Seminarium Spektroskopii Jądrowej, 12.11.2008

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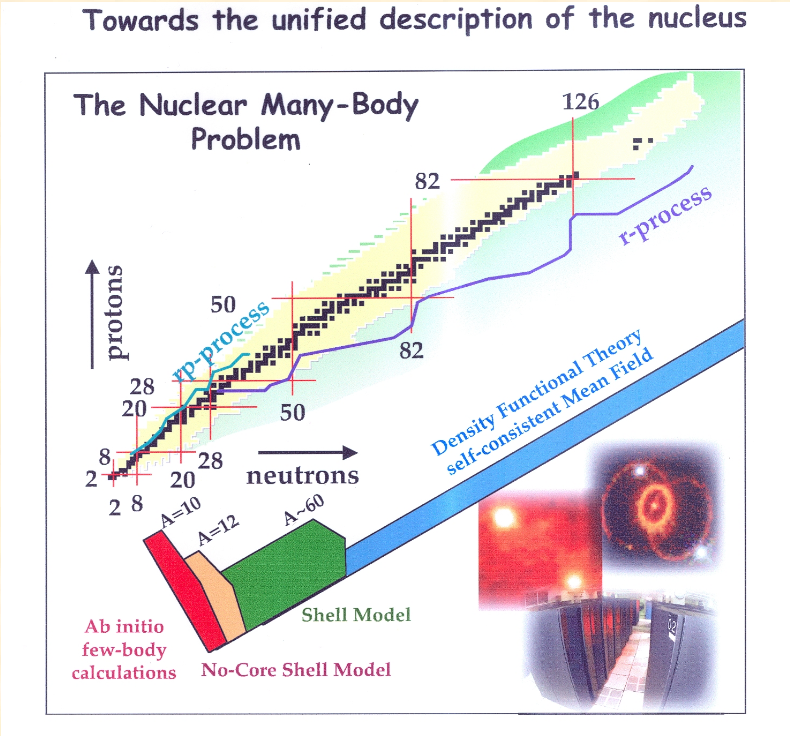
IFT

Wpływ oddziaływania tensorowego na strukturę jąder atomowych

współpraca
W. Satuła, J.Dobaczewski, P. Olbratowski, M.Rafalski, T.R. Werner, R.A. Wyss

Plan:
- Jądrowy funkcjonał gęstości – kilka słów przypomnienia.
- Jak konstruować potencjał i jak określić stałe sprzężenia?
- Część tensorowa funkcjonału gęstości
- Wpływ na masy i strukturę jąder atomowych.



- Hohenberg-Kohn-Sham theorems – energy is a functional of density,
- They don't tell how to construct this functional,
- We have to construct a functional which incorporates important physical acpects of our system

$$E = E[\rho]$$

$$V = \delta E/\delta\rho$$

densities → one-body hamiltonian

diagonalization

s.p. wave functions ← diagonalization

Local Energy Density Functional

Let assume that wave function is a Slater determinant (independent particles).
By calculating expectation value of the hamiltonian with two-body Skyrme interaction one obtain following expression for the energy of a nucleus.

$$\langle \Psi \mid H \mid \Psi \rangle$$

Slater determinant

$$E = E_{\rm kin} + \int d^3 r \, \mathcal{E}_{\rm Sk} + E_{\rm Coul} + E_{\rm pair} - E_{\rm corr} \,.$$

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

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

$$C_t^{j} = -C_t^{\tau}, \quad C_t^{J} = -C_t^{T} \quad C_t^{\nabla j} = C_t^{\nabla J}$$

Different densities are needed to describe nuclei: ρ, τ, J, s, j, T

one-body density matrix:

$$\rho(x,x') = \int \Psi^*(x,x_2,\cdots,x_N)\Psi(x',x_2,\cdots,x_N)dx_2\cdots dx_N$$
$$x = \{\vec{r},s,t\}$$

$\rho_0(\vec{r}) = \rho_0(\vec{r},\vec{r}) = \sum_{\sigma\tau}\rho(\vec{r}\sigma\tau;\vec{r}\sigma\tau)$	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
$\vec{j}_T(\vec{r}) = \frac{i}{2}(\vec{\nabla}'-\vec{\nabla})\rho_T(\vec{r},\vec{r}')\vert_{\vec{r}'=\vec{r}}$	current density
$\vec{J}_T(\vec{r}) = \frac{i}{2}(\vec{\nabla}'-\vec{\nabla})\otimes\vec{s}_T(\vec{r},\vec{r}')\vert_{\vec{r}'=\vec{r}}$	spin-current tensor density
$\tau_T(\vec{r}) = \vec{\nabla}\cdot\vec{\nabla}'\rho_T(\vec{r},\vec{r}')\vert_{\vec{r}'=\vec{r}}$	kinetic density
$\vec{T}_T(\vec{r}) = \vec{\nabla}\cdot\vec{\nabla}'\,\vec{s}_T(\vec{r},\vec{r}')\vert_{\vec{r}'=\vec{r}}$	kinetic spin density

20 parameters are fitted to:

- **Symmetric NM:**
  - saturation density (~0.16fm^{-3})
  - energy per nucleon (-16±0.2MeV)
  - incompressibility modulus (210±20MeV)
  - isoscalar effective mass (0.8)
- **Asymmetric NM:**
  - symmetry energy (30±2MeV)
  - isovector effective mass (GDR sum-rule enhancement)
  - neutron-matter EOS (Wiringa, Friedmann-Pandharipande)
- **Finite, double-magic nuclei [masses,radii, rarely sp levels]:**
  - surface properties

Spin current tensor in case of the spheical symmetry:

$$J_q(r) = \frac{1}{4\pi r^3} \sum_{n,j,\ell} (2j+1)\, v^2_{nj\ell} \times \left[j(j+1) - \ell(\ell+1) - \tfrac{3}{4} \right] \psi^2_{nj\ell}(r)$$

Spin orbit current is a strong shell effect:
- vanishes if nuclei is spin saturated,
- large if only one from spin-orbit partners is occupied,

$$\mathcal{H}^{\text{even}}_t = C^\rho_t \rho^2_t + C^{\Delta\rho}_t \rho_t \Delta\rho_t + C^\tau_t \rho_t \tau_t + C^J_t \mathbb{J}^2_t + C^{\nabla J}_t \rho_t \nabla \cdot \mathbf{J}_t,$$

tensor ($C^J_t \mathbb{J}^2_t$)

standart spin-orbit ($C^{\nabla J}_t \rho_t \nabla \cdot \mathbf{J}_t$)

one-body spin-orbit potential (for neutrons):

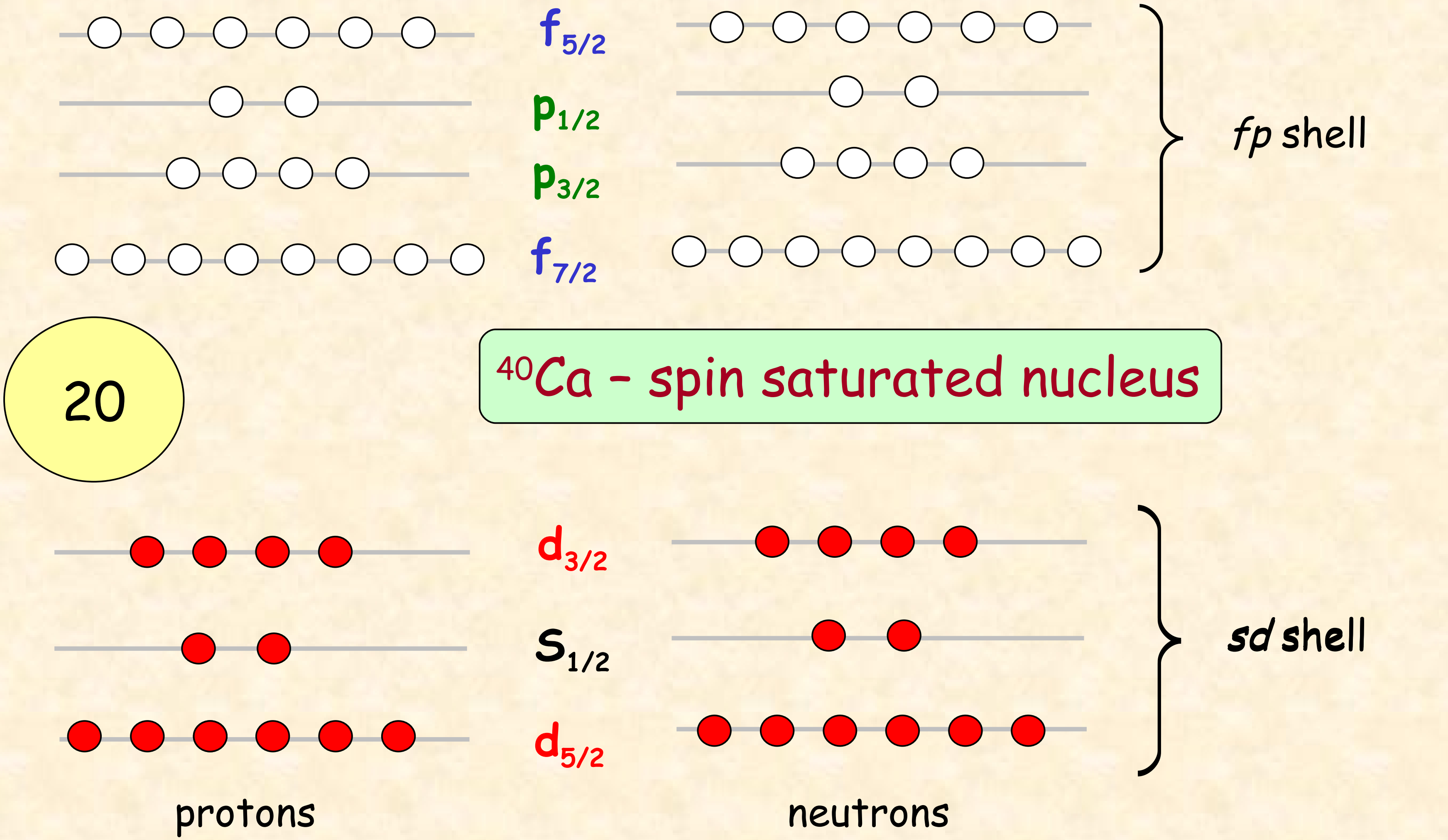
$$W_n(r) = \frac{\delta \mathcal{E}}{\delta \mathbf{J}_n(r)} \cdot \mathbf{e}_r = \frac{W_0}{2} (2\nabla\rho_n + \nabla\rho_p) + \alpha J_n + \beta J_p$$

