Towards spectroscopic quality energy density functionals.

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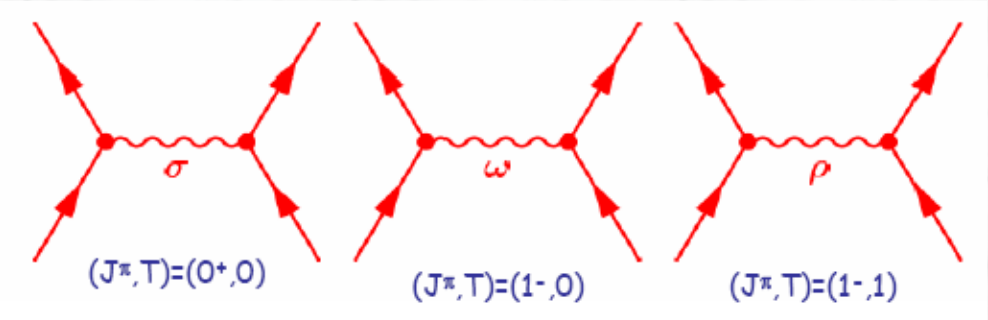
1. **Motivation: understand the possibilities and problems in achieving the spectroscopic quality covariant DFT**
2. **Deformed single(quasi)-particle configurations: successes and problems**
3. **Single-particle configurations in spherical nuclei: going beyond mean field by means of particle-vibration coupling.**
4. **Conclusions**

In collaboration with Elena Litvinova, GSI and Sheeren Shawaqfeh (MSU)

Covariant density functional theory (CDFT)

The nucleons interact via the exchange of effective mesons →
→ **effective Lagrangian**



Long-range attractive scalar field

Short-range repulsive vector field

Isovector field

$$E_{\mathrm{RMF}}[\hat{\rho}, \phi_m] = \mathrm{Tr}[(\boldsymbol{\alpha p} + \beta m)\hat{\rho}] \pm \int \left[\frac{1}{2}(\nabla\phi_m)^2 + U(\phi_m)\right] \mathrm{d}^3 r + \mathrm{Tr}[(\Gamma_m \phi_m)\hat{\rho}]$$

density matrix $\hat{\rho}$

$\phi_m \equiv \{\sigma, \omega^\mu, \vec{\rho}^\mu, A^\mu\}$ - meson fields

$$\hat{h} = \frac{\delta E}{\delta \hat{\rho}}$$

Mean field

$$\hat{h}|\varphi_i\rangle = \varepsilon_i |\varphi_i\rangle$$

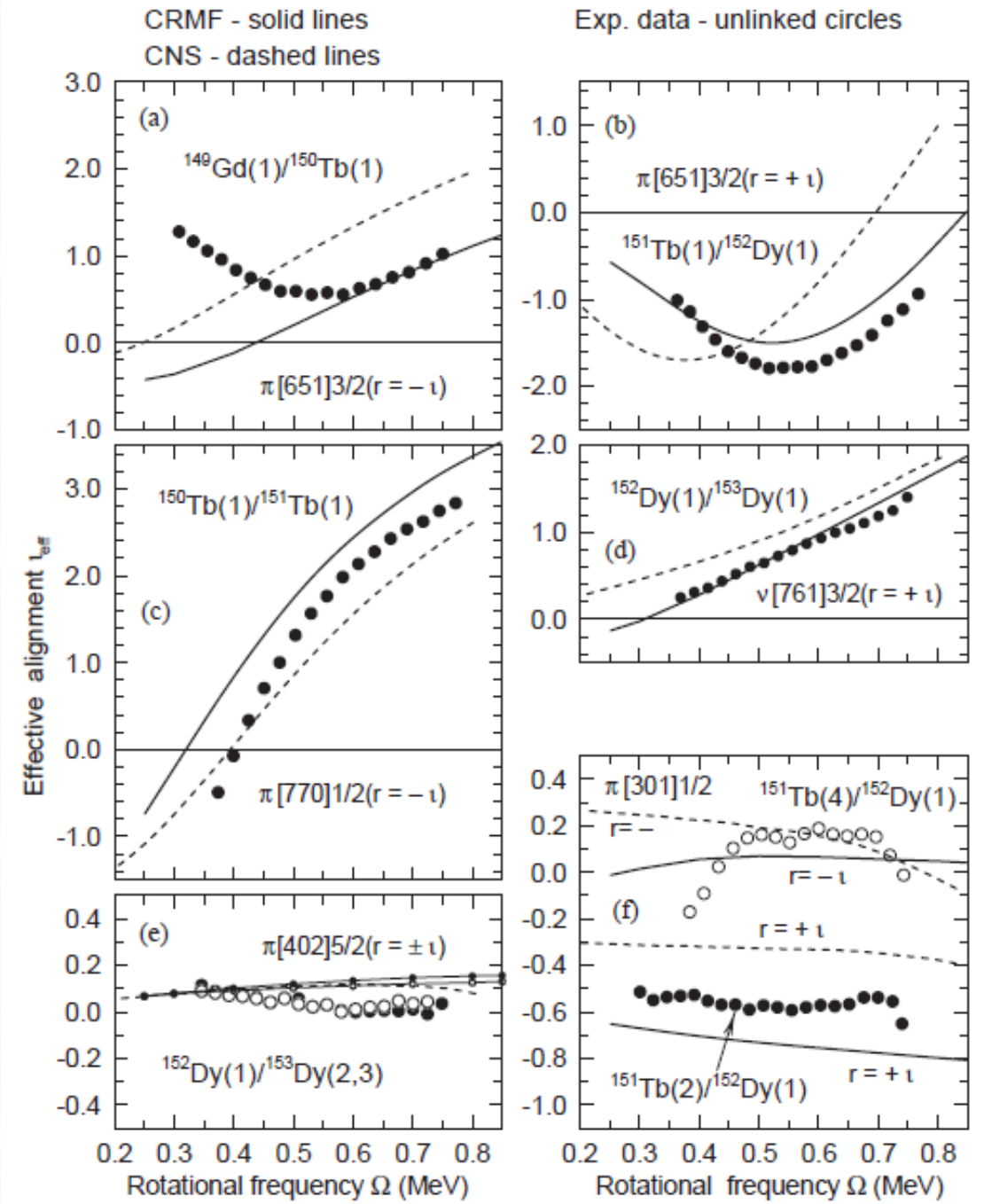
Eigenfunctions

Deformed single(quasi)-particle states: successes and problems

Different aspects of the single-particle motion:

1. deformation polarization effects induced by the particle(s) (test of time-even mean fields)
2. response to rotation (test of time-odd mean fields)
3. the energies of the single-(quasi)-particle configurations

Triaxial CRHB; fully self-consistent blocking, time-odd mean fields included, Gogny D1S pairing



Relative (effective) alignments of two rotational bands

$$i_{\rm eff}^{\rm B,A}(\Omega) = I_{\rm B}(\Omega) - I_{\rm A}(\Omega)$$

depends both **on the alignment properties of single-particle orbital(s)** by which the two bands differ and on **the polarization effects induced by the particles** in these orbitals

The impact of the particle(s) on kinematic and dynamic moments of inertia is well reproduced

