order of 10^6.

The limitations of applying the leptodermous expansion for finite nuclei are discussed. **While the leading terms in the macroscopic energy expansion can be extracted very precisely, the higher-order, isospin-dependent terms are prone to large uncertainties due to finite-size effects**.

$$\mathcal{E}^{(\mathrm{smooth})} = \frac{E}{A} - \delta\mathcal{E}^{(\mathrm{shell})}$$

From HF or RMF

Shell correction estimated using the Green's function method

Liquid-Drop Expansion

$$I = \frac{N-Z}{N+Z}$$

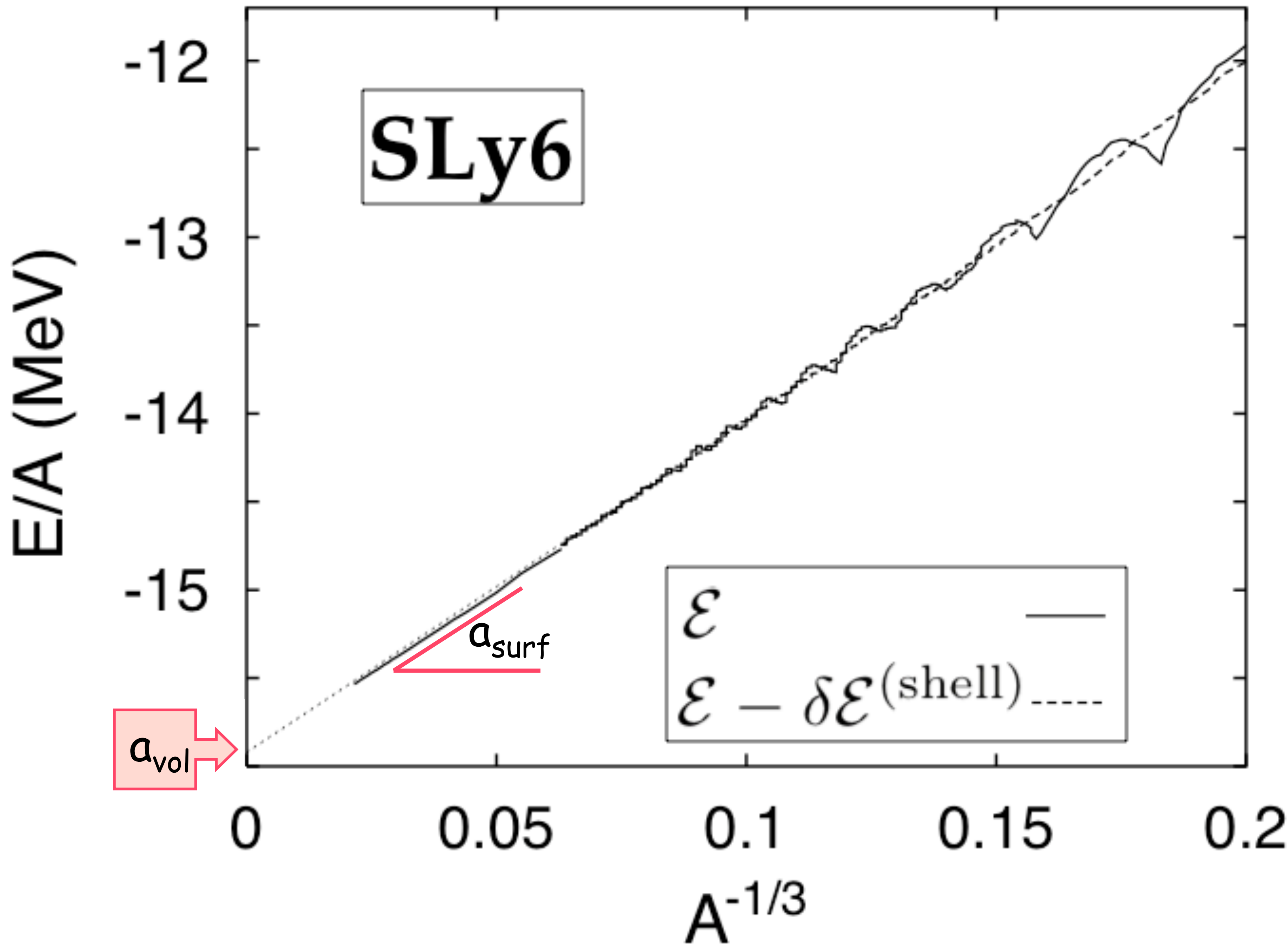
$$\begin{array}{rcl|cl|cl}
\mathcal{E}^{(\mathrm{LDM})} & = & \mathcal{E}^{(\mathrm{smooth})}(A,I) & & & & \\
& = & a_{\mathrm{vol}} & + & a_{\mathrm{surf}}A^{-1/3} & + & a_{\mathrm{curv}}A^{-2/3} \\
& & & + & a_{\mathrm{sym}}I^2 & + & a_{\mathrm{ssym}}I^2A^{-1/3} \\
& & & & & + & a_{\mathrm{sym}}^{(2)}I^4 \quad . \\
\hline
& & \mathrm{O(0)} & & \mathrm{O(1)} & & \mathrm{O(2)}
\end{array}$$