Standard spin-orbit potential

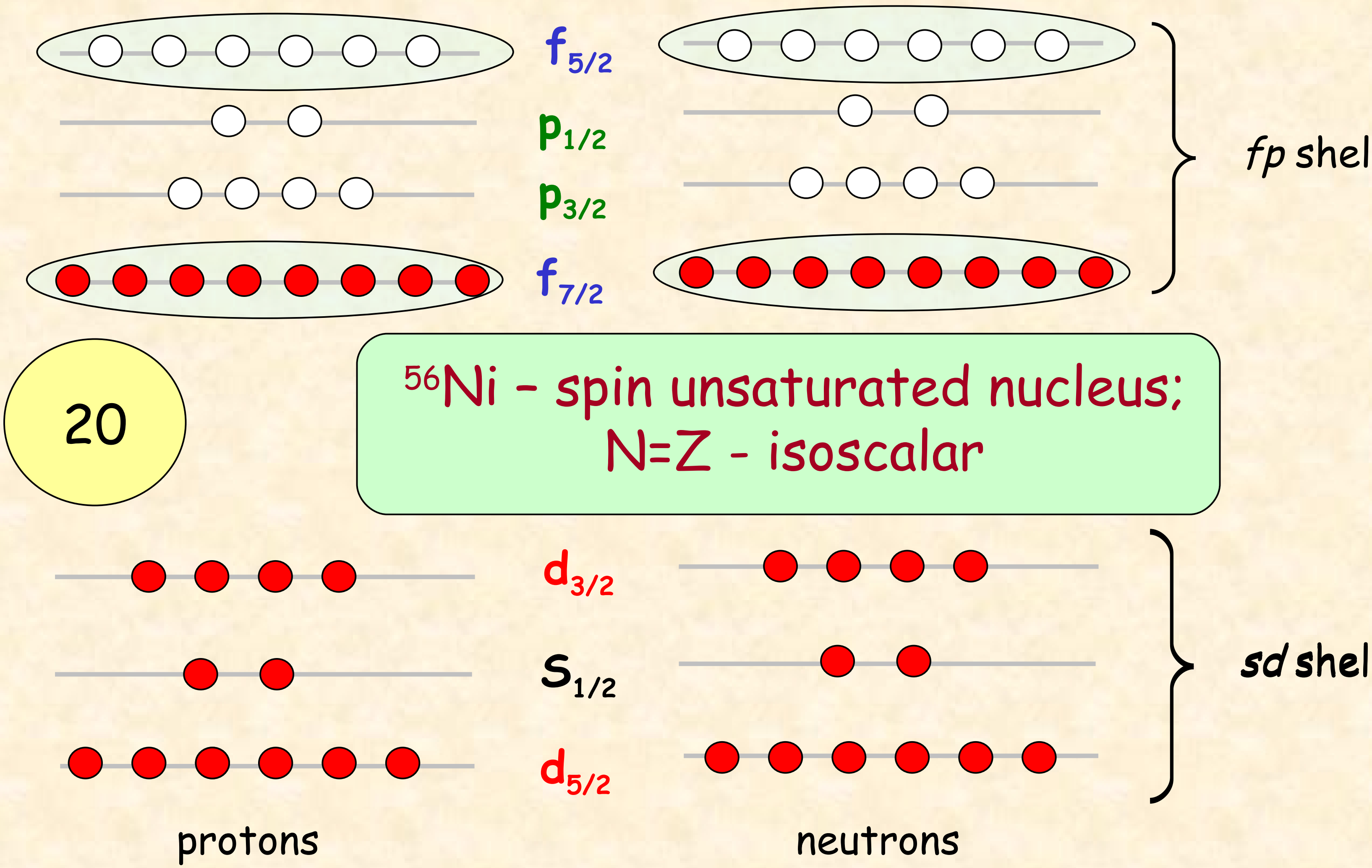
TENSOR: dependance on neutron AND proton spin-orbit currents

SHELL EFFECT!

How to determine spin-orbit and tensor coupling constants?



How to determine spin-orbit and tensor coupling constants?