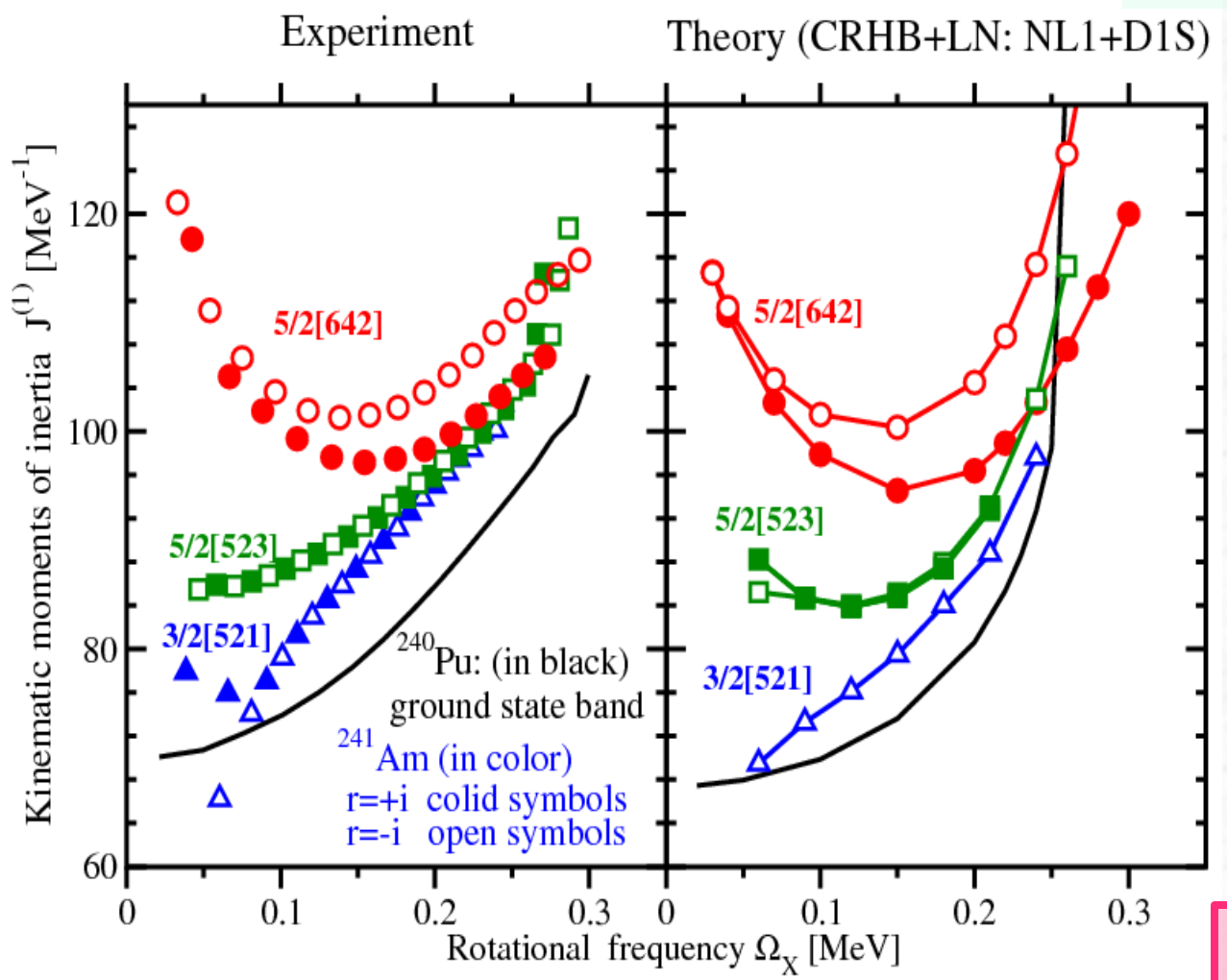
AA, G.A. Lalazissis, P. Ring, Nucl. Phys. A 634 (1998) 395.

AA and P.Ring, Phys. Scripta, T88, 10 (2000)

^{241}Am: the dependence of the rotational properties on the single-particle state.

AA,…P.Ring, … J. Physics: Conference series, in press

$^{241}Am = ^{240}Pu + \pi$



Increase of $J^{(1)}$ in odd-proton nucleus as compared with even-even ^{240}Pu is due to blocking which includes:

(a) Decrease of proton pairing

(b) Alignment properties of blocked proton state

Useful tool for configuration assignments

Data: K. Abu Saleem at al, PRC 70, 024310 (2004)

Impact of particle(s) on charge quadrupole moments: example of SD bands in the A~150 mass region

Experimental and calculated relative charge quadrupole moments $\Delta Q_0 = Q_0(\text{Band}) - Q_0(^{152}\text{Dy}(1))$ of the ^{149}Gd(1), ^{151}Tb(1) and ^{151}Dy(1).

Band	Configuration	ΔQ_0^{exp} (*e*b)	ΔQ_0^{th} (*e*b)
^{149}Gd(1)	$\nu[770]\frac{1}{2}(r=-i)^{-1}(\pi[651]\frac{3}{2})^{-2}$	−2.5(0.3)	−2.41
^{151}Tb(1)	$\pi[651]\frac{3}{2}(r=+i)^{-1}$	−0.7(0.7)	−1.01
^{151}Dy(1)	$\nu[770]\frac{1}{2}(r=-i)^{-1}$	−0.6(0.4)	−0.53

The detailed structure of the configurations of these bands relative to the doubly magic ^{152}Dy core is given in column 2.

AA, G.A. Lalazissis, P. Ring, Nucl. Phys. A 634 (1998) 395.

This impact is rather well reproduced in non-relativistic and relativistic DFT

Satula et al, PRL 88, 5182 (1996)

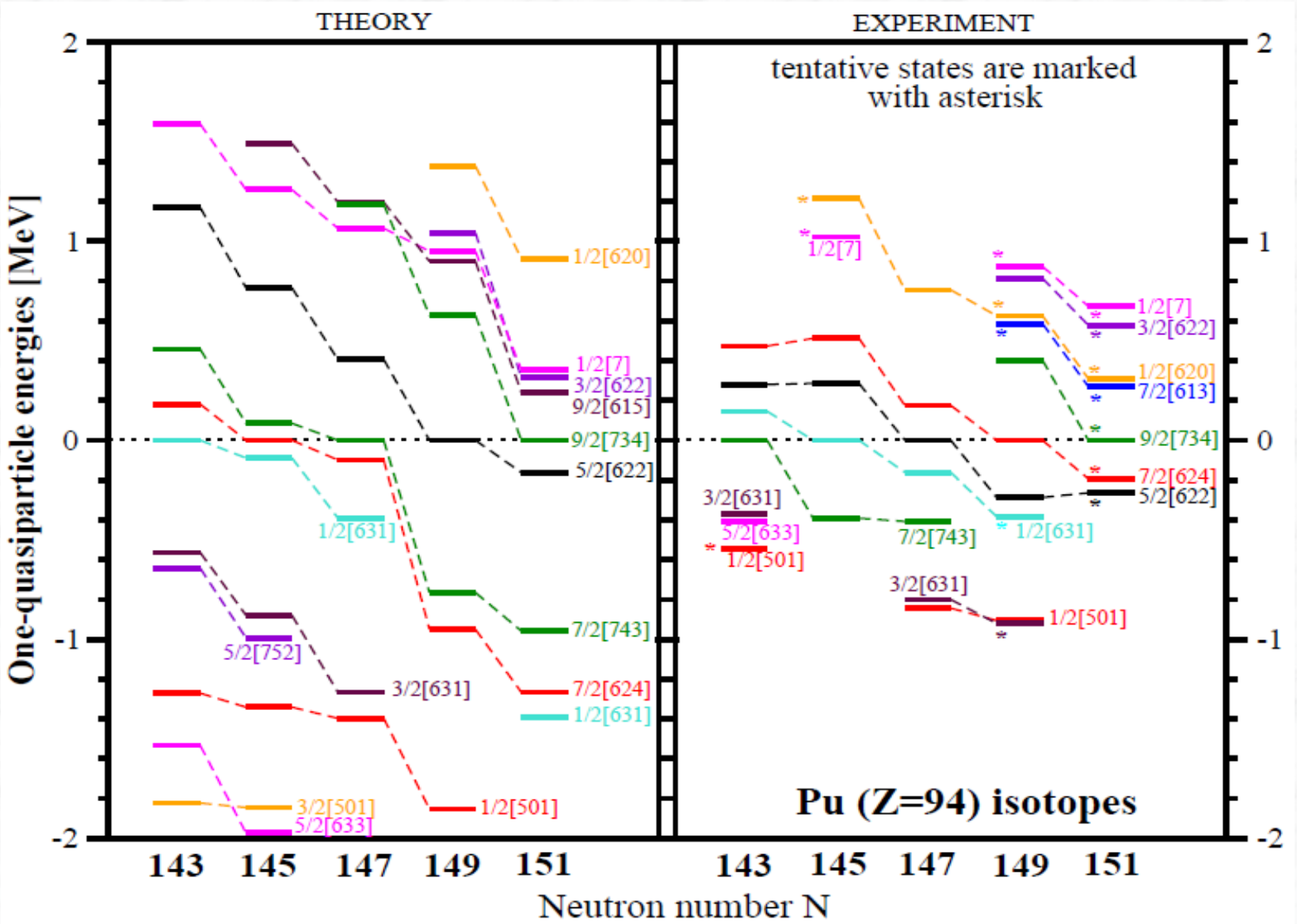
M.Matev et al, PRC 76, 034304 (2007)

R.W. Laird et al, PRL 88, 152501(2002)