Droplet Model Expansion

Myers, Swiatecki 1974

$$\begin{aligned}
\mathcal{E}^{(\mathrm{drop})} &= \mathcal{E}^{(\mathrm{drop})}(A,I,\epsilon,d) \\
&= a_{\mathrm{vol}} + a_{\mathrm{surf}}A^{-1/3} + \tilde{a}_{\mathrm{curv}}A^{-2/3} + 2a_{\mathrm{surf}}A^{-1/3}\epsilon + \tfrac{K}{2}\epsilon^2 \\
&\quad + a_{\mathrm{sym}}I^2 + \tilde{a}_{\mathrm{ssym}}A^{-1/3}f(I,d) - 3a'_{\mathrm{sym}}I^2\epsilon \\
&\quad + \tilde{a}_{\mathrm{sym}}^{(2)}I^4
\end{aligned}$$

$$K \equiv 9\rho_0^2 \frac{d^2}{d\rho^2}\frac{E}{A}\bigg|_{\rho=\rho_0} \qquad a'_{\mathrm{sym}} = \frac{\partial a_{\mathrm{sym}}}{\partial\rho}\bigg|_{\rho=\rho_0} \qquad a_{\mathrm{sym}}^{(2)} = \tilde{a}_{\mathrm{sym}}^{(2)} - \frac{9}{2}(a'_{\mathrm{sym}})^2\frac{\rho_0^2}{K}$$