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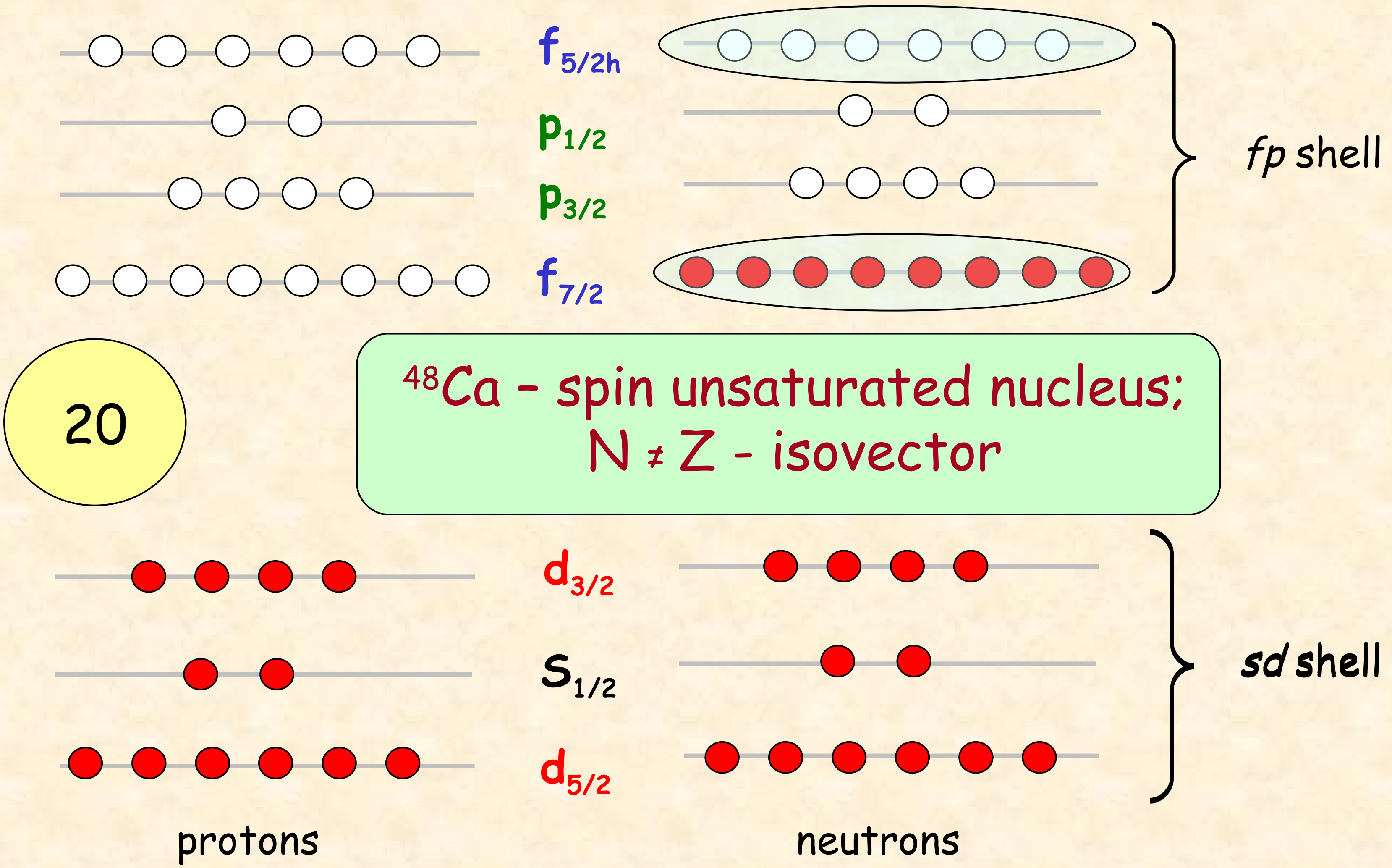
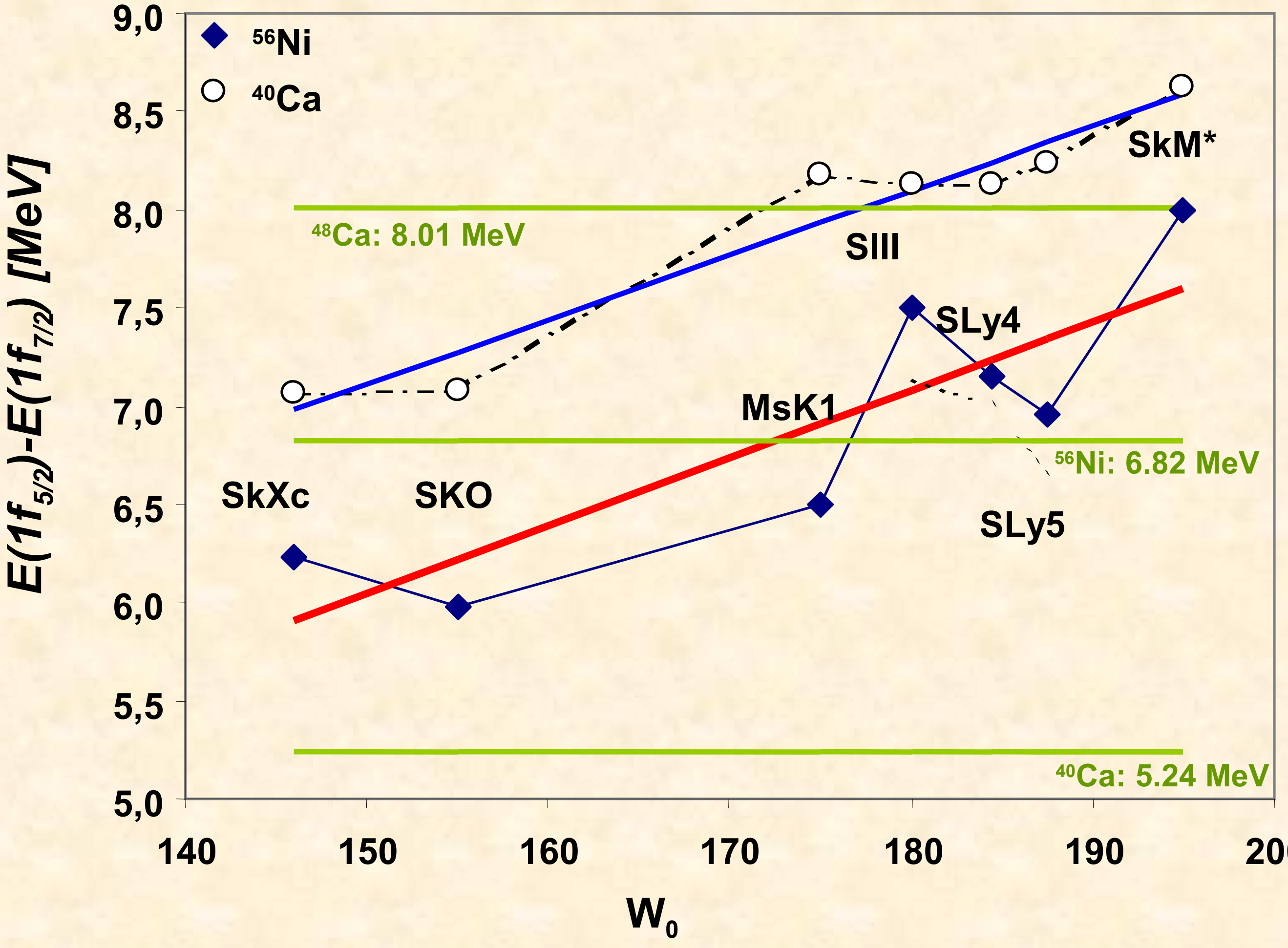
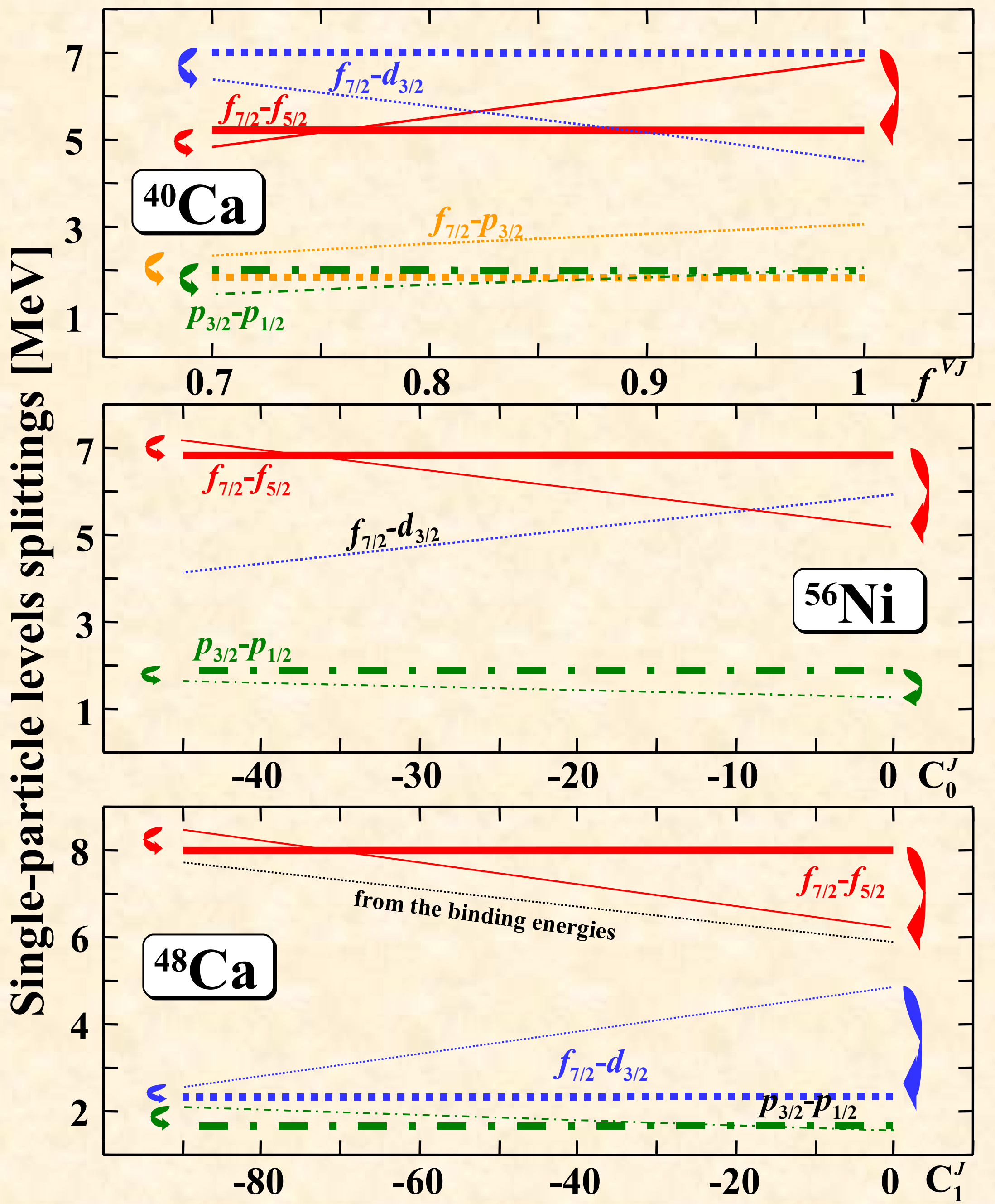


1f spin-orbit splitting



Spin-orbit splitting of *f* orbitals is completely wrong in ^{40}Ca!



1) Fit isoscalar strength of the two-body SO interaction

↓

2) Fit isoscalar strength of the tensor interaction

↓

3) Fit isovector strength of the tensor interaction

VALUES OF COUPLING CONSTANTS:

	m^*/m	$C_0^{\nabla J}$	C_0^J	C_1^J
SLy4	0,67	-60	-45	-60
SKO	0,90	-62	-33	-92
SKP	1,00	-60	-38	-61
SIII	0,76	-58	-51	-65
SkM*	0,67	-56	-42	-68

isoscalar isovector

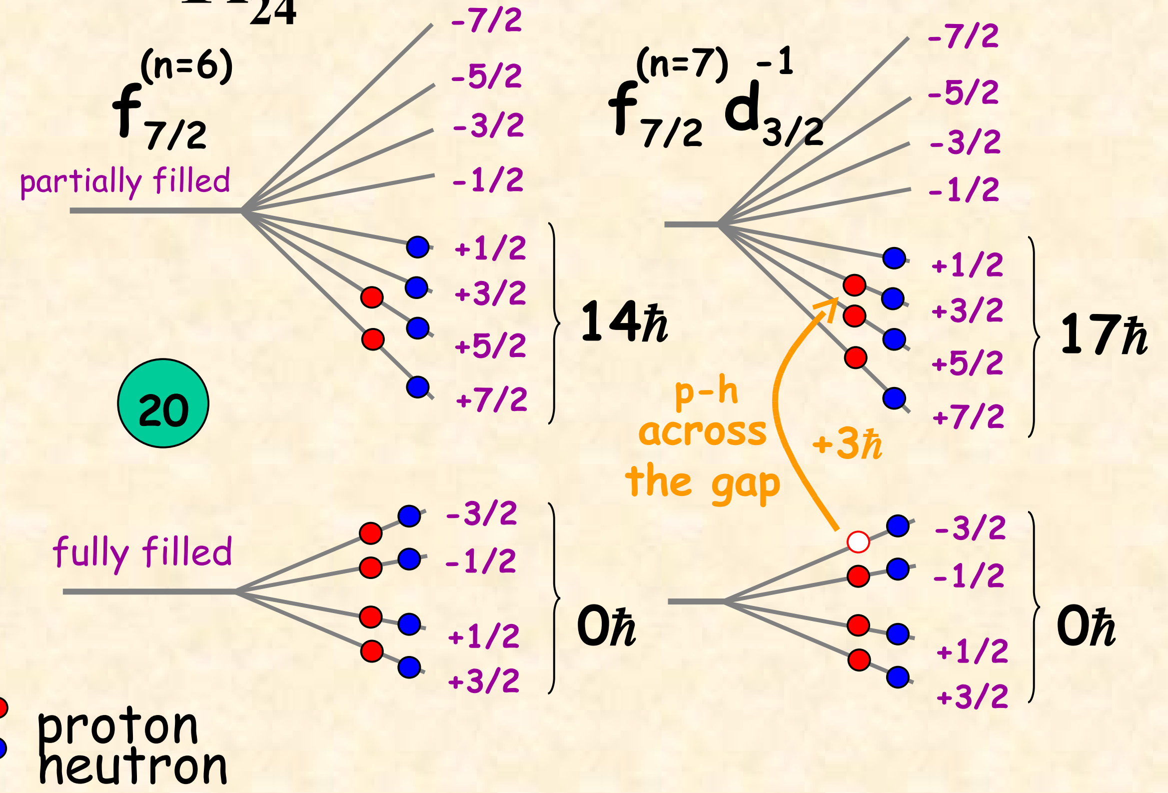
spin-orbit tensor

Coupling constant more or less the same for completly different forces.