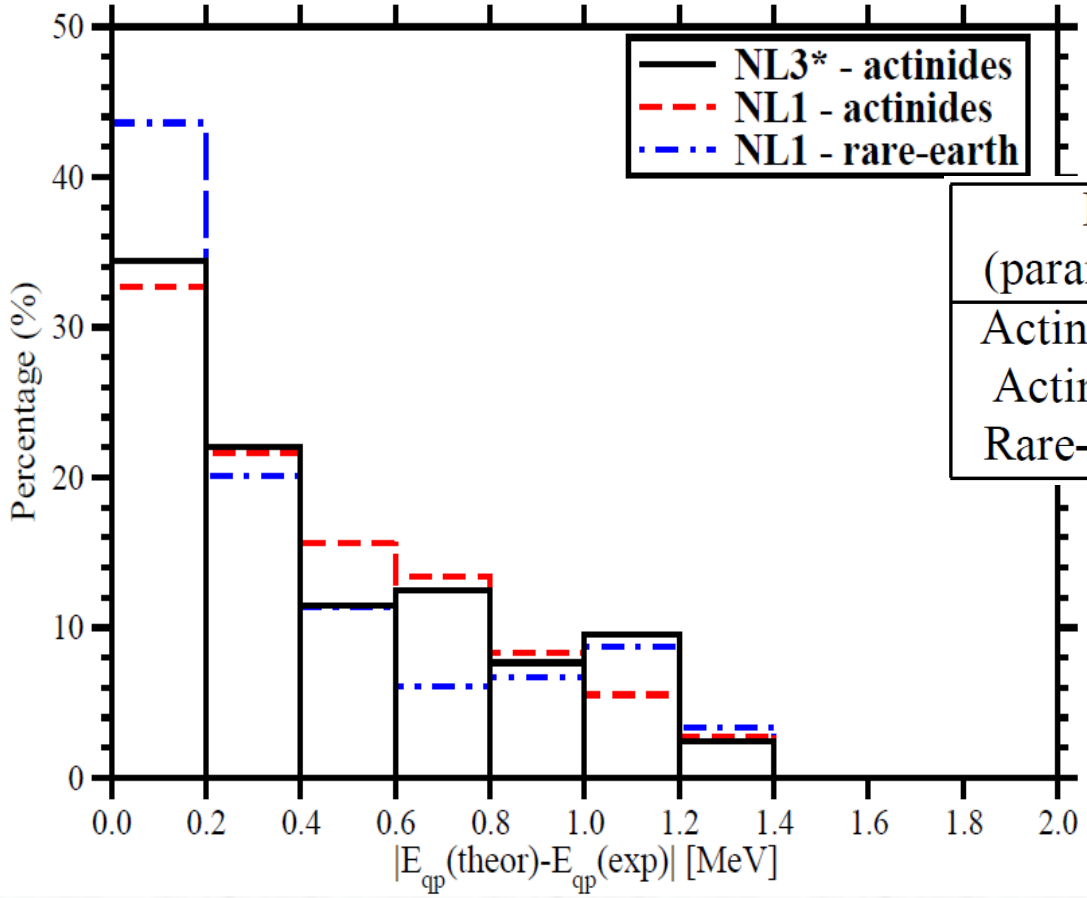
On the contrary, the ΔQ_0 quantity is not uniquely defined in phenomenological models based on the Nilsson or Woods-Saxon potentials

Systematics of one-quasiparticle configurations in actinides

Binding energies are calculated for each one-quasiparticle configuration and only then the spectra are built.



Statistical distribution of deviations of the energies of one-quasiparticle states from experiment



1. ~ 5% of calculated states have triaxial deformation

Region (parametrization)	calculated states (#)	compared states (#)
Actinides (NL3*)	415	209
Actinides (NL1)	444	217
Rare-earth (NL1)	360	149

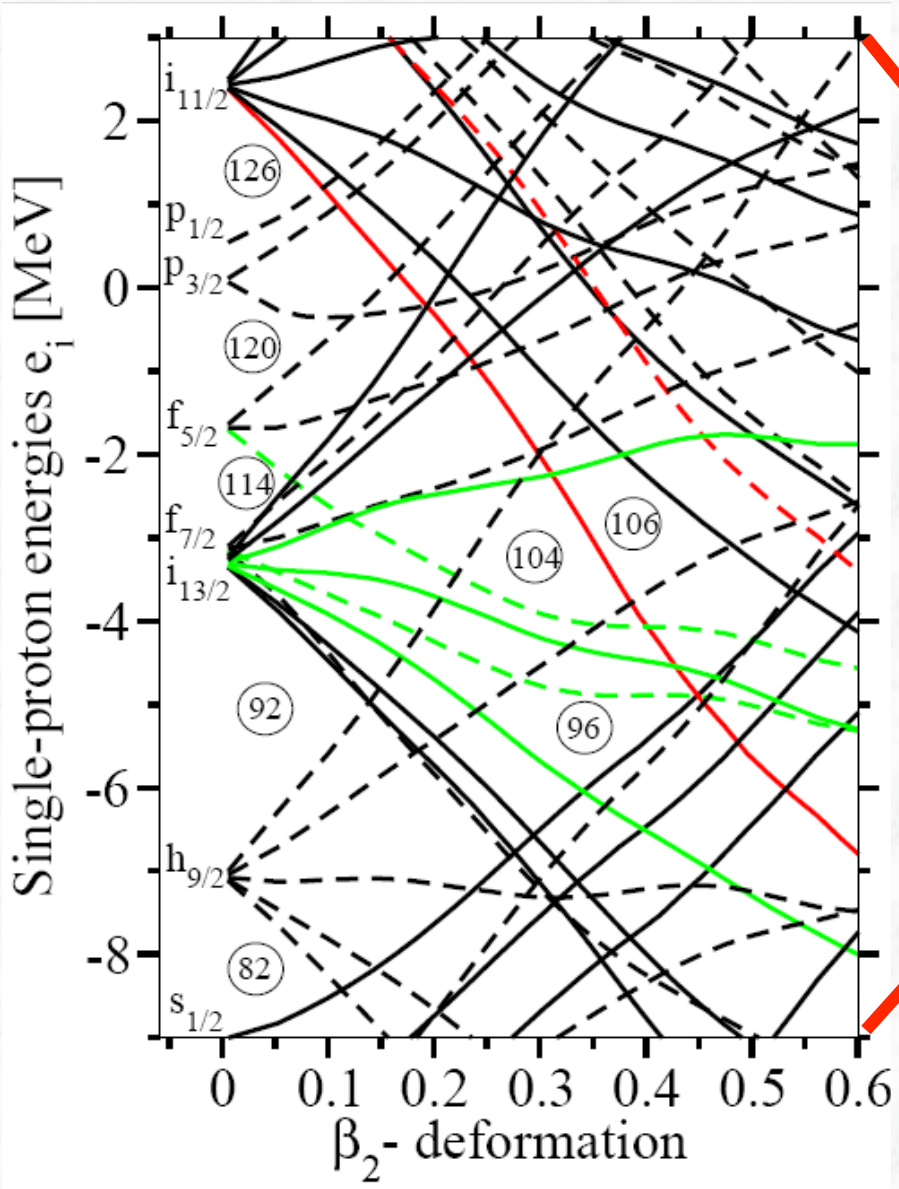
2. For a given state, the deviation from experiment depends on particle number (consequence of the stretching out of energy scale due to low effective mass)
3. For some of the states, there is persistent deviation from experiment (due to wrong placement of subshell at spherical shape).

Two sources of deviations:

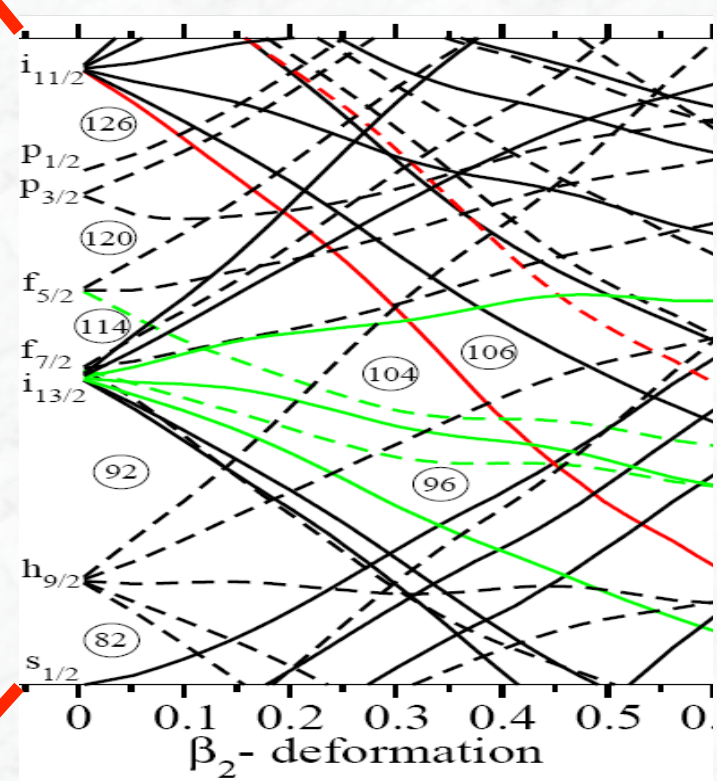
1. Low effective mass (stretching of the energy scale)
2. Wrong relative energies of the states