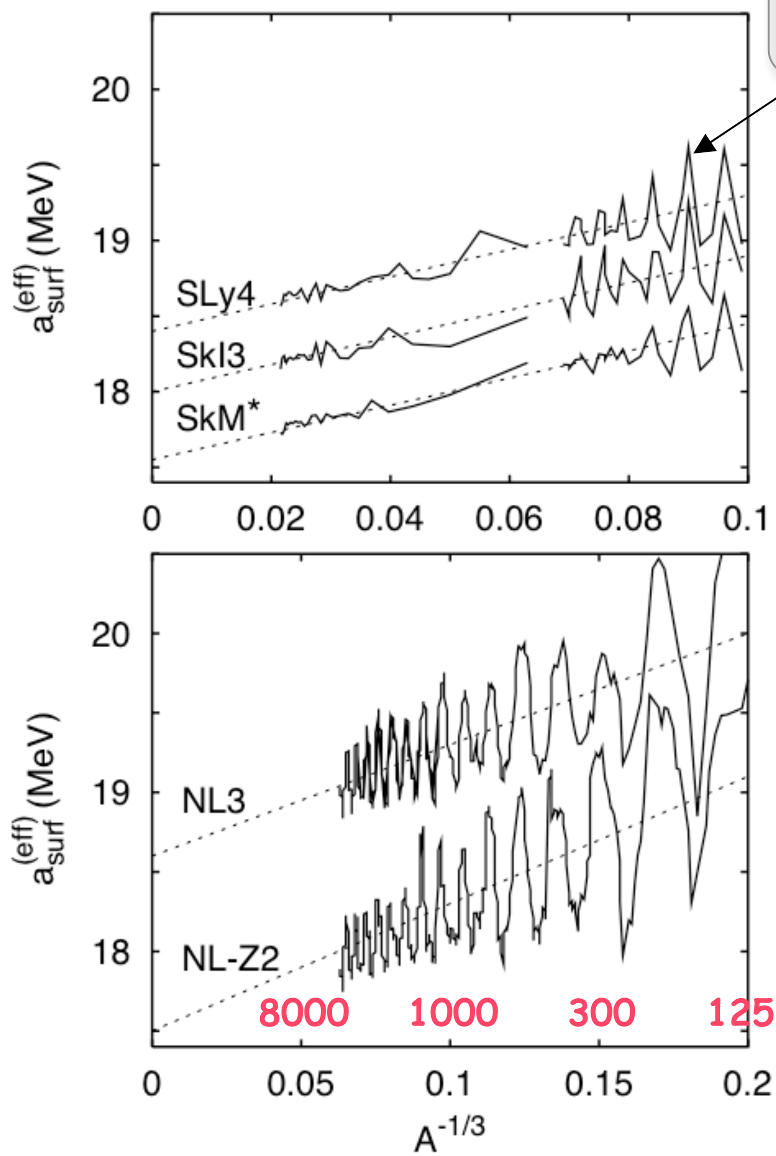
SLy6
E/A (MeV)
-12
-13
-14
-15
0
0.05
0.1
0.15
0.2
$A^{-1/3}$
$\mathcal{E}$
$\mathcal{E} - \delta\mathcal{E}^{(\mathrm{shell})}$
a_{surf}
