Spectroscopic quality energy density functionals: problems and solutions.

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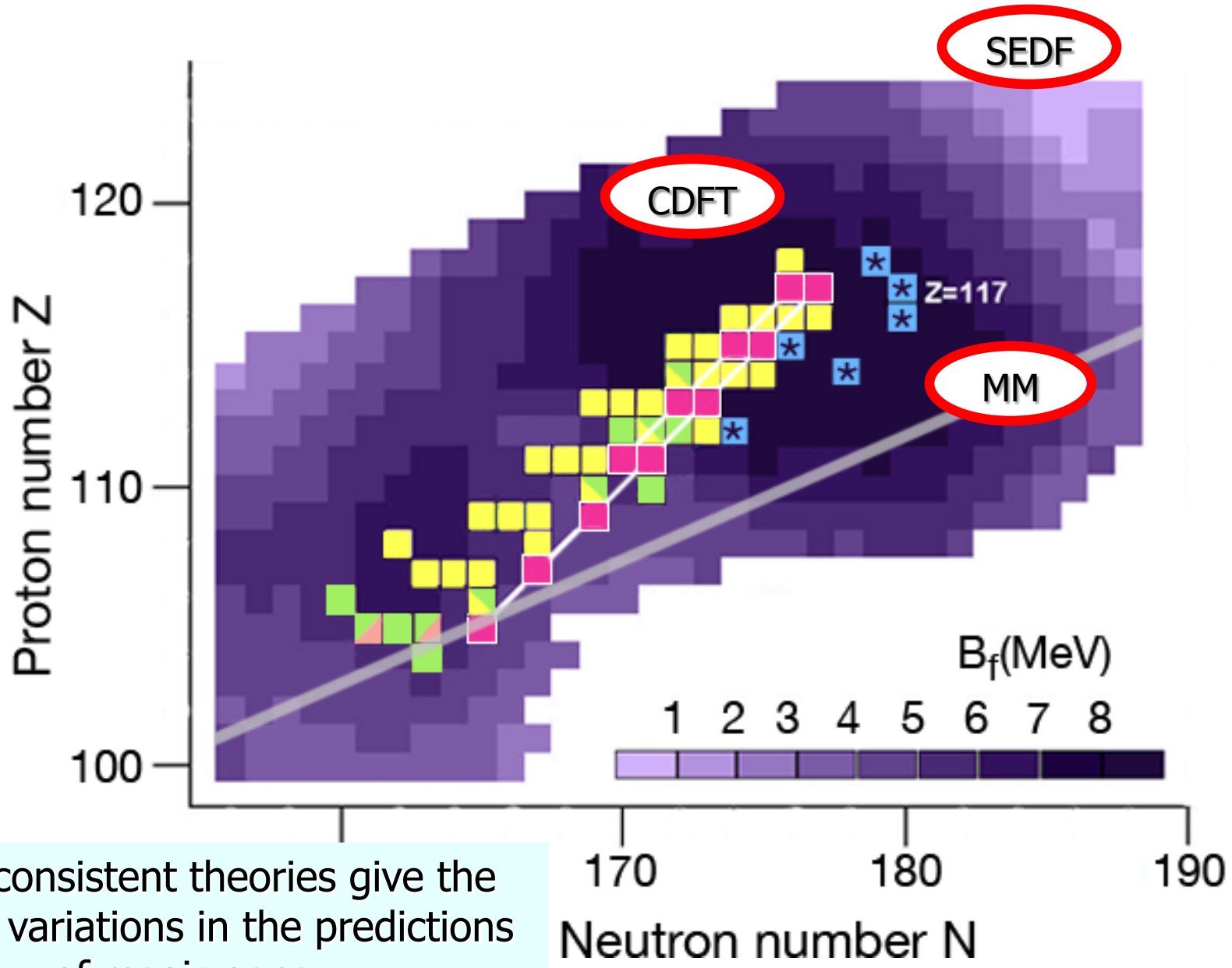
1. **Motivation: understand the possibilities and problems in achieving the spectroscopic quality covariant DFT**
2. **Deformed single(quasi)-particle states: successes and problems**
3. **Single-particle states in spherical nuclei: going beyond mean field by means of particle-vibration coupling.**
4.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