Illustration of energy scale stretching due to low effective mass

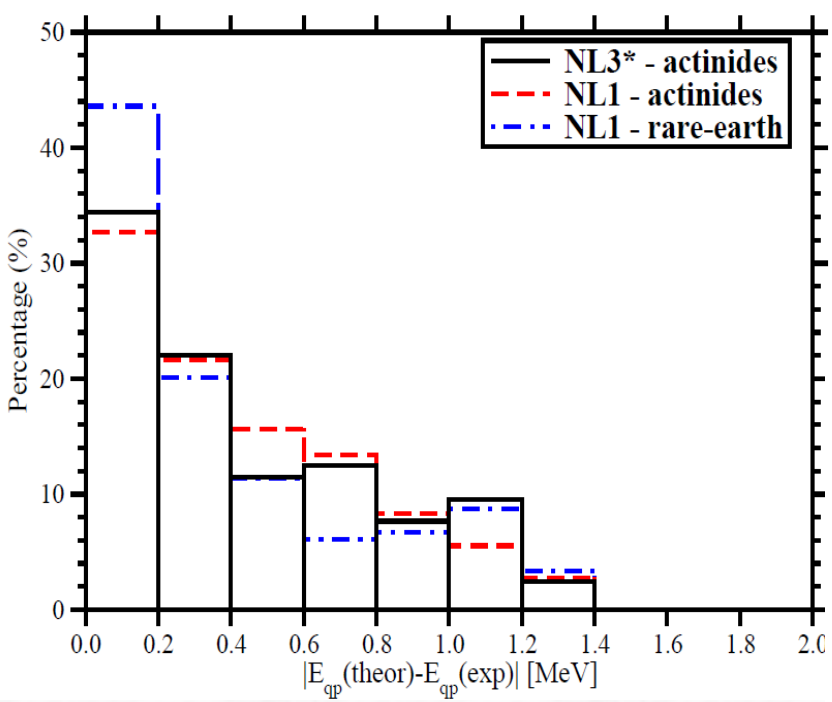
Low effective mass (~0.65)



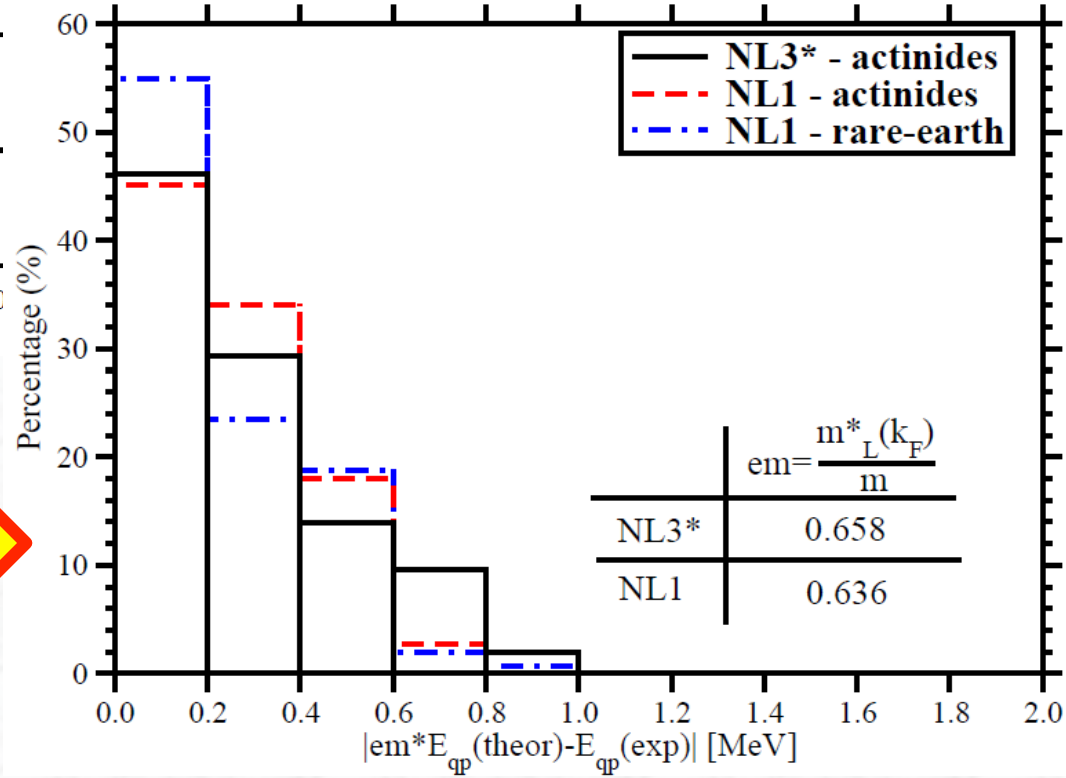
High effective mass (1.0)



Accuracy of the description of the energies of deformed one-quasiparticle states in actinides in RHB calculations: **correction for low Lorentz effective mass**



Energy scale is corrected for low effective mass



1. 75-80% of the states are described with an accuracy of phenomenological (Nilsson, Woods-Saxon) models
2. The remaining differences are due to incorrect relative energies of the single-particle states

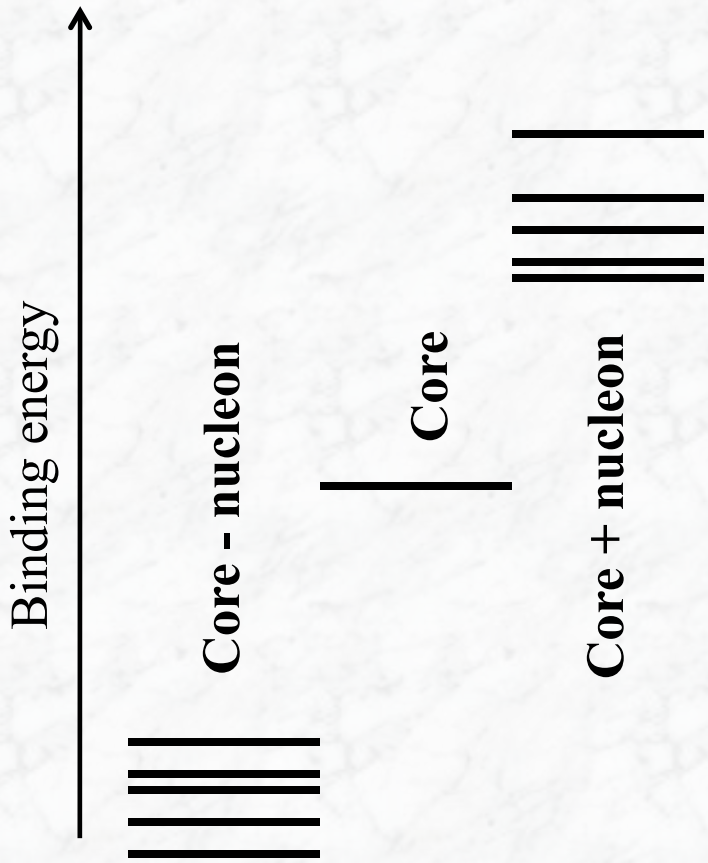
Single-particle configurations in spherical nuclei: going beyond mean field by means of particle-vibration coupling.