Examples of band terminating states in $^{46}\mathrm{Ti}_{24}$

Terminating states:

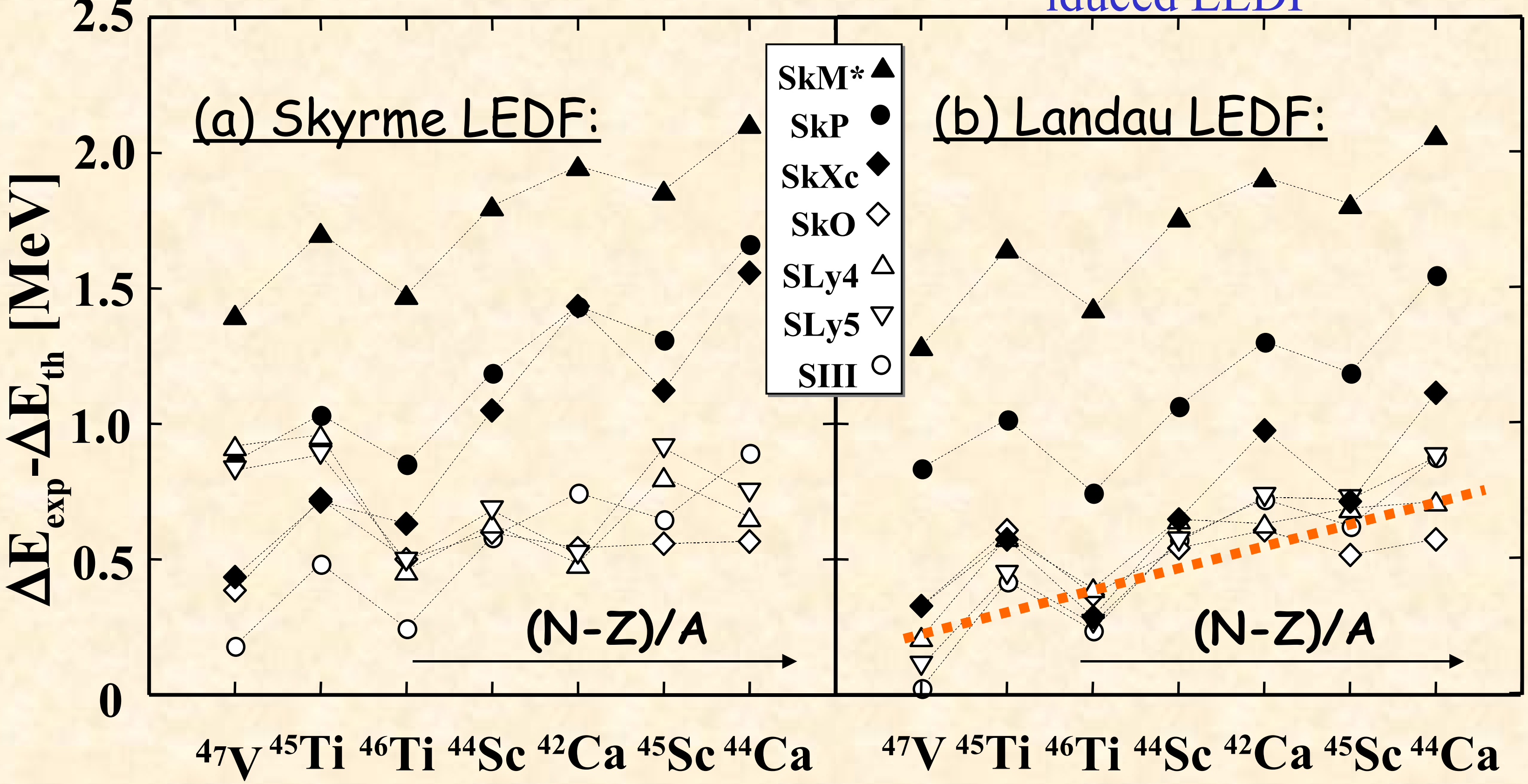
- -the best example of almost unperturbed single particle motion,
- -uniquely defined (N≠Z),
- -configuration mixing beyond mean-field expected to be marginal,
- -shape-polarization effects included already at the level of the SHF,
- -good to test badly known time-odd fields,
- -seem to be ideal for fine tuning of particle-hole interaction.



$$\Delta E = E(f_{7/2}^{n+1} d_{3/2}^{-1}) - E(f_{7/2}^{n})$$

Original Skyrme force induced LEDF

Landau parameters: $g_0=0.4$; $g_1=0.19$ iduced LEDF



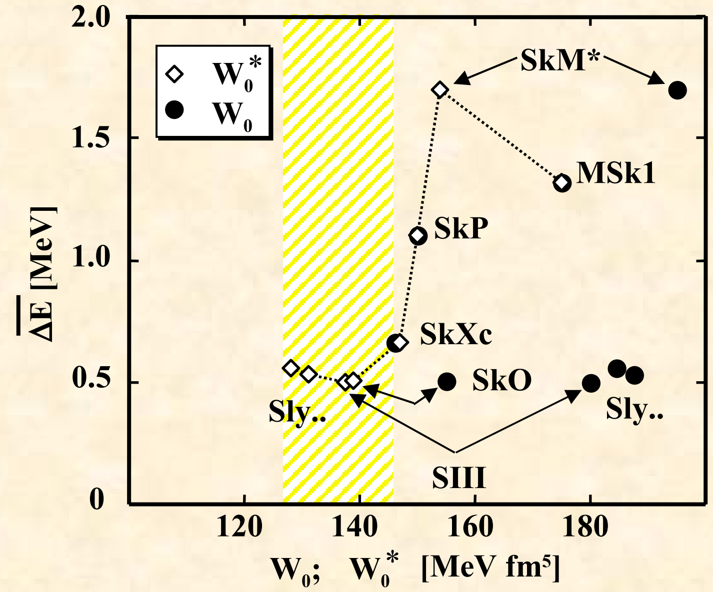
H. Zduńczuk, W. Satuła, R. Wyss, Phys. Rev. C58 (2005) 024305

In some sense it is a wrong result:
- level density is scaled with an effective mass
- we should expect that ΔE grows when m*/m decreases.

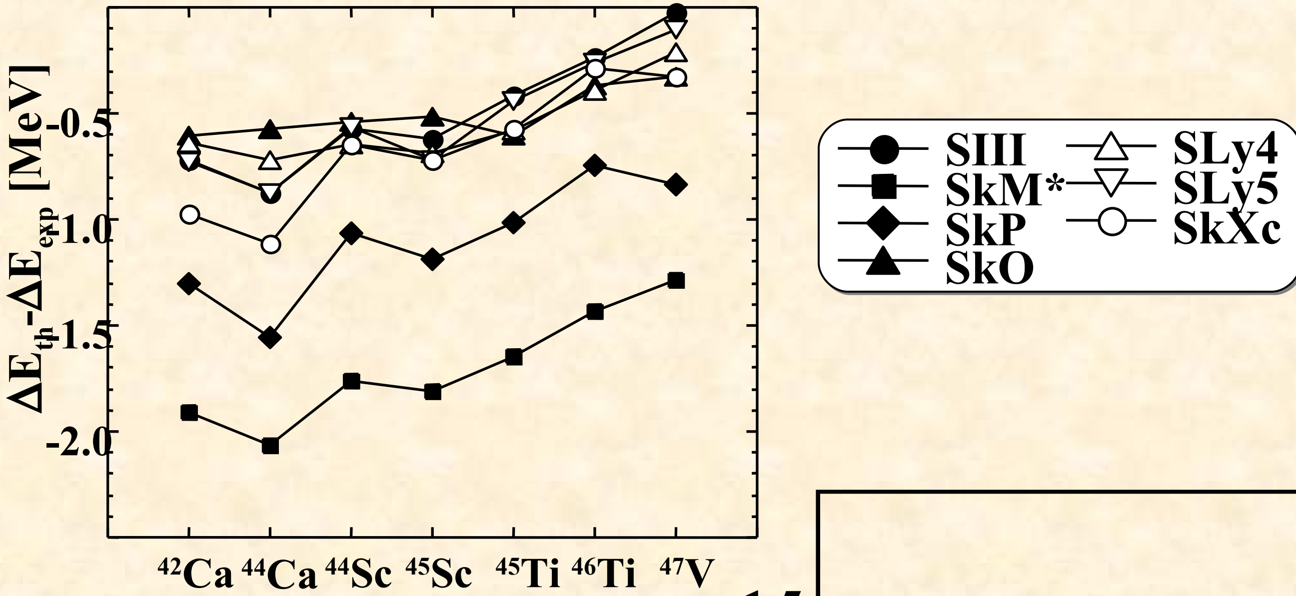
Why nearly all force give the same ΔE?