a_{vol}

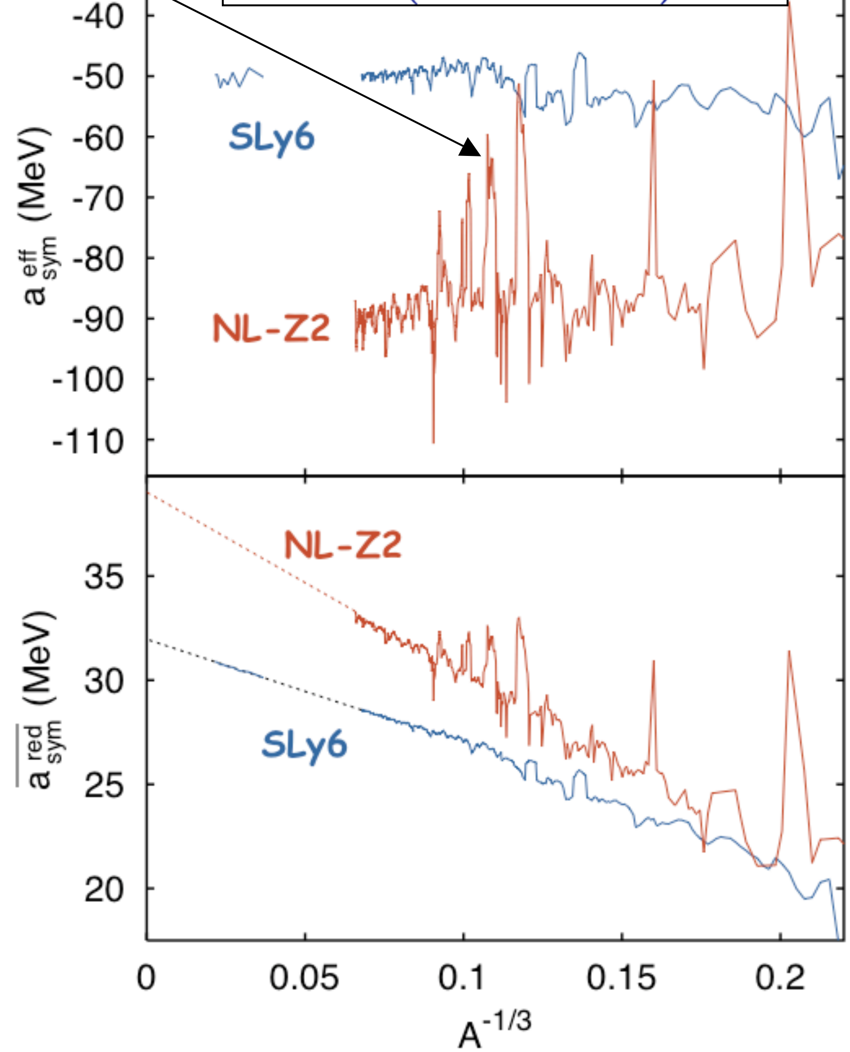
$$a_{\rm surf}^{\rm (eff)} = [\mathcal{E}^{\rm (smooth)}(A,0) - a_{\rm vol}]A^{1/3} = a_{\rm surf} + a_{\rm curv}A^{-1/3}$$