Hybrid approach

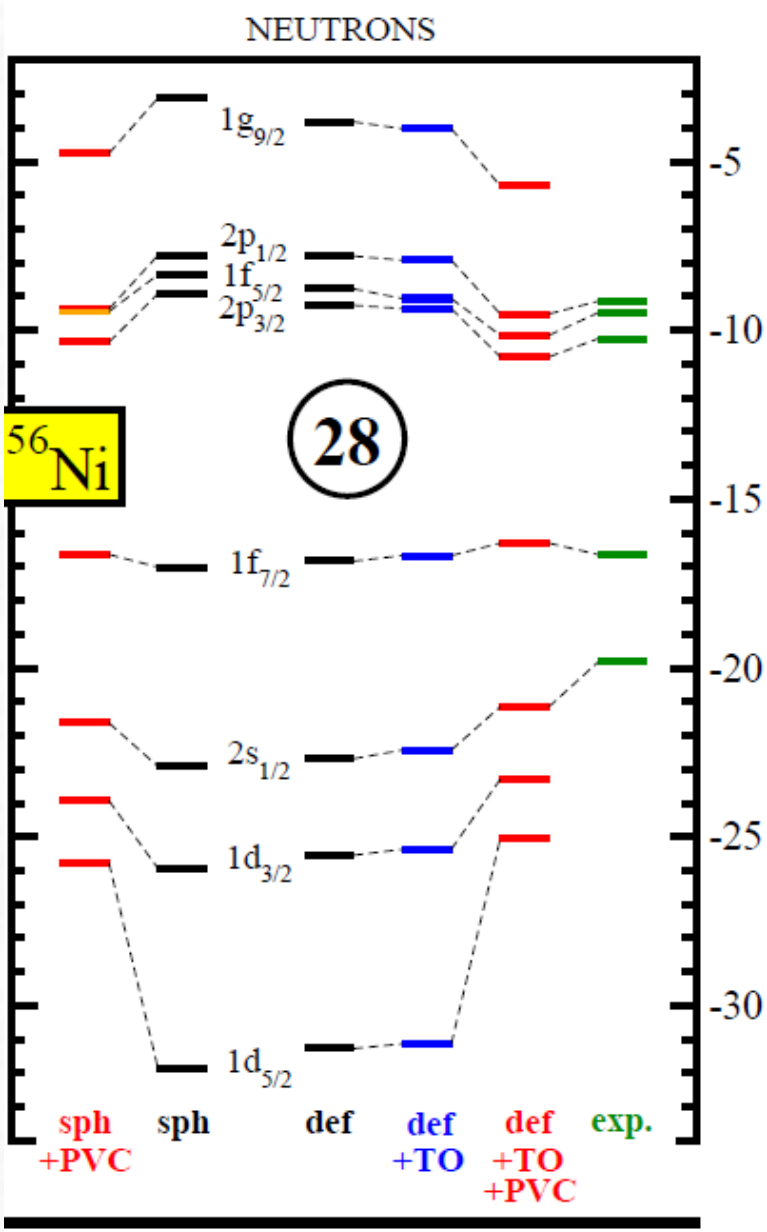
Treat

1. the polarization effects due to deformation and time-odd mean fields in the triaxial relativistic mean field approach (AA, H.Abusara, PRC 81, 014309 (2010))
2. energy corrections due to PVC in the relativistic particle-vibration coupling model for spherical nuclei (according to E.Litvinova and P.Ring, PRC73, 044328 [2006])
3. In both approaches
   - NL3* parametrization [G.Lalazissis, et al PLB 671, 36 (2009)]
   - pairing is neglected

How single-particle spectra are obtained in experiment



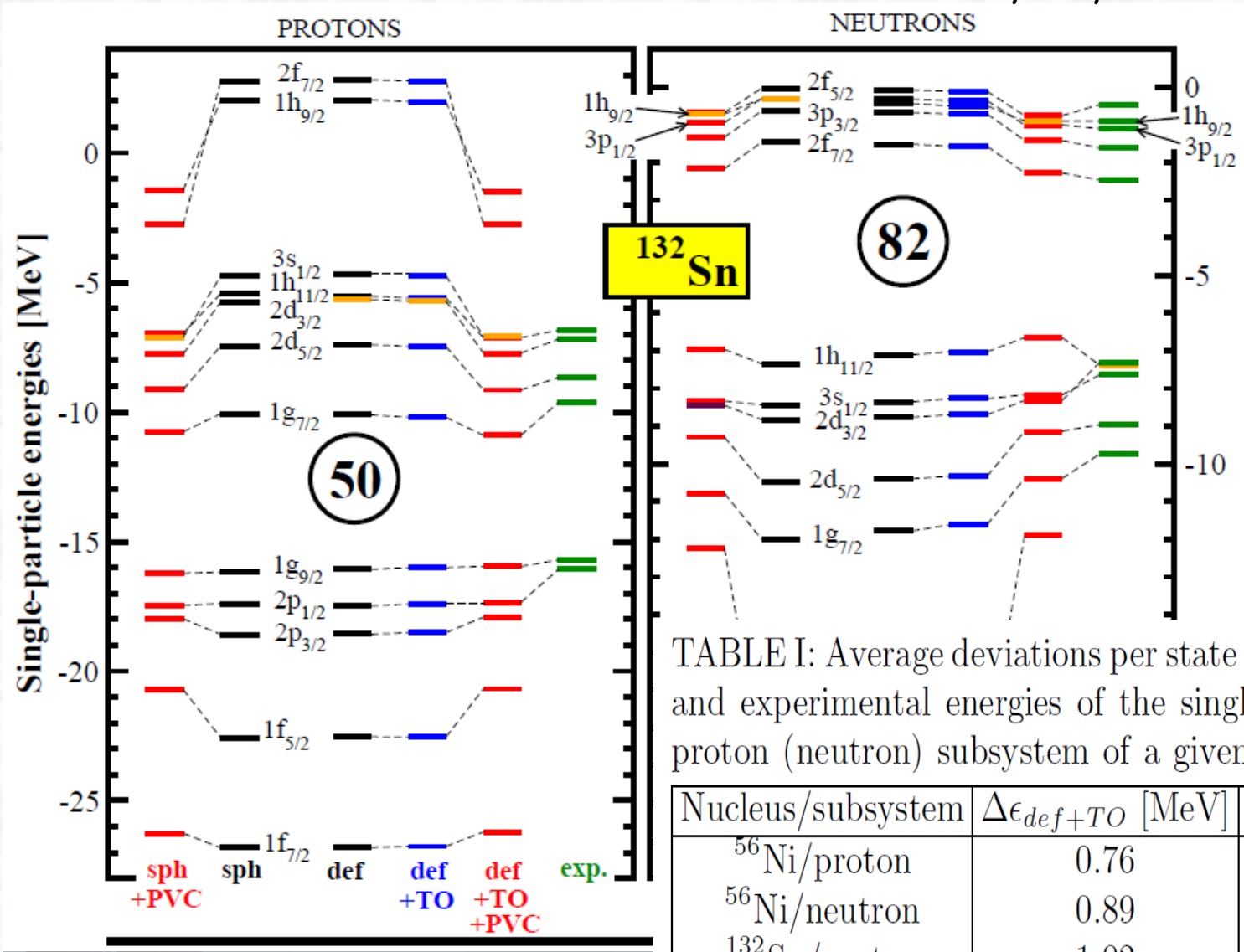
$$\varepsilon(\text{particle}) = B(\text{core}) - B(\text{core} + \text{nucleon})$$
$$\varepsilon(\text{hole}) = B(\text{core} - \text{nucleon}) - B(\text{core}).$$



Include **polarization effects due to**

1. **deformation (def) and**
2. **time-odd (TO) mean fields as well as**
3. **energy corrections due to particle-vibration coupling (PVC)**

E. Litvinova, AA, PRC 84, 014305 (2011)



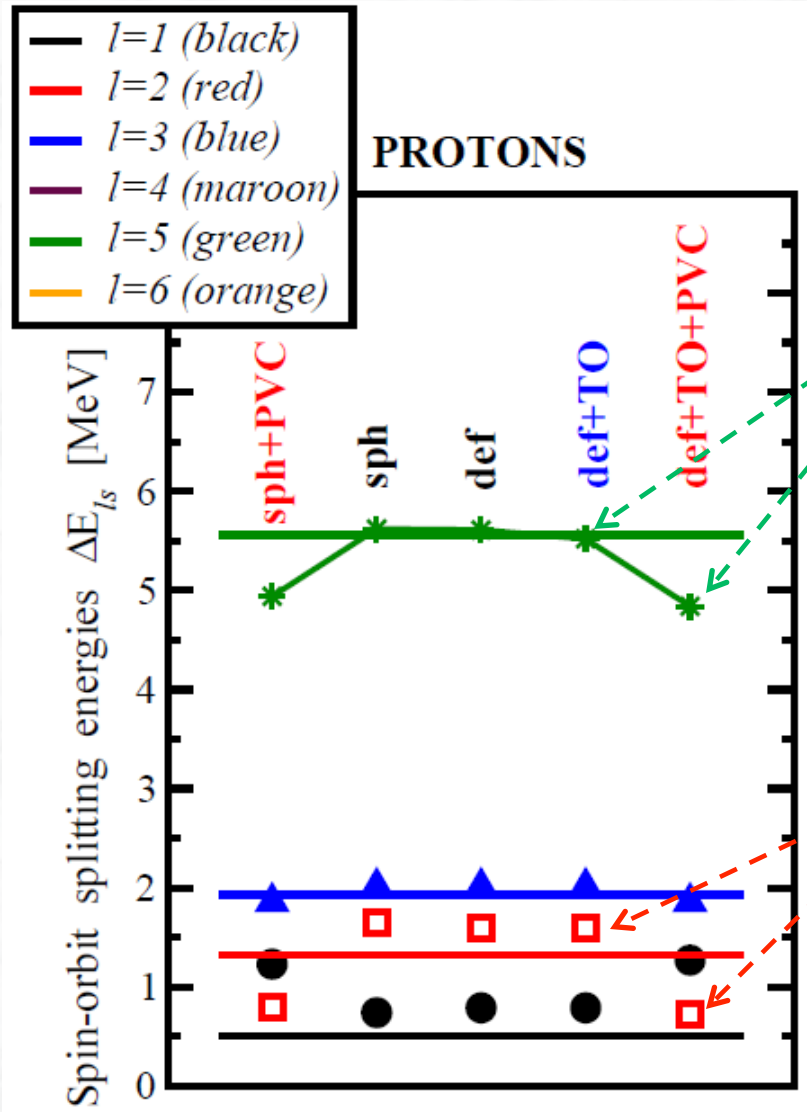
Detailed calculations are also performed for ^{100}Sn, ^{208}Pb and ^{56}Ni