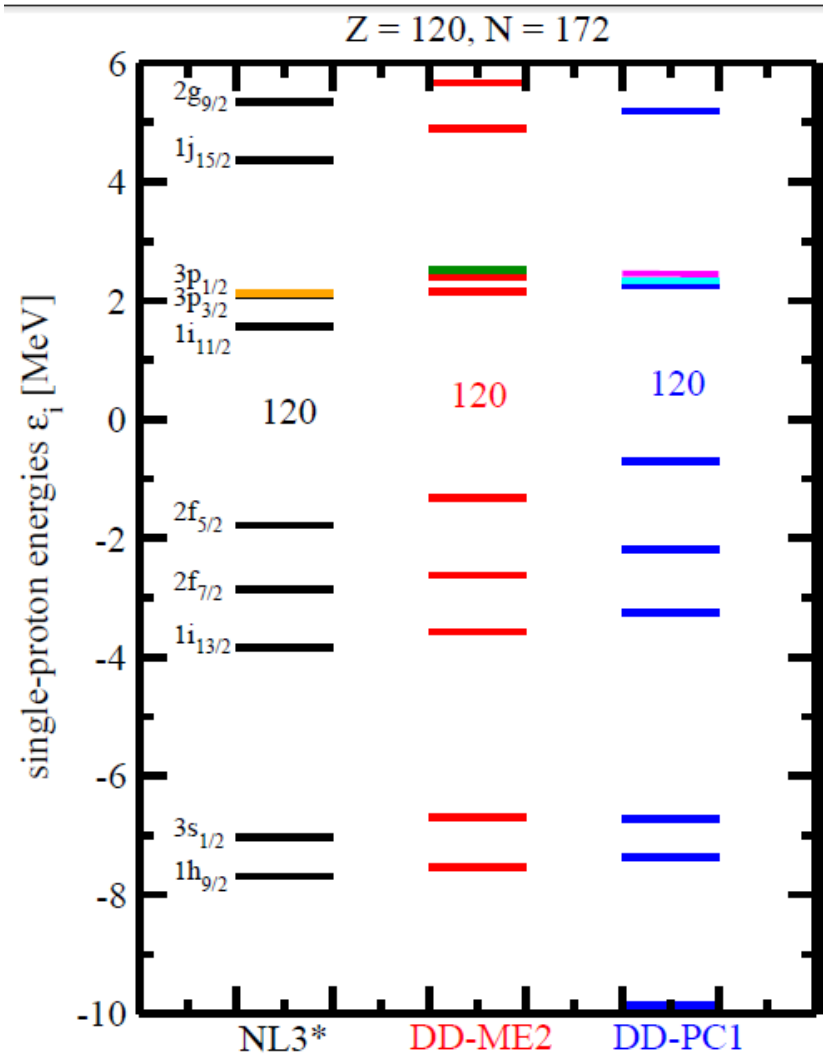
In collaboration with Elena Litvinova, GSI and Sheeren Shawaqfeh (MSU)

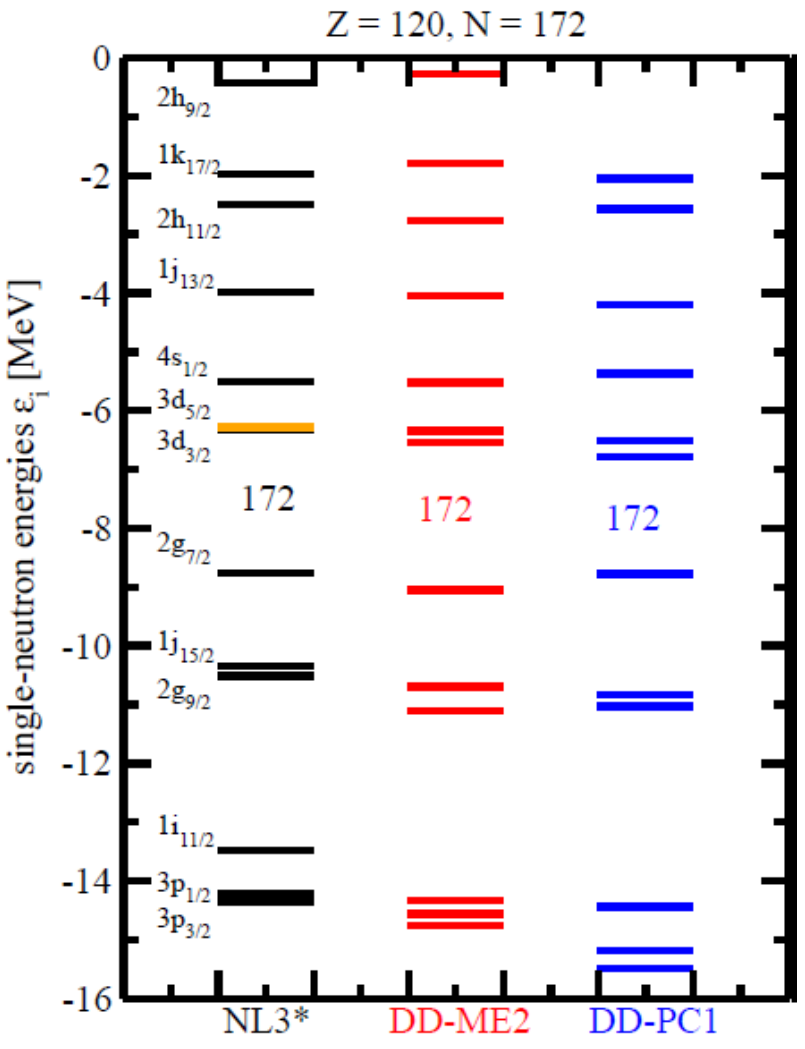


Self-consistent theories give the largest variations in the predictions of magic gaps