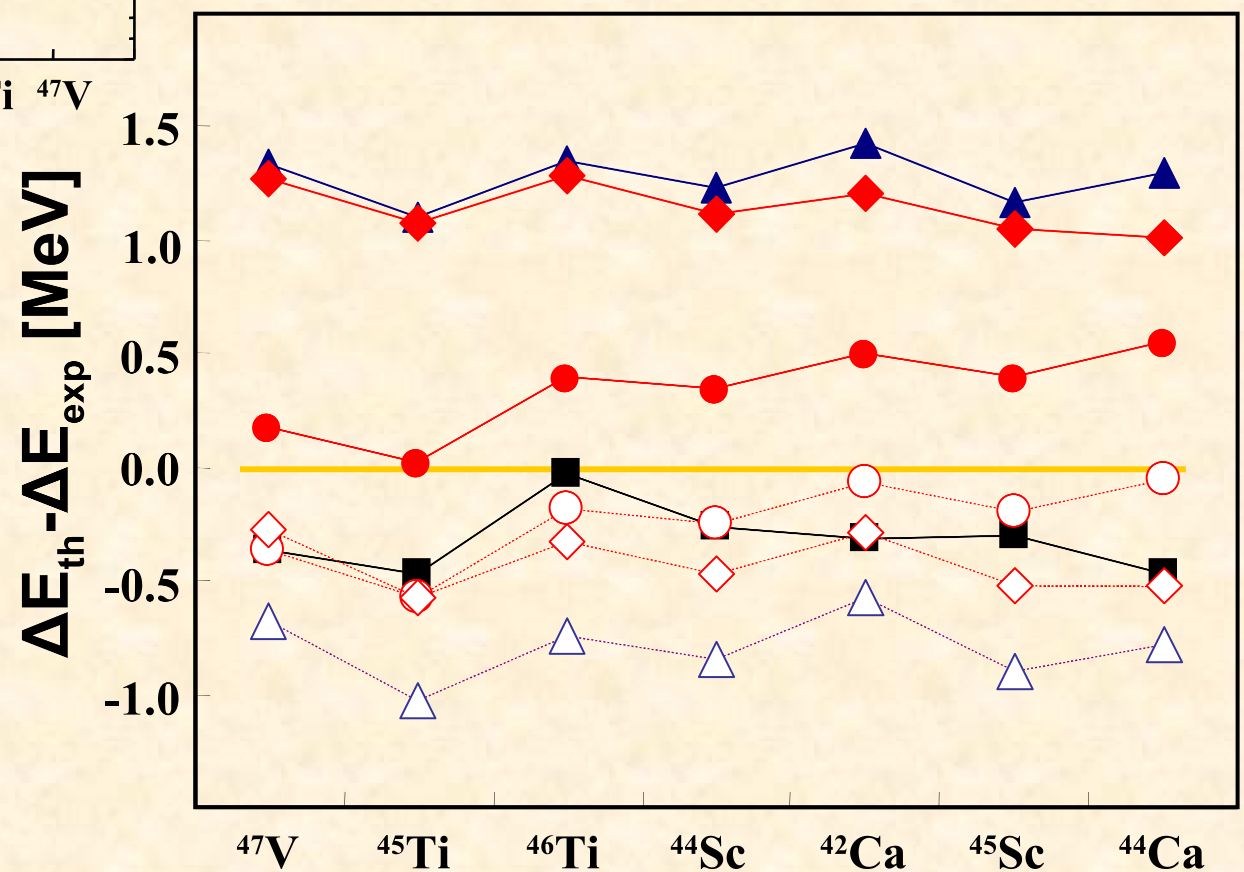
This is due to the fact that parameters are fitted to masses and not to spectroscopic data.
Large spin orbit coupling constant counterbalance the influence of small m* on ΔE.

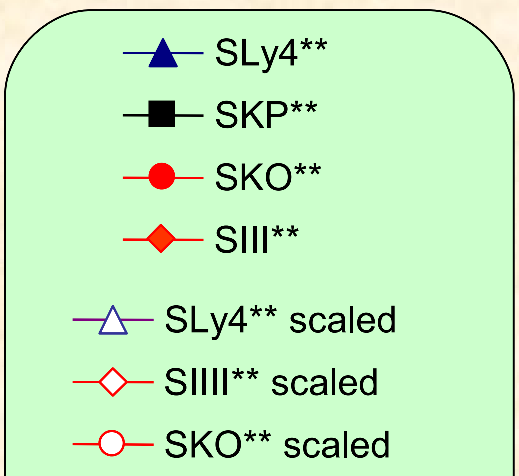
$$W_0^* = \frac{m}{m^*} W_0$$



H. Zduńczuk, W. Satuła, R. Wyss,
Int. Jour. of Mod. Phys.A422







$$\Delta E^{(sc)}_{th} = \Delta E_{th} \frac{m^*}{m}$$

How does tensor influence masses?

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

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- negative coupling constant,
- this term provides more binding,
- depend on which shells are filled,

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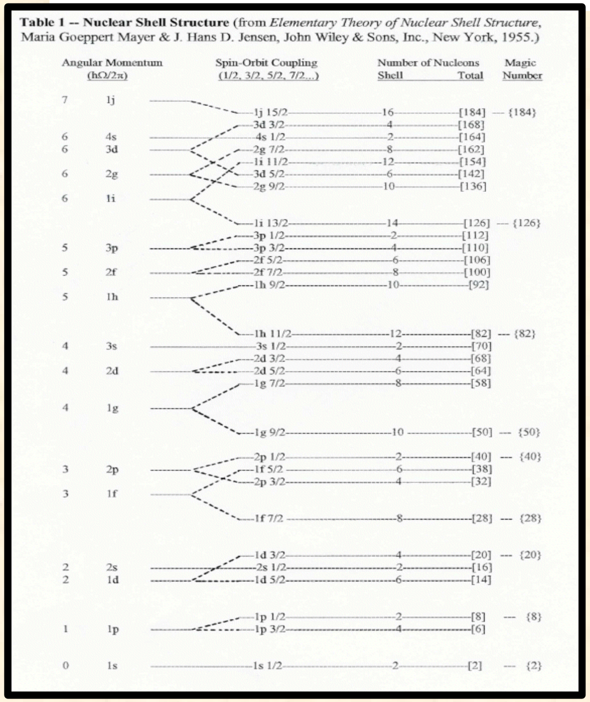

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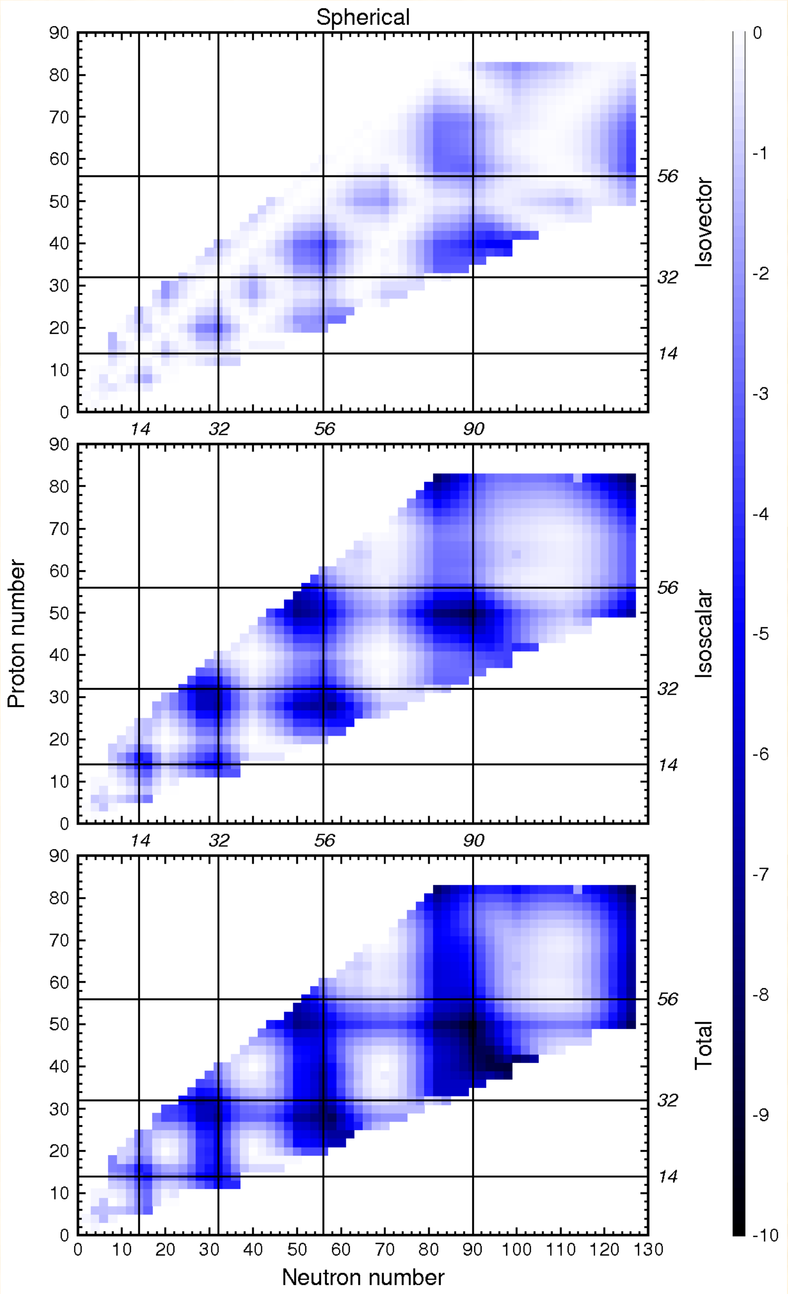
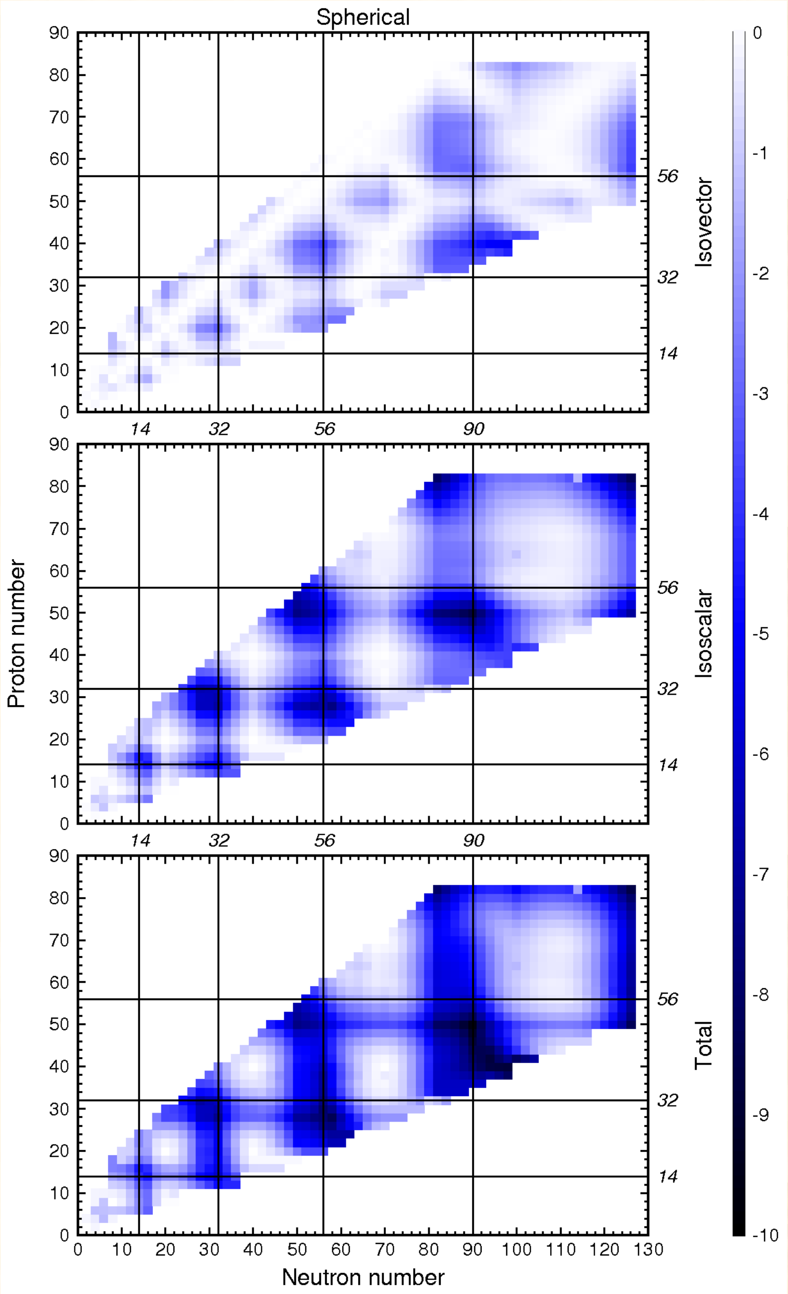