TABLE I: Average deviations per state $\Delta\epsilon$ between calculated and experimental energies of the single-particle states for a proton (neutron) subsystem of a given nucleus. The results

Nucleus/subsystem	$\Delta\epsilon_{def+TO}$ [MeV]	$\Delta\epsilon_{def+TO+PVC}$ [MeV]
^{56}Ni/proton	0.76	0.77
^{56}Ni/neutron	0.89	0.71
^{132}Sn/proton	1.02	0.68
^{132}Sn/neutron	0.89	0.39
^{208}Pb/proton	1.53	0.84
^{208}Pb/neutron	1.00	0.47

PVC – particle-vibration coupling

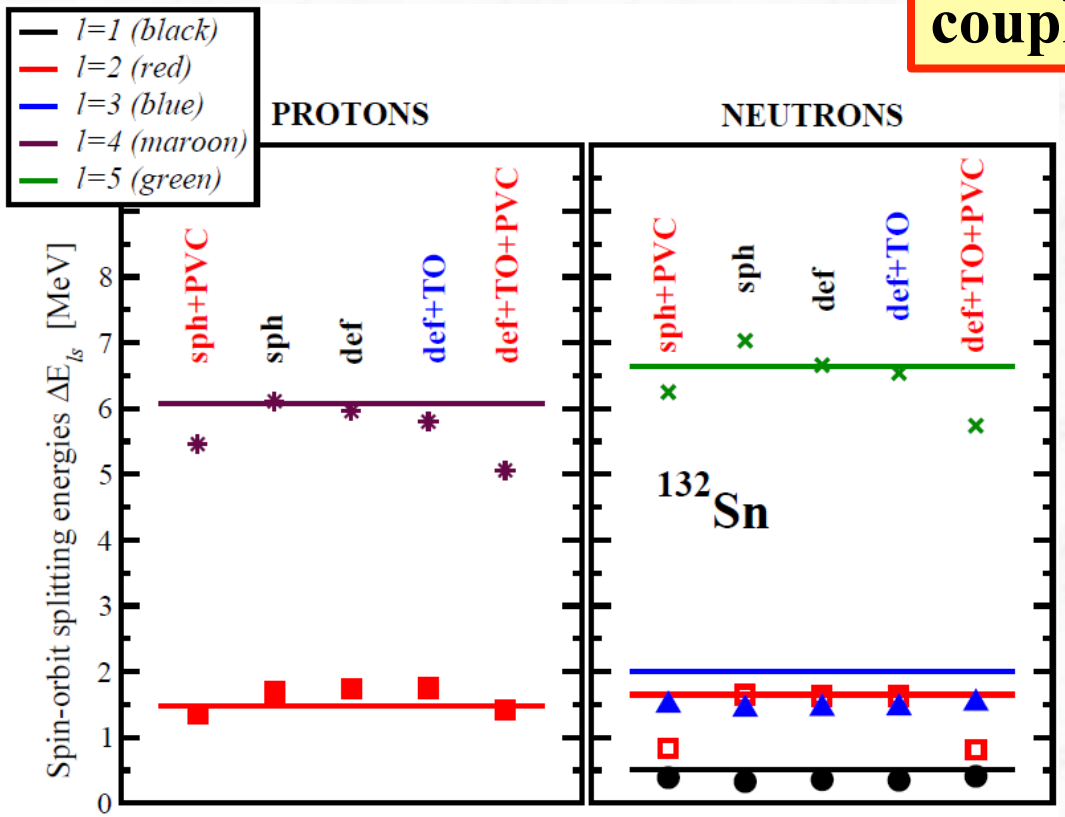
The impact of particle-vibration coupling on spin-orbit splittings.



The members of the spin-orbit doublet are located on both sides of the shell gap.

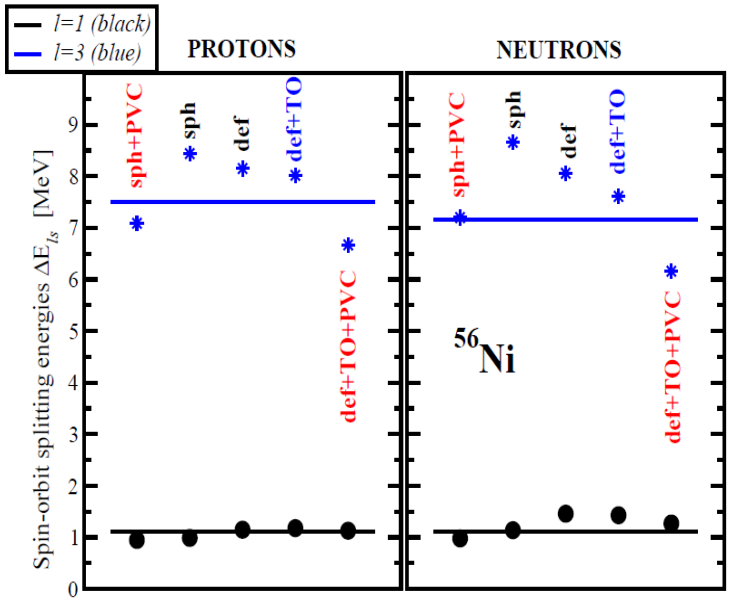
Both members of the spin-orbit doublets are located below the shell gap.

The impact of particle-vibration coupling on spin-orbit splittings.