at Z=120, 126 and 172, 184

Dependence of proton Z=120 and neutron N=172 gaps on CDFT parametrization

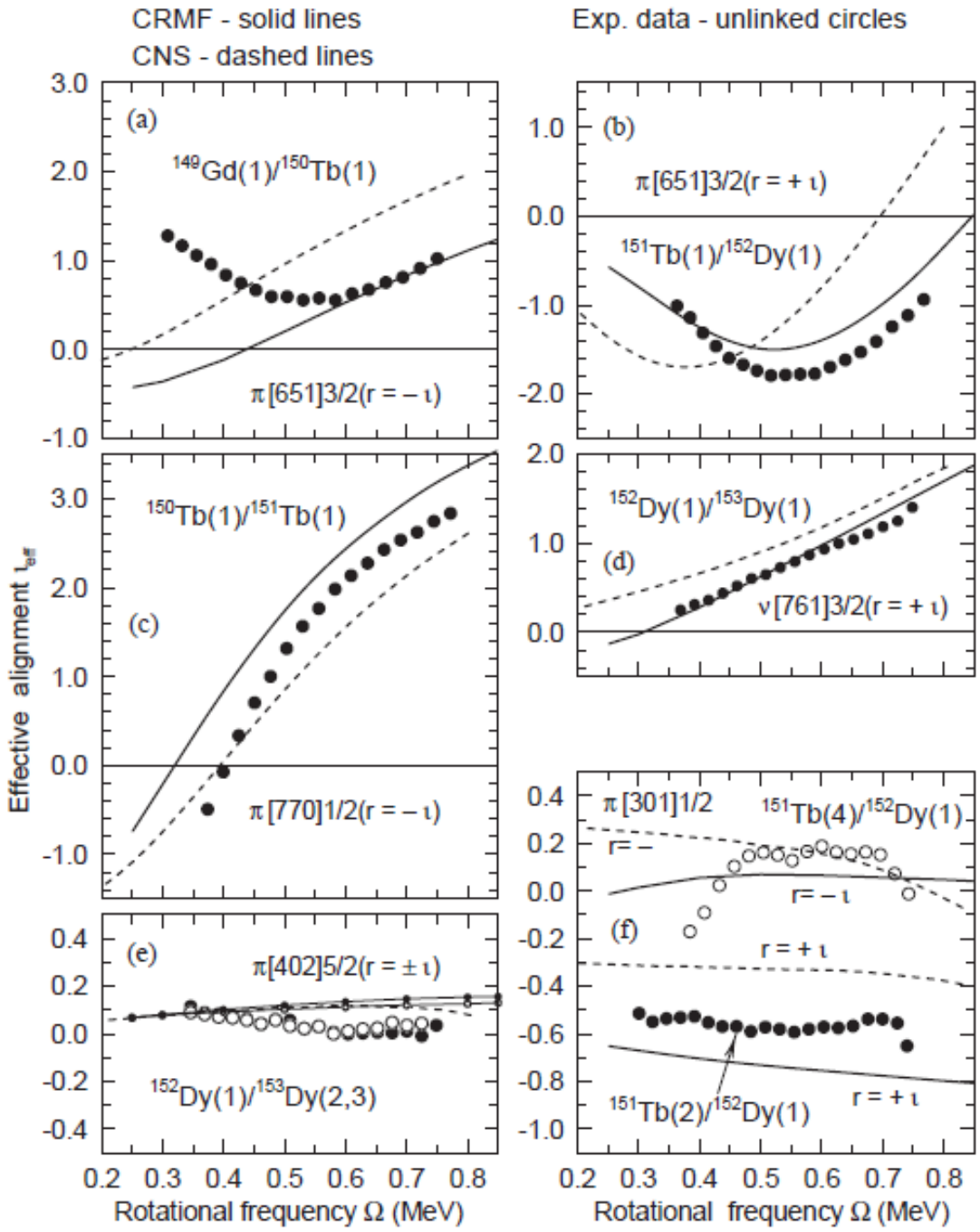




Different aspects of the single-particle motion:

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 states

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



Relative (effective) alignments of two rotational bands

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

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

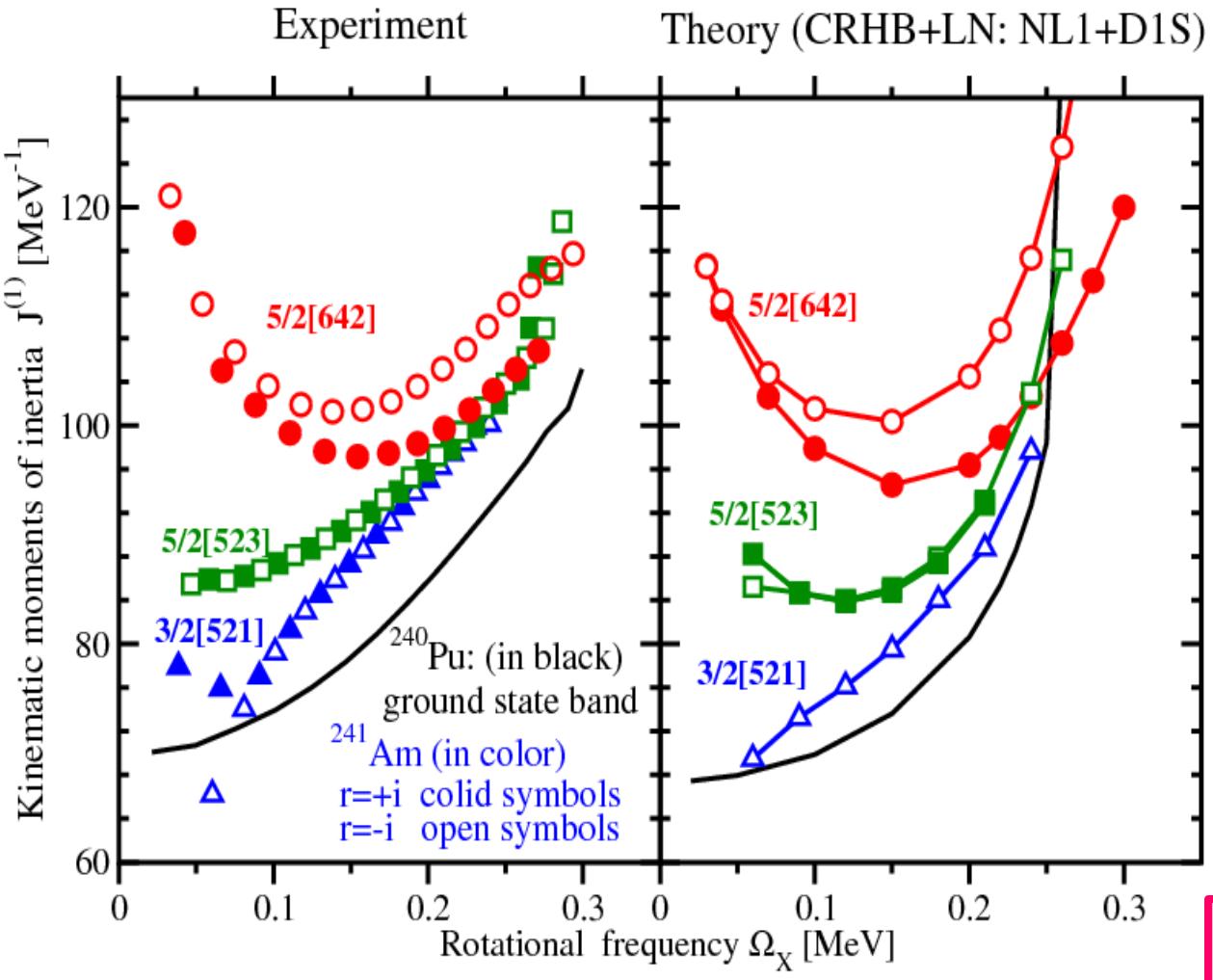
AA, G.A. Lalazissis, P. Ring, Nucl. Phys. A 634 (1998) 395.