$$a_{\rm sym}^{\rm red}(A,I) = \frac{\mathcal{E}^{\rm (smooth)}(A,I) - \mathcal{E}^{\rm (smooth)}(A,0) + \frac{9(a'_{\rm sym})^2\rho_0^2}{2K}I^4}{I^2}$$

residual shell effects

$$a_{\rm ssym}^{\rm (eff)} = \left(\overline{a_{\rm sym}^{\rm red}} - a_{\rm sym}\right)A^{1/3}$$



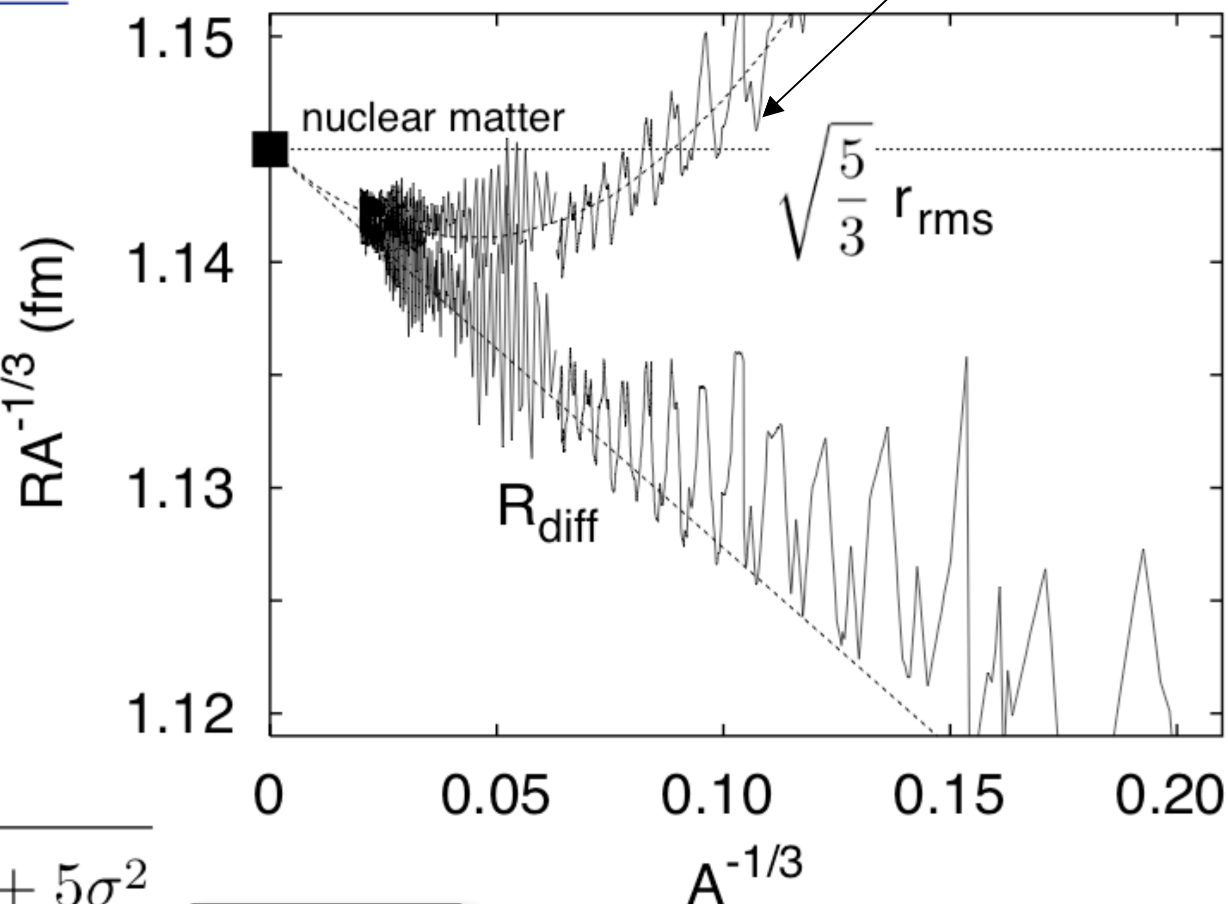


Macroscopic Droplet Model Radii

$$R = R_0(1-\epsilon)$$

$$\epsilon = -\frac{\rho-\rho_0}{3\rho_0} = \frac{-2a_{\mathrm{surf}}A^{-1/3}+3a'_{\mathrm{sym}}I^2}{K}$$

residual shell effects

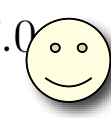


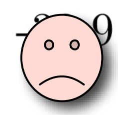
$$r_{\mathrm{rms}} = \sqrt{\frac{3}{5}}\sqrt{R_{\mathrm{diff}}^2 + 5\sigma^2}$$