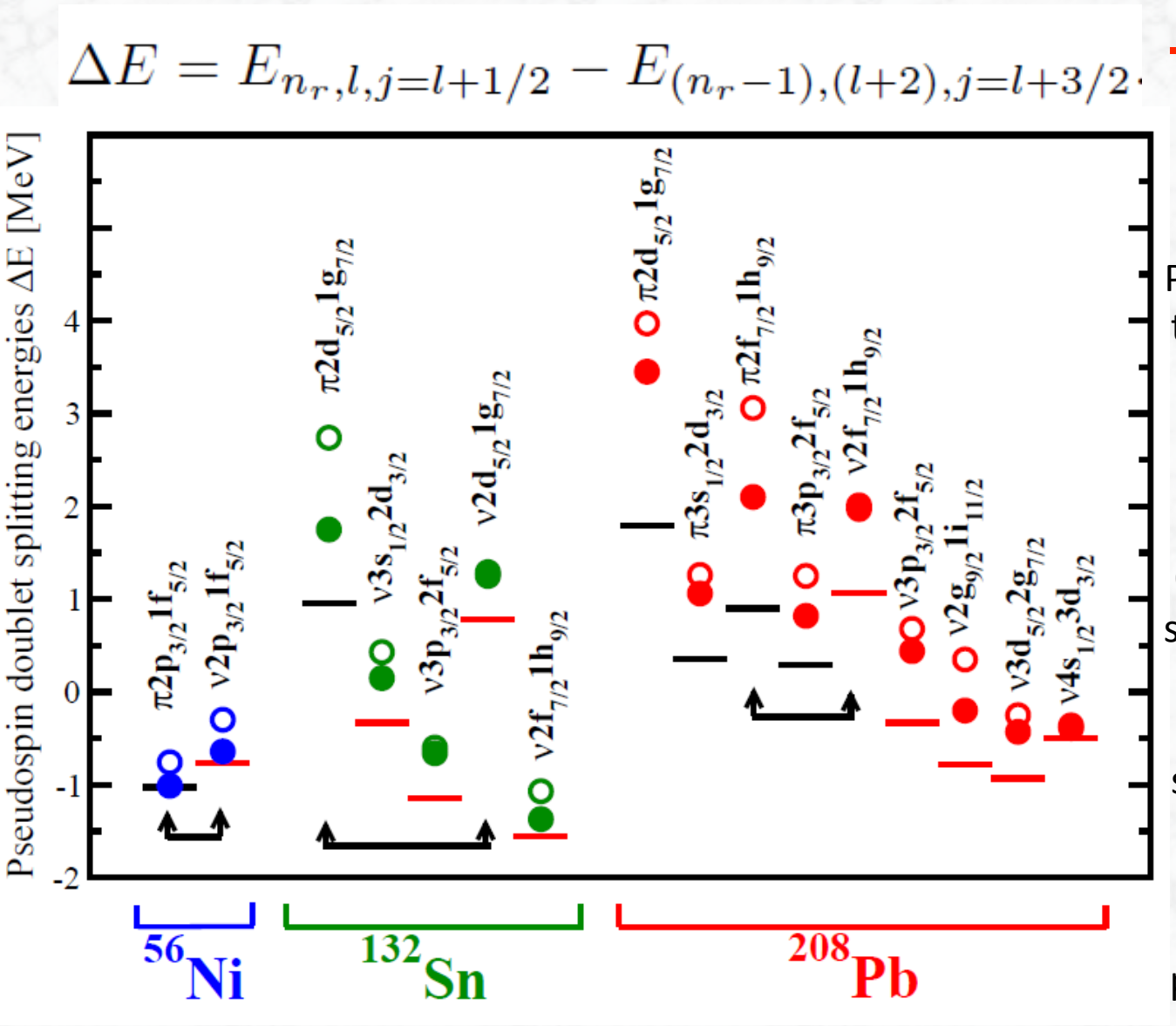


The inclusion of particle-vibration coupling **decreases** the accuracy of the description of spin-orbit splittings.

The absolute deviations per doublet are **0.34 MeV [0.50 MeV], 0.23 MeV [0.56 MeV]** and **0.26 MeV [0.45 MeV] in the mean field** ("def+TO") **[particle-vibration coupling** ("def+TO+PVC")] calculations in ^{56}Ni, ^{132}Sn and ^{208}Pb, respectively.



The impact of particle-vibration coupling on pseudospin doublets.



Exp (protons)

Exp (neutrons)

def+TO

def+TO+PVC

PVC substantially improves the description of splitting energies in pseudospin doublets as compared with mean field calculations.

Observed similarity of the splitting energies of proton and neutron pseudospin doublets with the same single-particle structure in medium and heavy mass nuclei can only be reproduced when the particle-vibration coupling is taken into account.

Spectroscopic factors

The absolute values of experimental spectroscopic factors are characterized by large ambiguities and depend strongly on the reaction employed in experiment and the reaction model used in the analysis

Nucleus	State	S_{th}	S_{exp}	S_{exp}
^{209}Pb	$2g_{9/2}$	0.85	0.78±0.1 [76]	0.94 [80]
	$1i_{11/2}$	0.89	0.96±0.2 [76]	1.05 [80]
	$1j_{15/2}$	0.66	0.53±0.2 [76]	0.57 [80]
	$3d_{5/2}$	0.89	0.88±0.1 [76]	
	$4s_{1/2}$	0.92	0.88±0.1 [76]	
	$2g_{7/2}$	0.87	0.78±0.1 [76]	
	$3d_{3/2}$	0.89	0.88±0.1 [76]	
^{209}Bi	$1h_{9/2}$	0.88	1.17 [75]	0.80 [69]
	$2f_{7/2}$	0.78	0.78 [75]	0.76 [69]
	$1i_{13/2}$	0.63	0.56 [75]	0.74 [69]
	$2f_{5/2}$	0.61	0.88 [75]	0.57 [69]
	$3p_{3/2}$	0.62	0.67 [75]	0.44 [69]
	$3p_{1/2}$	0.37	0.49 [75]	0.20 [69]
^{207}Pb	$3p_{1/2}$	0.90		1.08 [83]
	$2f_{5/2}$	0.87	1.13 [78]	1.05 [83]
	$3p_{3/2}$	0.86	1.00 [78]	0.95 [83]
	$1i_{13/2}$	0.82	1.04 [78]	0.61 [83]
	$2f_{7/2}$	0.64	0.89 [78]	0.64 [83]
	$1h_{9/2}$	0.38		
^{207}Tl	$3s_{1/2}$	0.84	0.95 [77]	0.85 [68]
	$2d_{3/2}$	0.86	1.15 [77]	0.90 [68]
	$1h_{11/2}$	0.80	0.89 [77]	0.88 [68]
	$2d_{5/2}$	0.68	0.62 [77]	0.63 [68]
	$1g_{7/2}$	0.22	0.40 [77]	0.27 [68]

Conclusions:

1. Rotational response (alignment properties) of particle(s) and polarization effects [in time-even (deformation) and time-odd mean fields] induced by them are well reproduced in CDFT.

2. The accuracy of the description of the energies of deformed one-quasiparticle configurations on the CDFT level is insufficient due to low effective mass and wrong relative energies of some subshells at spherical shape.

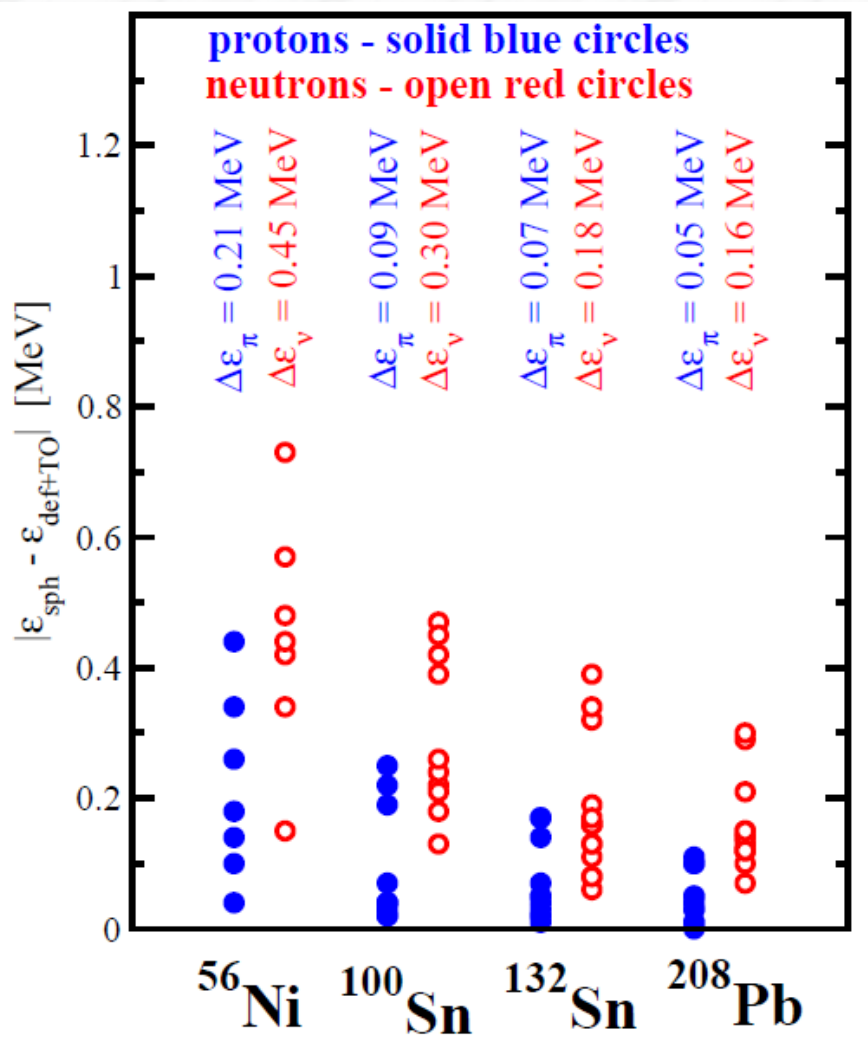
3. **The improvement of spectroscopic properties (energies of single-particle configurations, wave functions) on the DFT level has its own limits.**
It ultimately requires the accounting of particle-vibration coupling which
- substantially improves the accuracy of the description of the energies of the single-particle configurations and pseudospin doublets in spherical nuclei
- somewhat decreases the accuracy of the description of spin-orbit splittings

4. **The reparametrization of CDFT on the PVC level will be needed to further improve the accuracy of the description of the energies of single-particle config.**

The PVC results for spherical nuclei are published in
E.V. Litvinova and AA, PRC 84, 014305 (2011)
Statistical analysis of deformed one-quasiparticle states
AA and S.Shawaqfeh, PLB 706 (2011) 177