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} (eb)	ΔQ_0^{th} (eb)
^{149}Gd(1)	$\nu[770]\frac{1}{2}(r=-\mathrm{i})^{-1}(\pi[651]\frac{3}{2})^{-2}$	−2.5(0.3)	−2.41
^{151}Tb(1)	$\pi[651]\frac{3}{2}(r=+\mathrm{i})^{-1}$	−0.7(0.7)	−1.01
^{151}Dy(1)	$\nu[770]\frac{1}{2}(r=-\mathrm{i})^{-1}$	−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)

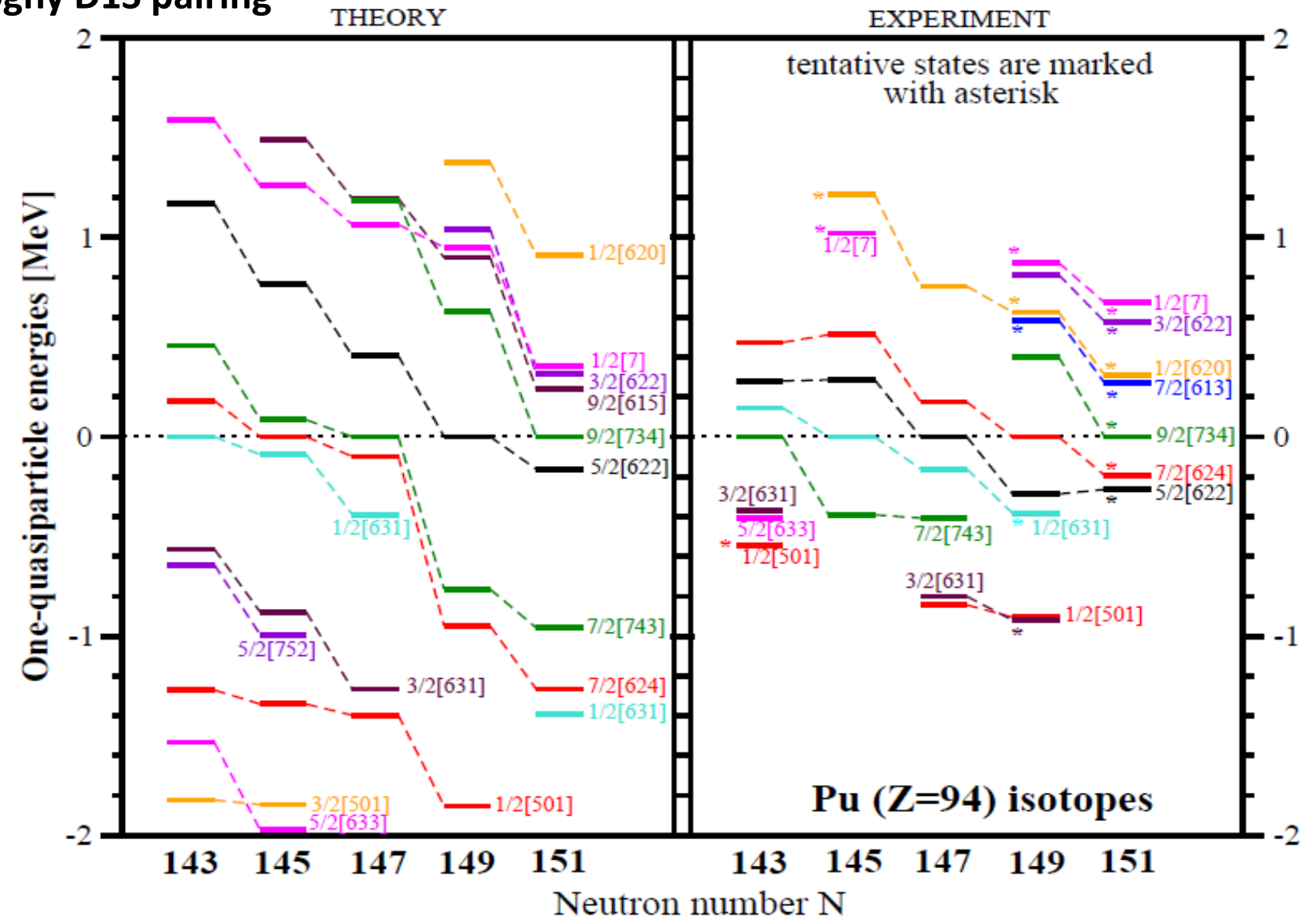
M.Matev et al, PRC 76, 034304 (2007)