around 1fm

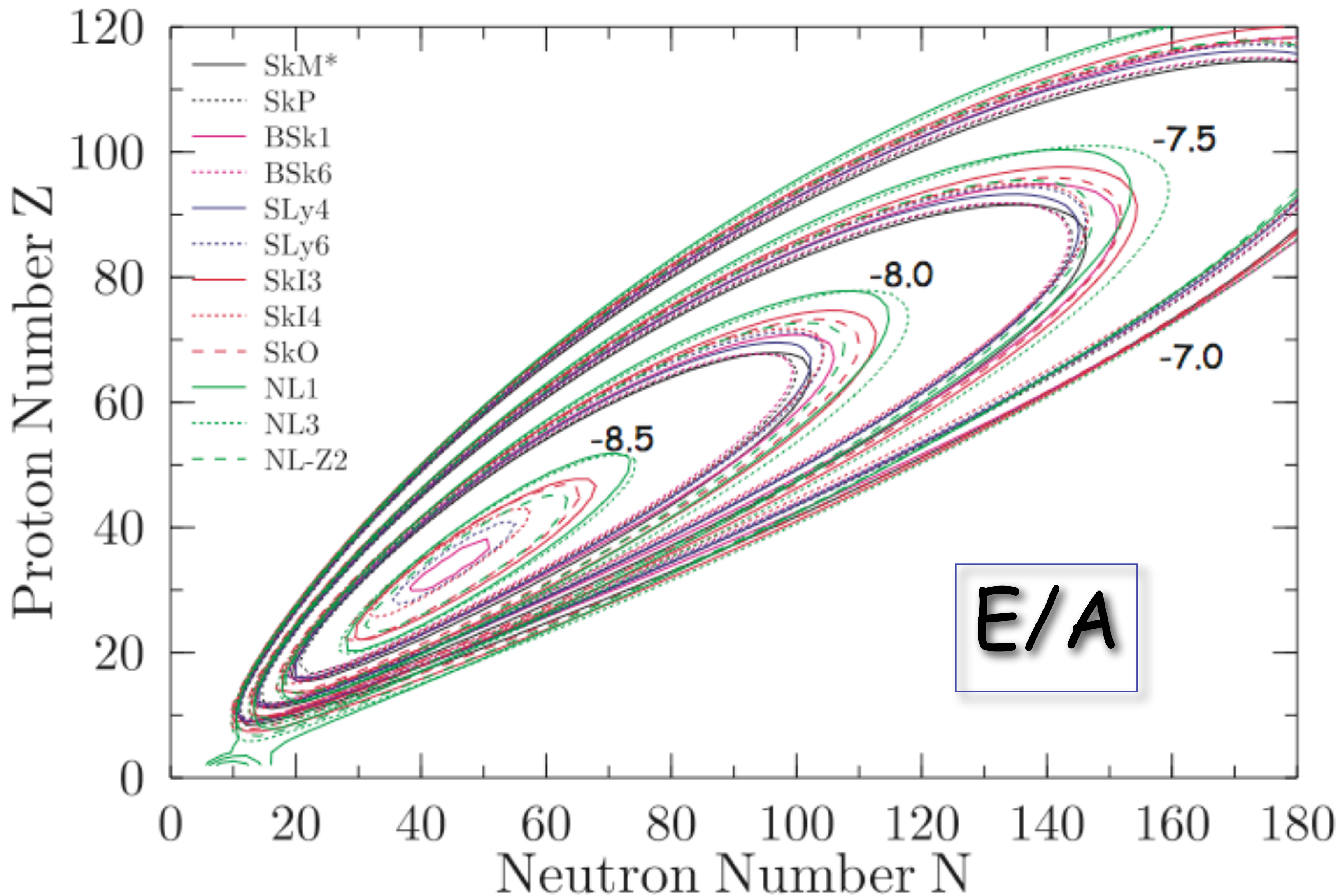
LDM and Droplet Model Coefficients

	bulk properties					semi bulk	from finite nuclei		
Model	ρ_0	K	a_{vol}	a_{sym}	a'_{sym}	$a^{(NM)}_{\mathrm{surf}}$	a_{surf}	a_{curv}	a_{ssym}
SkM*	0.1603	216.6	-15.752	30.04	95.25	17.70	17.6	9	-52
SkP	0.1625	201.0	-15.930	30.01	40.43	18.22	18.2	9.5	-45
BSk1	0.1572	231.4	-15.804	27.81	15.76	17.54	17.5	9.5	-36
BSk6	0.1575	229.2	-15.748	28.00	35.67		17.3	10	-33
SLy4	0.1596	230.1	-15.972	32.01	95.97		18.4	9	-54
SLy6	0.1590	230.0	-15.920	31.96	99.48	17.74	17.7	10	-51
SkI3	0.1577	258.1	-15.962	34.84	212.47		18.0	9	-75
SkI4	0.1601	247.9	-15.925	29.51	125.80		17.7	9	-34
SkO	0.1605	223.5	-15.835	31.98	163.50		17.3	9	-58
NL1	0.1518	211.3	-16.425	43.48	311.18		18.8	9	-110
NL3	0.1482	271.7	-16.242	37.40	269.16	18.5	18.6	7	-86
NL-Z	0.1509	173.0	-16.187	41.74	299.51		17.8	9	$<$ -125
NL-Z2	0.1510	172.4	-16.067	39.03	281.40	17.7	17.4	10	-90
LDM	0.153		-16.00	30.56			21.1		-48.6
LDM	0.1611	234.4	-16.24	32.65			18.6	12	
LDM	0.1417		-15.848	29.28			19.4		-38.4
LSD	0.1324		-15.492	28.82			17.0	3.9	[illegible]