N = 14 $d_{5/2}$

N = 32 $f_{7/2}$ $p_{3/2}$

N = 56 $g_{9/2}$ $d_{5/2}$

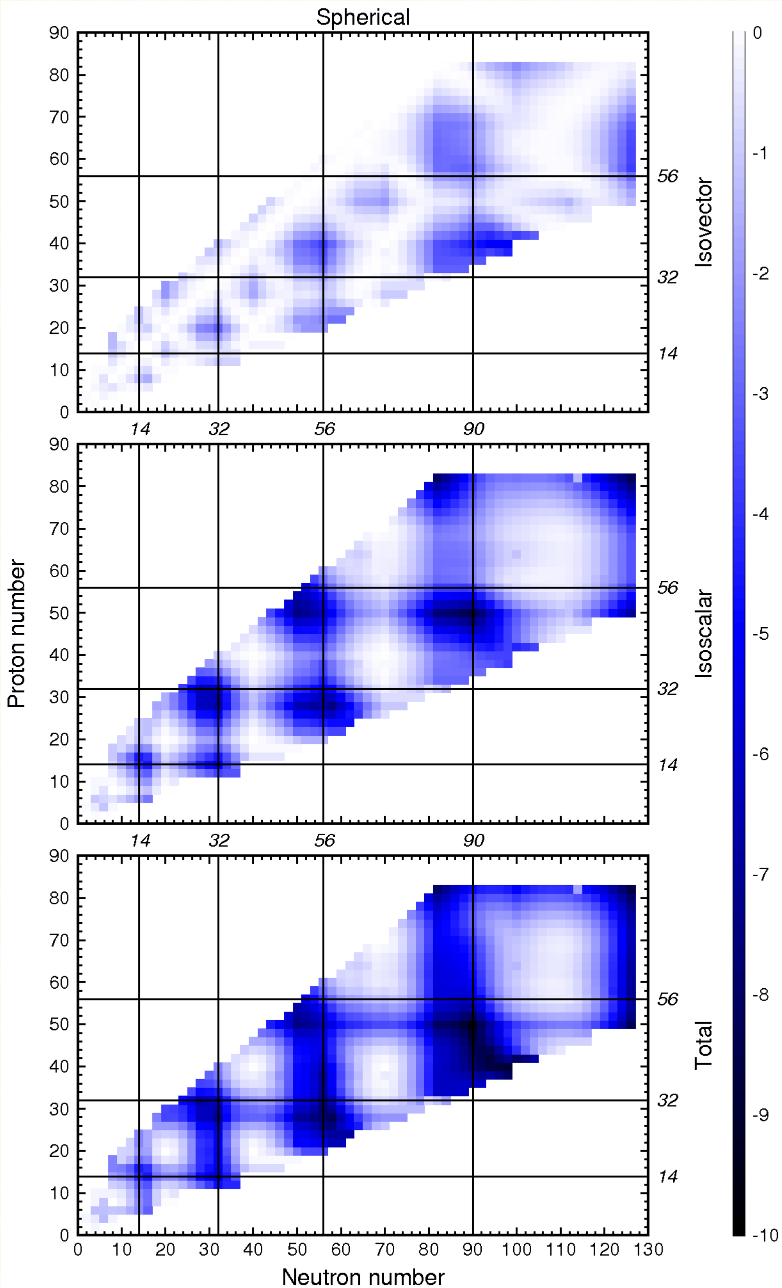
N = 90 $h_{11/2}$ $f_{7/2}$



Z = 14 $d_{5/2}$

Z = 32 $f_{7/2}$ ~~$p_{3/2}$~~

Z = 50 $g_{9/2}$ ~~$d_{5/2}$~~



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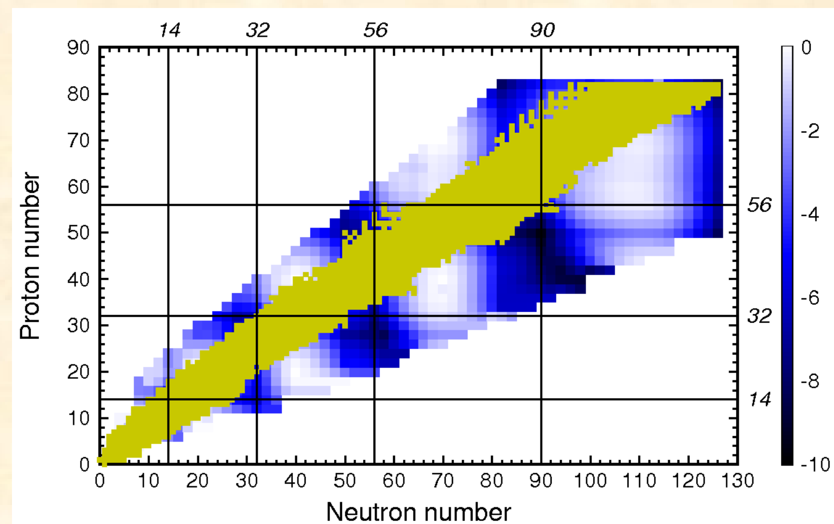
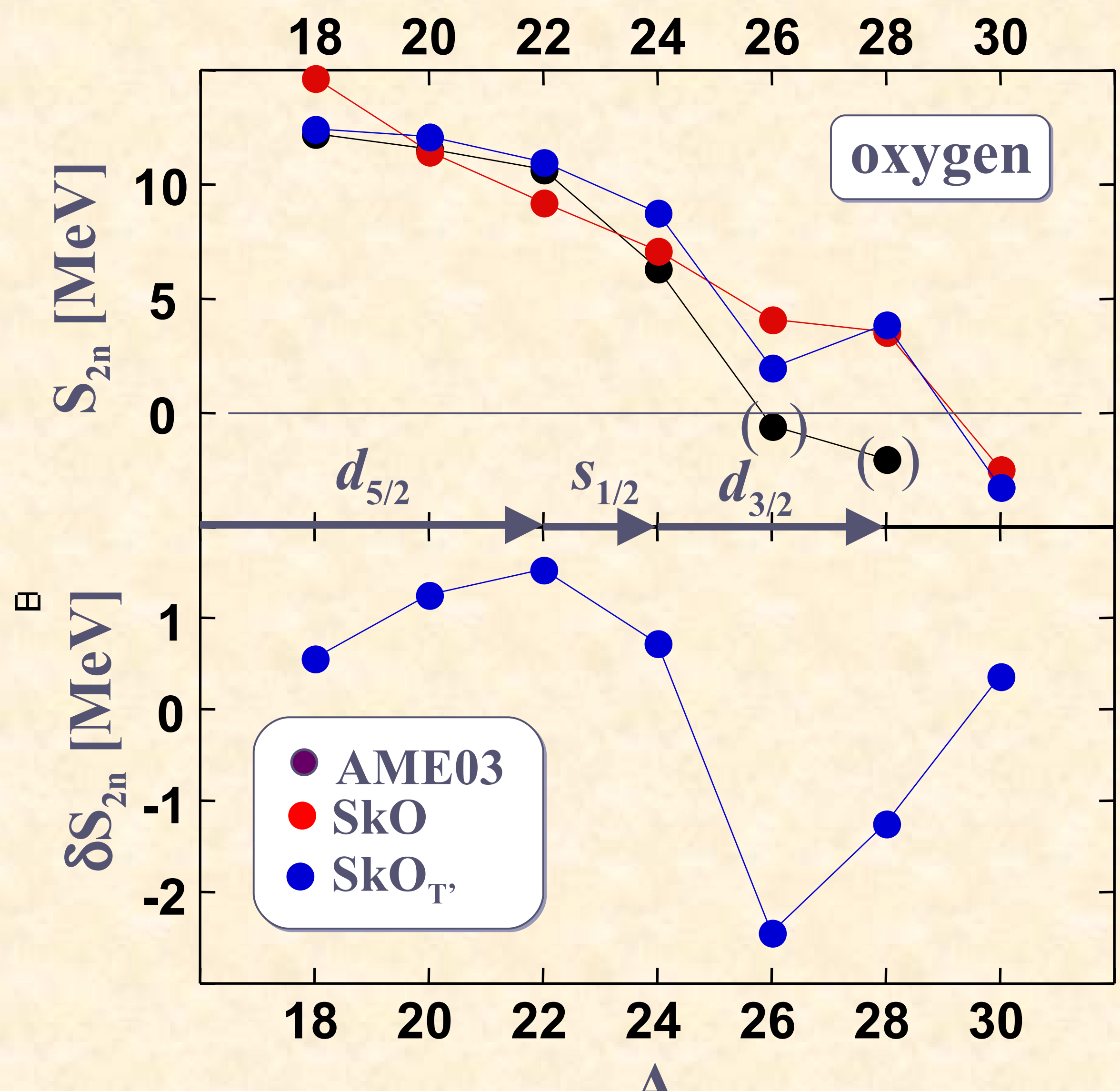