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

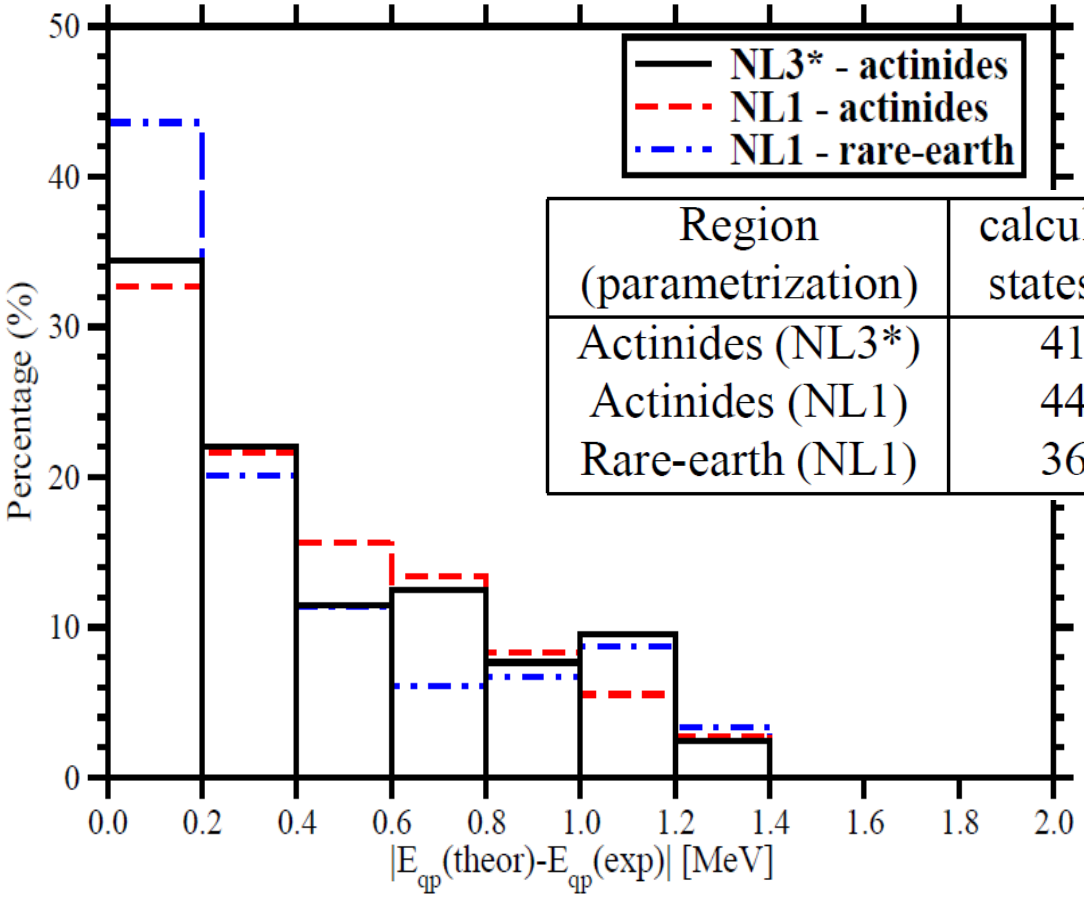
On the contrary, the ΔQ_0 quantity is not uniquely defined in phenomenological models based on the Nilsson or Woods-Saxon potentials

Systematics of one-quasiparticle states in actinides: the CRHB study

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



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



Region (parametrization)	calculated states (#)	compared states (#)	correct ground states (%)
Actinides (NL3*)	415	209	38 %
Actinides (NL1)	444	217	45 %
Rare-earth (NL1)	360	149	48 %