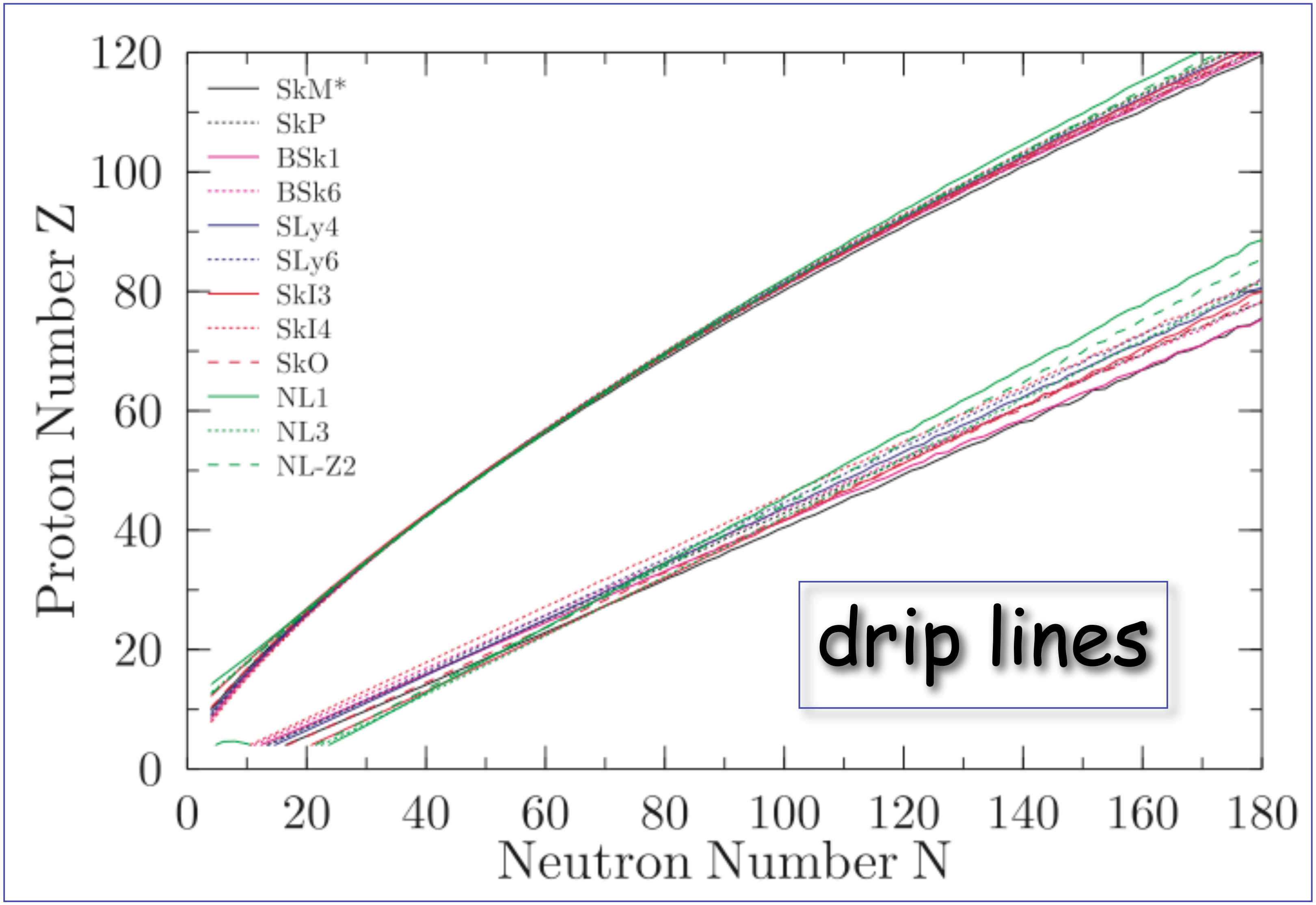




“Microscopic” LDM with Coulomb term
close (5%) to SHF energies



See Bertsch et al. PRC71, 054311 (2005) for the fitting strategy



… discussed by Michael Bender

THE END