EXTRA

Combined polarization effects due to deformation and time-odd mean fields



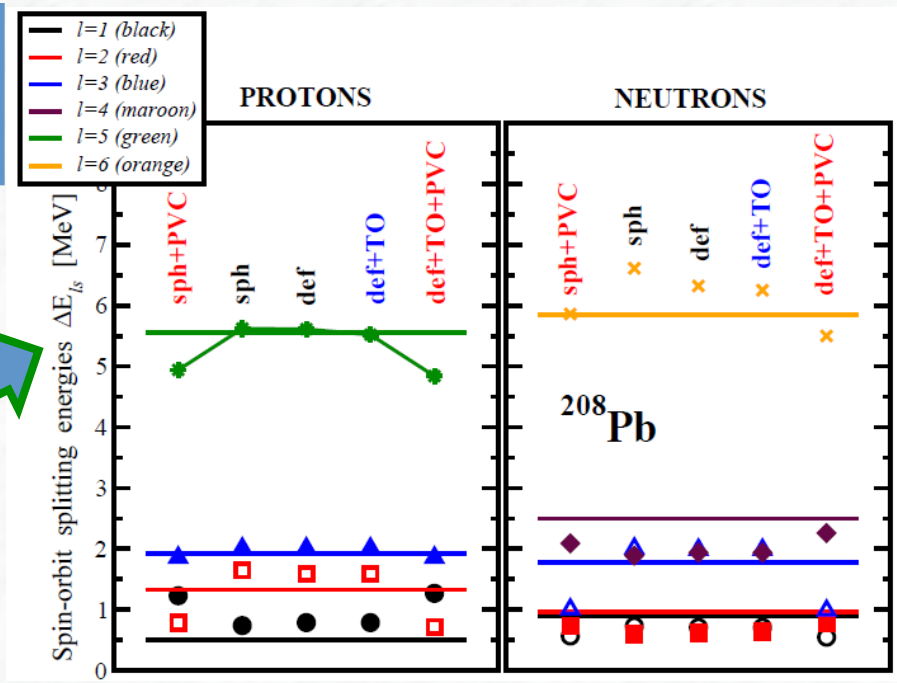
The polarization effects in odd-mass nuclei due to deformation and time-odd mean fields induced by odd particle are important. They have to be taken into account when experimental and calculated single-particle energies are compared.

Their neglect (as usually done in PVC calculations) is more or less justified only for heavy nuclei, and it is more justified for proton subsystem than for neutron one.

Why relativistic treatment based on Dirac equation?

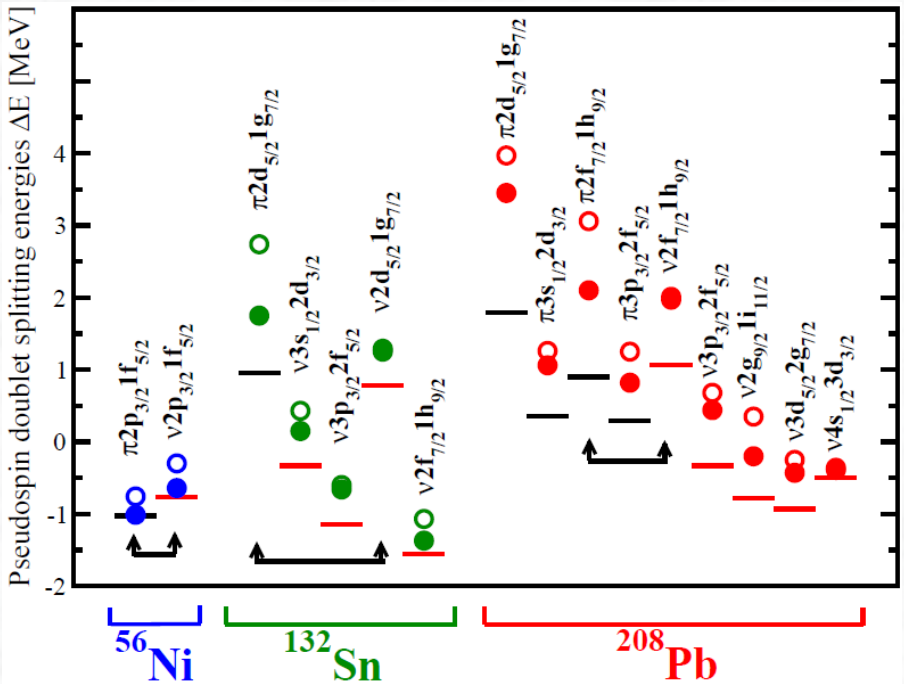
No relativistic kinematics,
HOWEVER

1. **Spin** degrees of freedom as well as **spin-orbit interaction** are obtained in a natural way (no extra parameters). Spin-orbit splittings are properly described.

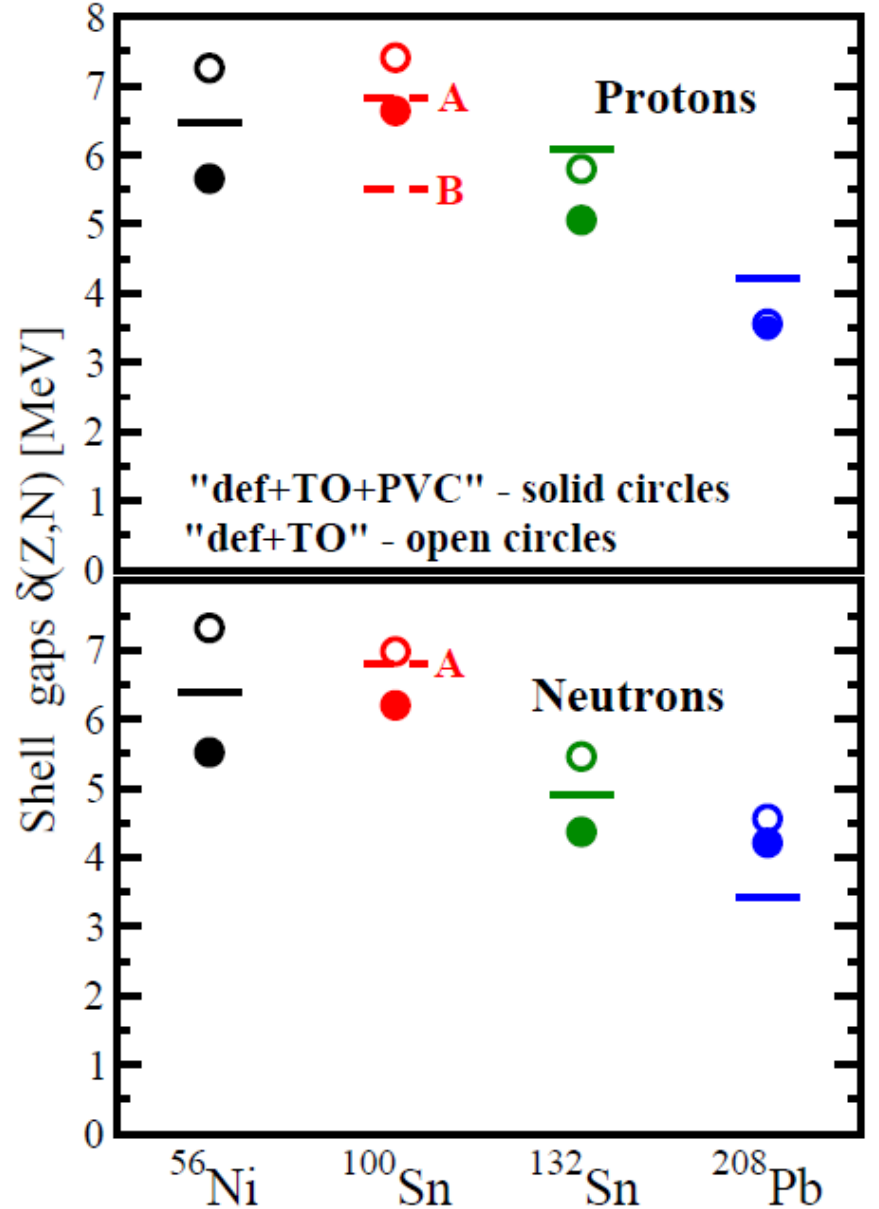


2. **Pseudospin symmetry** is a relativistic effect. J.Ginocchio, PRL 78, 436 (1997)

3. **Time-odd mean fields** are defined via Lorentz covariance → very weak dependence on the RMF parametrization. AA, H. Abusara, PRC 81, 014309 (2010)



The size of proton and neutron shell gaps.



Particle-vibration coupling leads to a shrinkage of the shell gaps. The size of the shell gaps is typically underestimated in the PVC calculations as compared with experiment and overestimated in the mean field calculations.