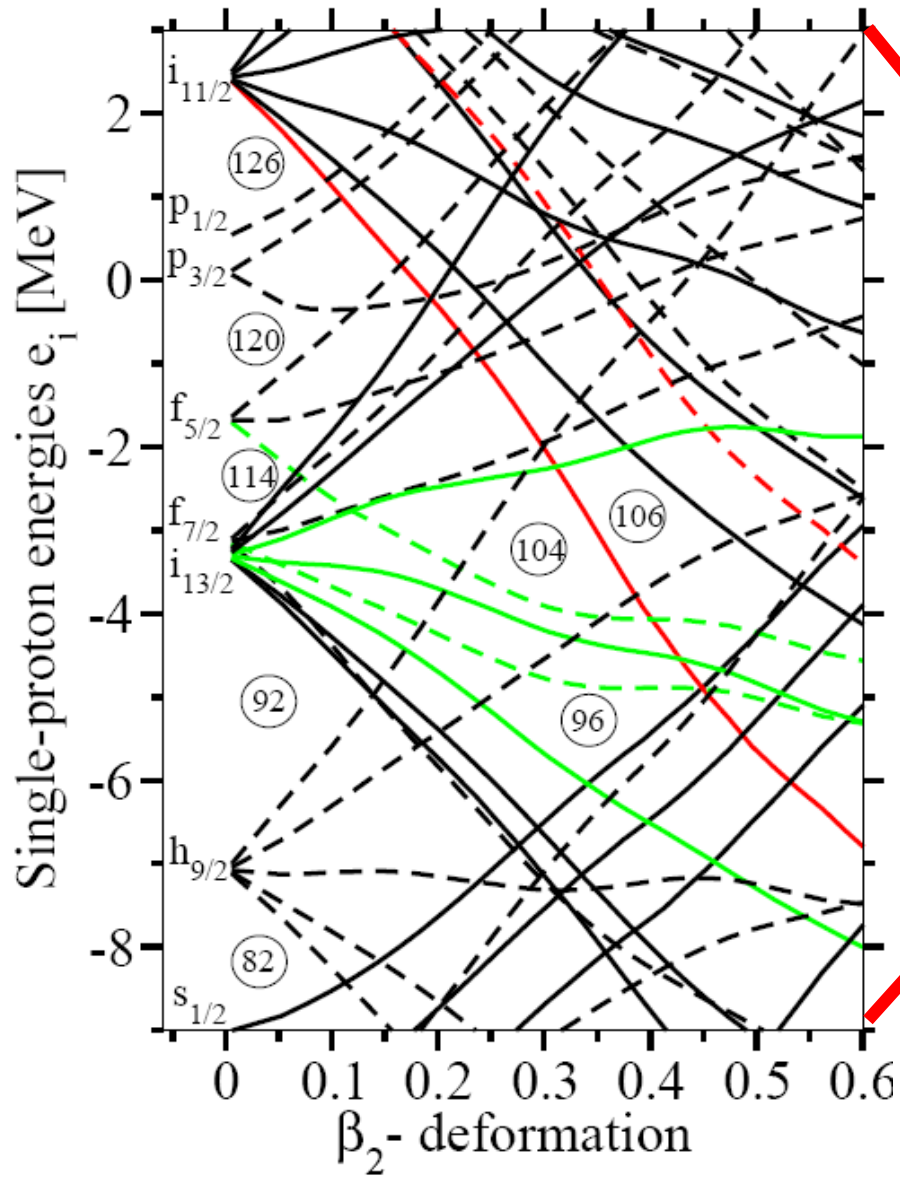
1. ~ 5% of calculated states have triaxial deformation
2. For a given state, the deviation from experiment depends on particle number (consequence of the stretching out of energy scale due to low effective mass)
3. For some of the states, there is persistent deviation from experiment (due to wrong placement of subshell at spherical shape).

Two sources of deviations:

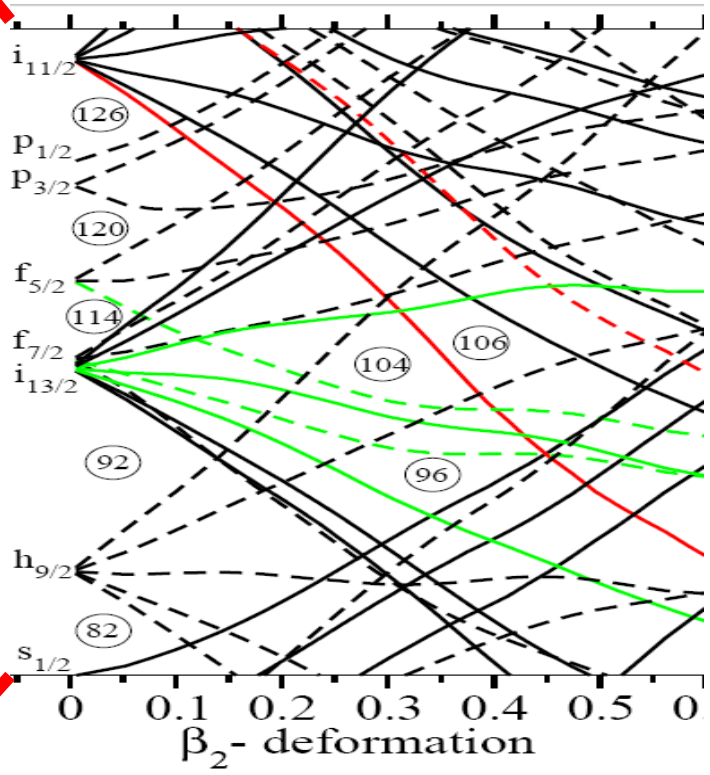
1. Low effective mass (stretching of the energy scale)
2. Wrong relative energies of the states

Illustration of energy scale stretching due to low effective mass

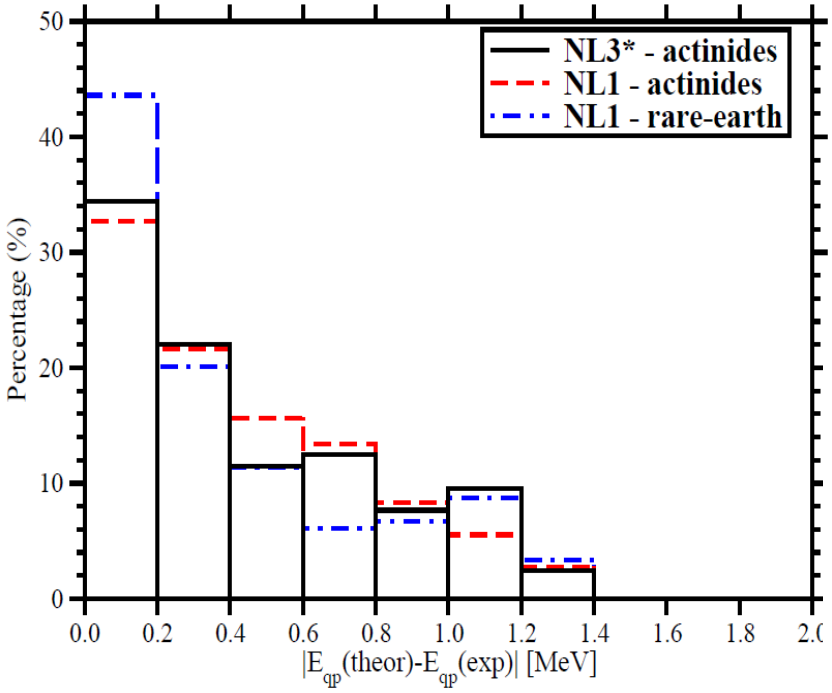
Low effective mass (~0.6)