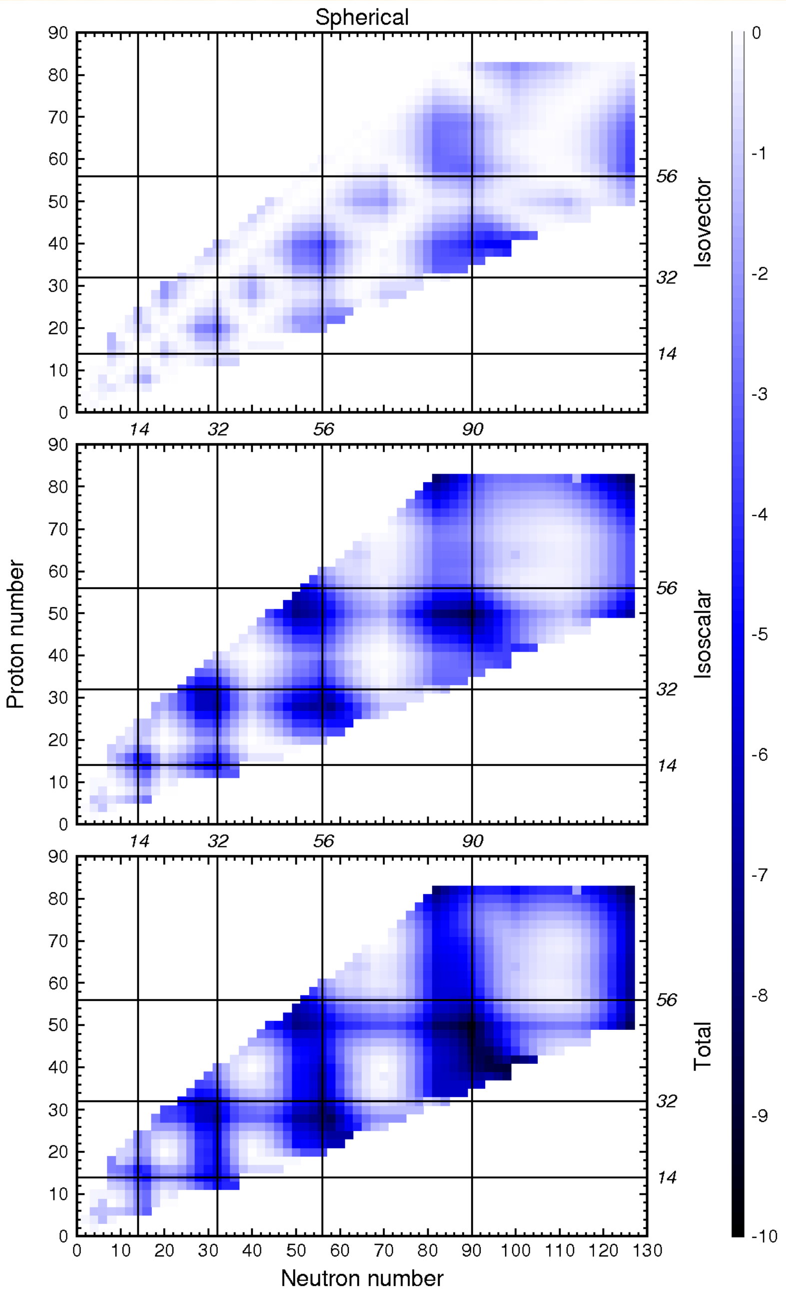




oxygen
S_{2n} [MeV]
δS_{2n} [MeV]
$d_{5/2}$
$s_{1/2}$
$d_{3/2}$
AME03
SkO
$SkO_{T'}$
A
18 20 22 24 26 28 30
10
5
0
1
0
-1
-2



Spherical
Isovector
Isoscalar
Total
Proton number
Neutron number
14
32
56
90
0
-1
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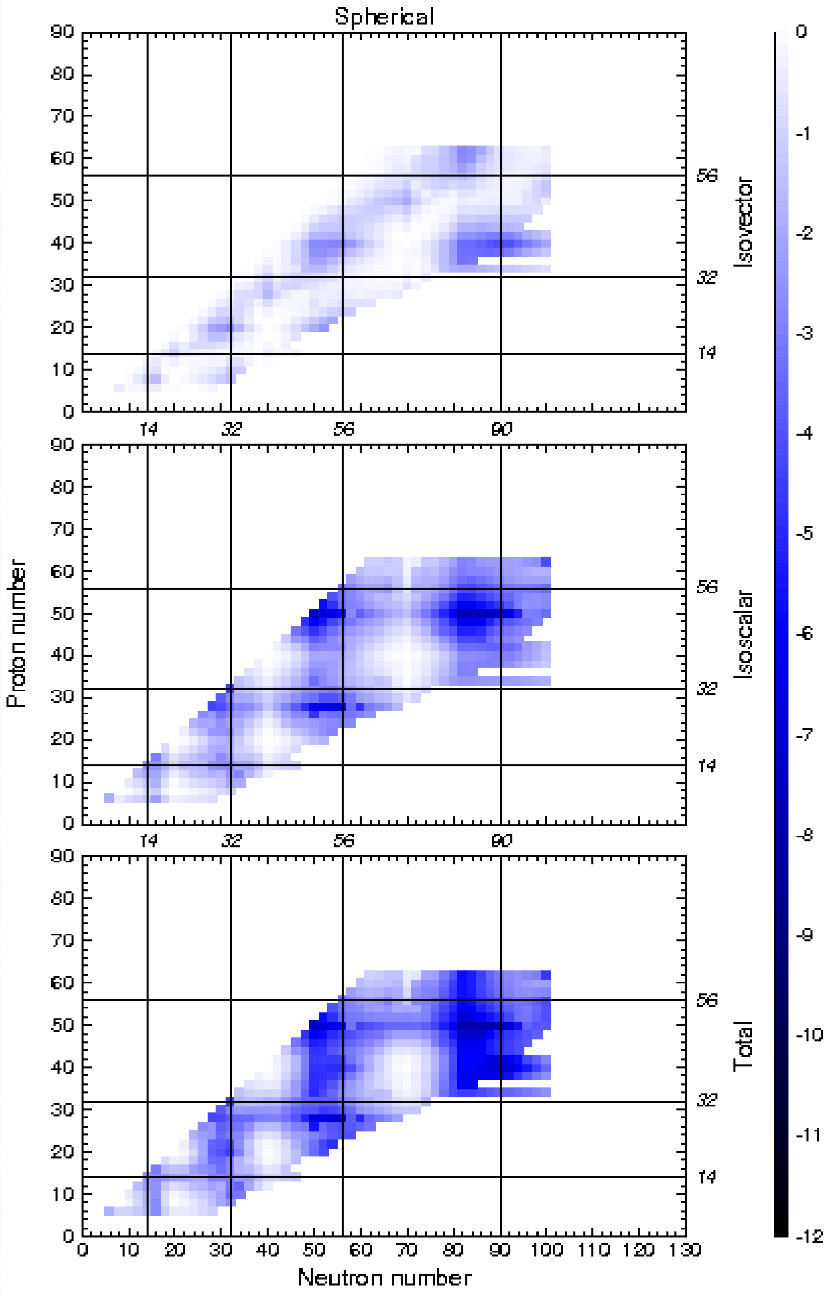
-4
-5
-6
-7
-8
-9
-10