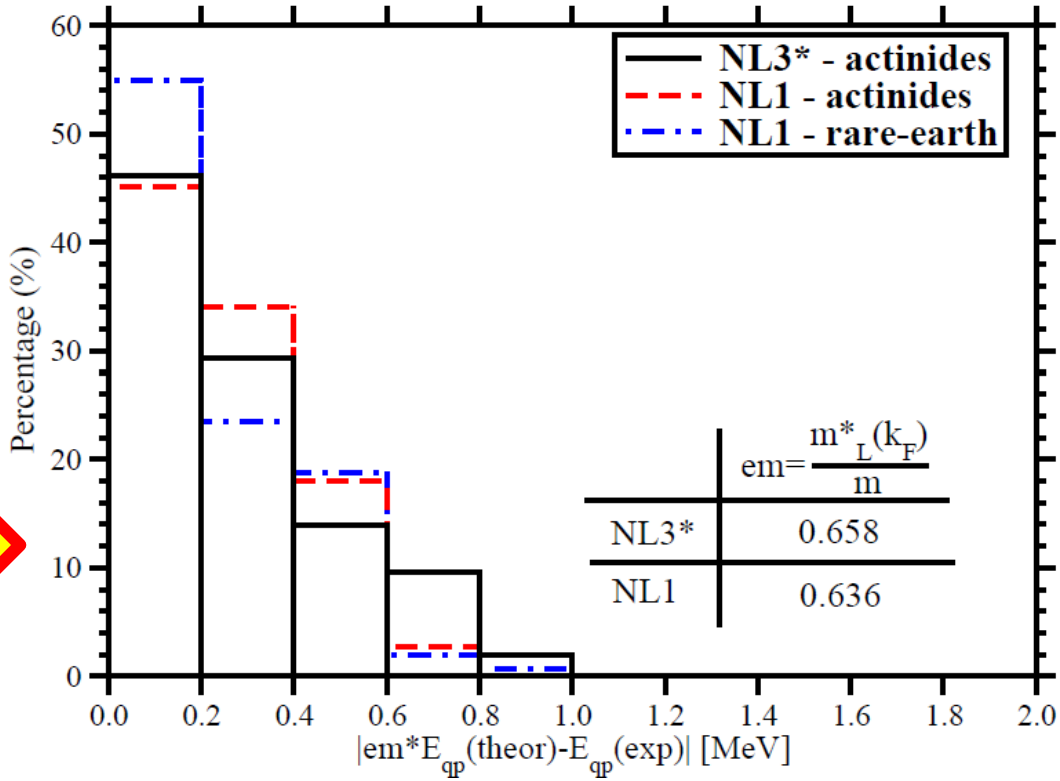
High effective mass (1.0)



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



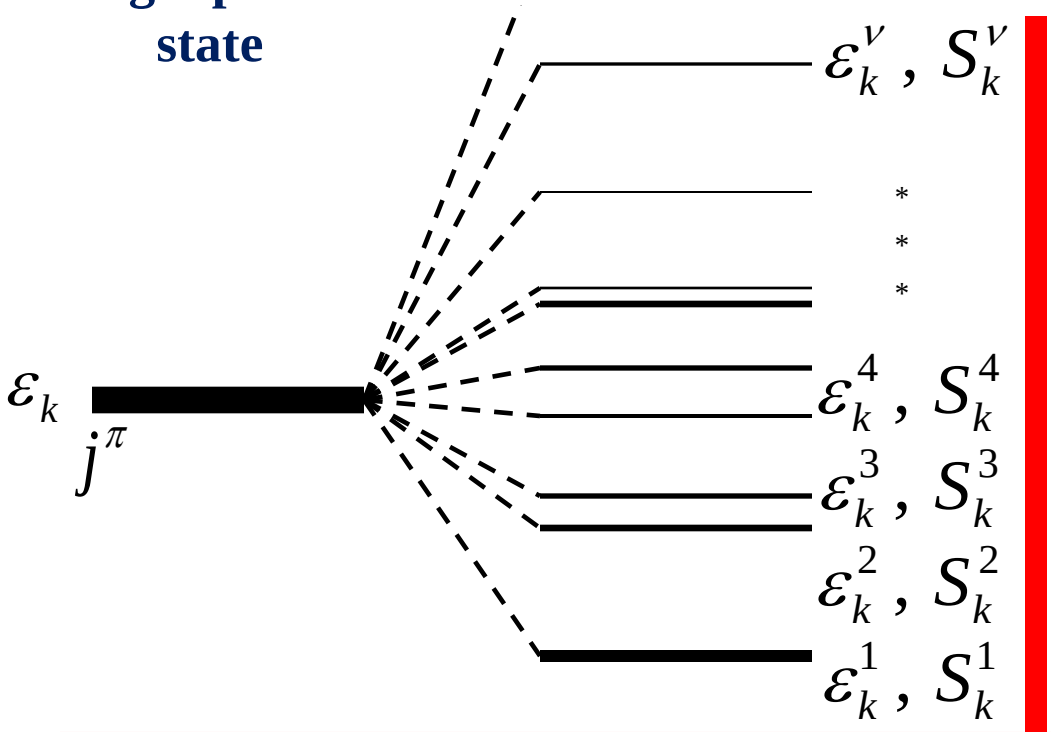
1. 75-80% of the states are described with an accuracy of phenomenological (Nilsson, Woods-Saxon) models
2. The remaining differences are due to incorrect relative energies of the single-particle states

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

Can we obtain "bare" single-particle energies that can be used for comparison with plain DFT?