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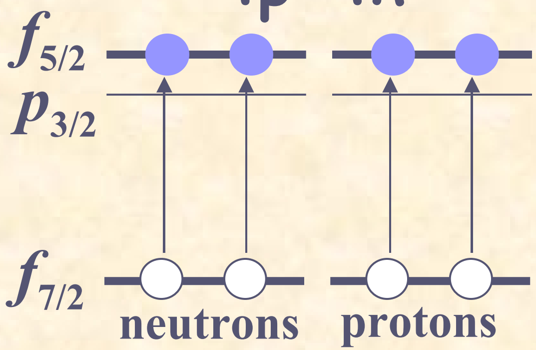
-11
-12

4p-4h

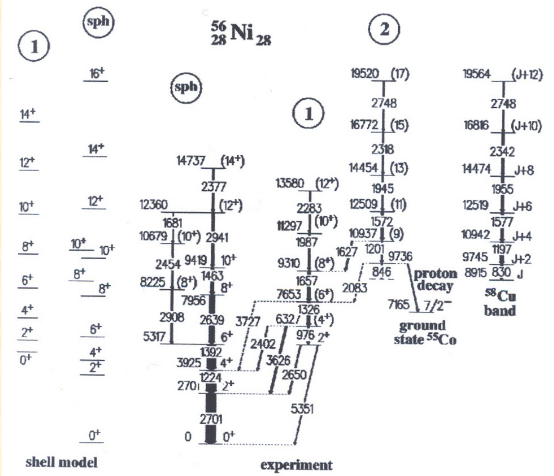


Nilsson

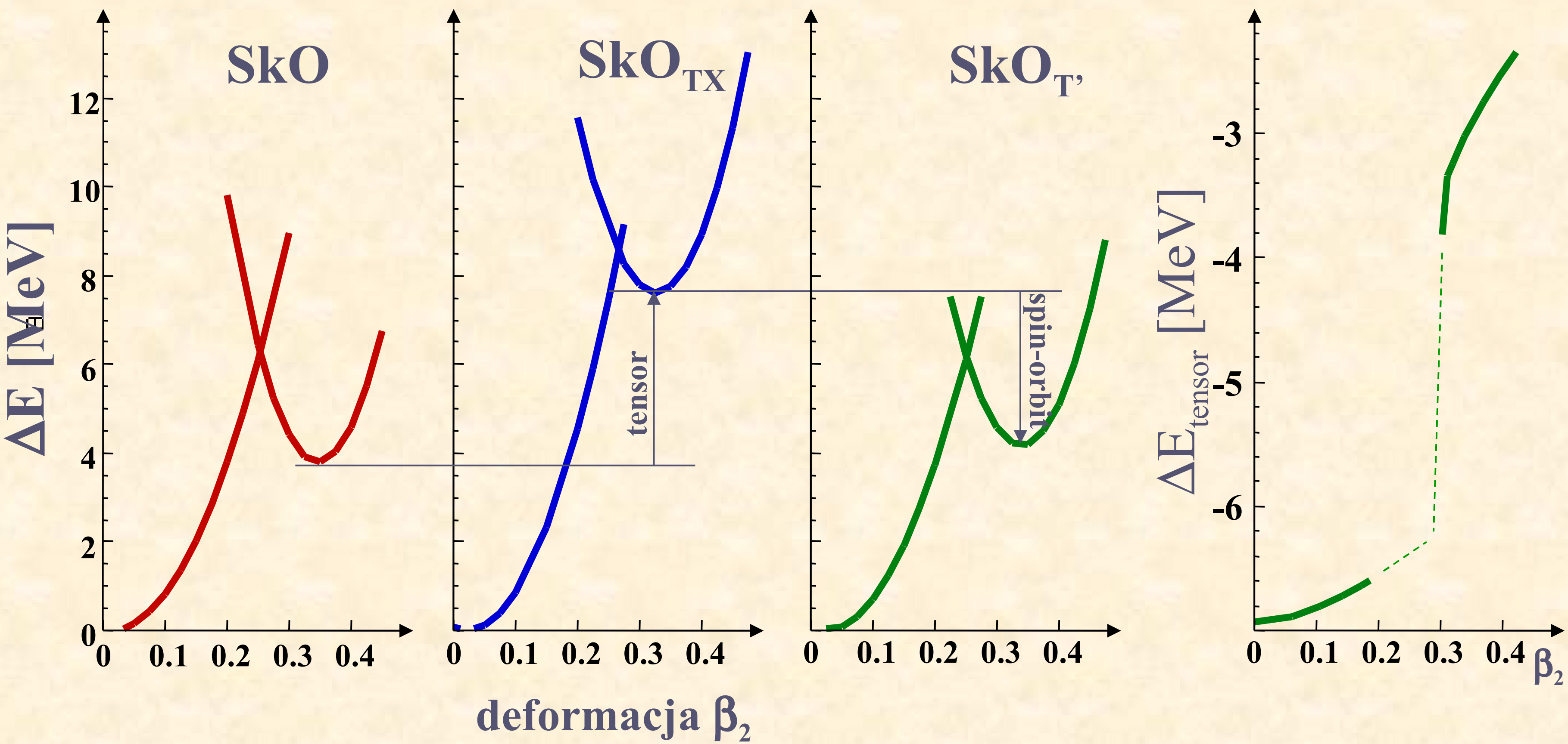
[321]1/2

↑

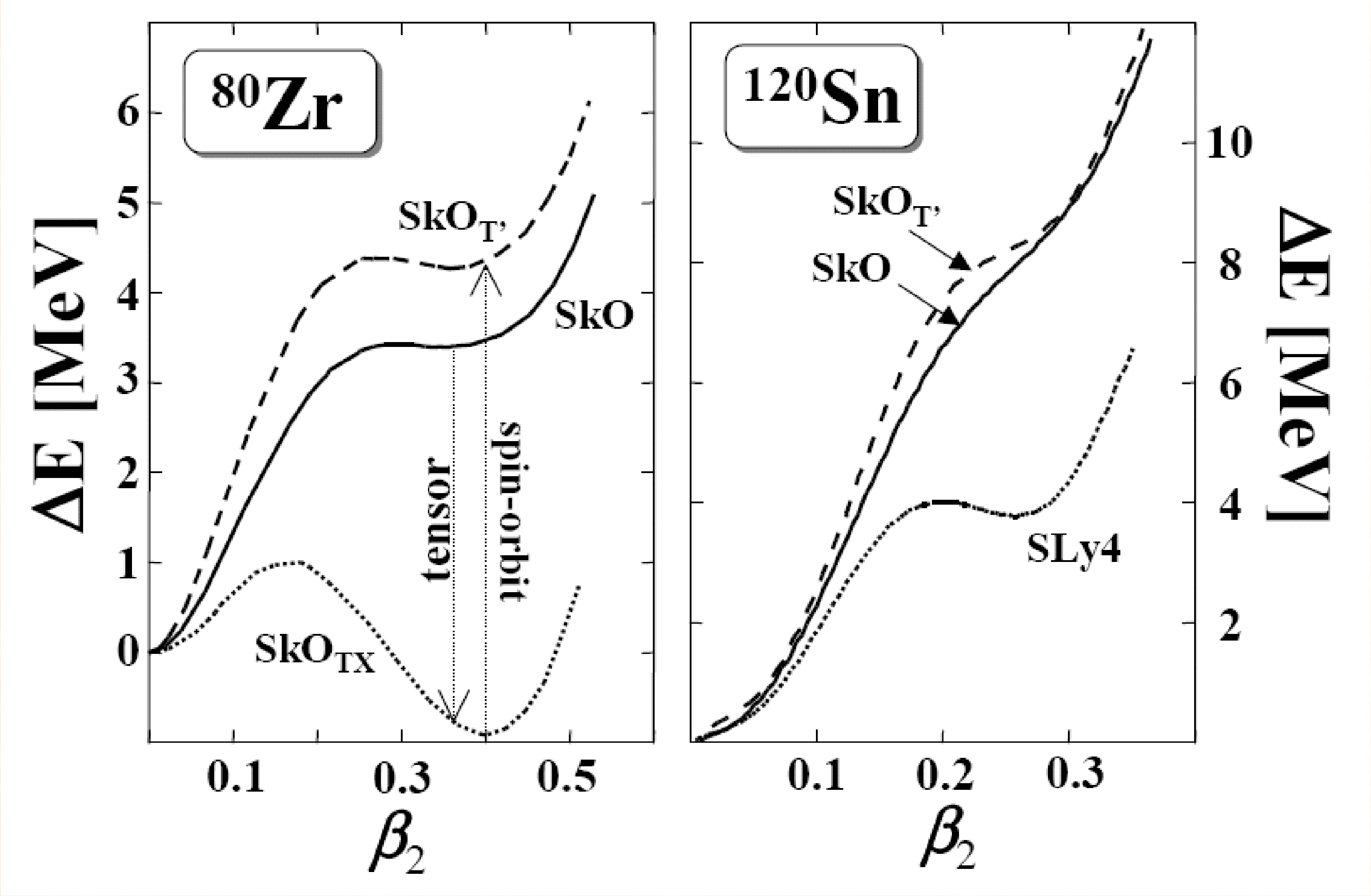
[303]7/2



Rudolph et al. PRL82, 3763 (1999)



constrained HFB calculations in spin-saturated ^{80}Zr



Summary

- Tensor part of the functional is necessary to describe single-particle properties,
- We have proposed a way to constrain tensor coupling constants.
- Tensor contribution to energy features strong shell-dependance.
- Subtle interpley between spin-orbit and tensor terms.