Mean-field single-particle state

Fragmented levels (due to coupling to phonons)



METHOD 1.

$$\varepsilon_k^{grav} = \left[\sum_\nu S_k^\nu \cdot \varepsilon_k^\nu\right] / \left[\sum_\nu S_k^\nu\right]$$

This energy is associated with a "bare" single-particle energy.

1. Spectroscopic factors depend on reaction and method of extraction: example of spectroscopic factors in ^{209}Bi

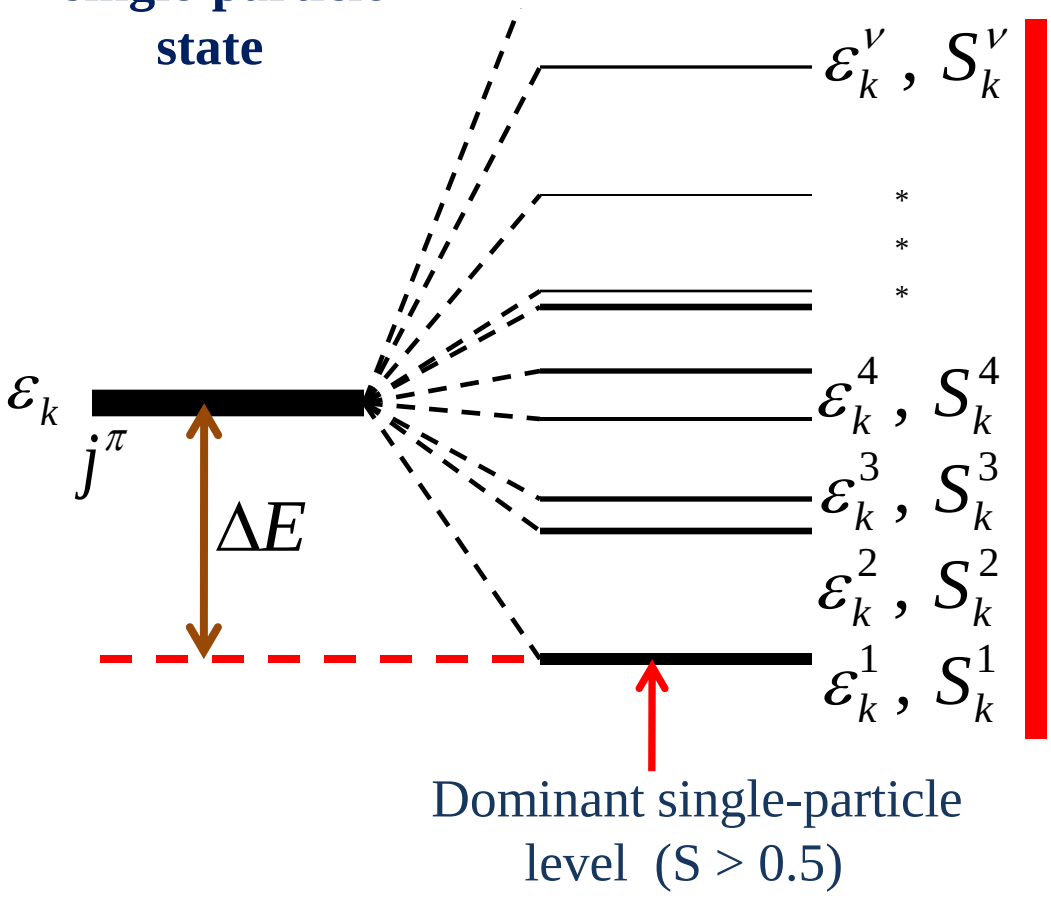
$1h_{9/2}$	1.17	0.80
$2f_{7/2}$	0.78	0.76
$1i_{13/2}$	0.56	0.74
$2f_{5/2}$	0.88	0.57
$3p_{3/2}$	0.67	0.44
$3p_{1/2}$	0.49	0.20
	(^{3}He,d)	(α,t) reactions

2. Spins and parities of fragments are frequently not measured.
3. Some fragments are not observed.
4. Sum rule $\sum_\nu S_k^\nu = 1$ is frequently violated.

Can we obtain "bare" single-particle energies that can be used for comparison with plain DFT?

Mean-field single-particle state

Fragmented levels (due to coupling to phonons)



METHOD 2.

$$\varepsilon_k = \varepsilon_k^1 + \Delta E$$

Model –dependent procedure

Neutrons in ^{208}Pb

	$\Delta\varepsilon = \varepsilon_i - \varepsilon_i^{(0}$	
	[9]	[10]
$3d_{3/2}$	−0.61	−0.32
$4s_{1/2}$	−0.56	−0.21
$3d_{5/2}$	−0.76	−0.43
$1j_{15/2}$	−1.36	−0.55
$2g_{9/2}$	−0.79	−0.40
$1i_{11/2}$	−0.31	−0.37

From P.F. Bortignon et, JPG 37 (2010) 064013

[9] Relativistic PVC, E.Litvinova and P.Ring, PRC C73, 044328 [2006]

[10] Skyrme PVC model, Colo et al, AIP conf. proc. vol. 1165, p. 267

Can we obtain “bare” single-particle energies that can be used for comparison with plain DFT?

it is clear that “bare” single-particle energies cannot be defined with controllable precision in spherical nuclei under study

Two ways to compare with the experimental data

“business as usual”

With mean field calculations

realistic

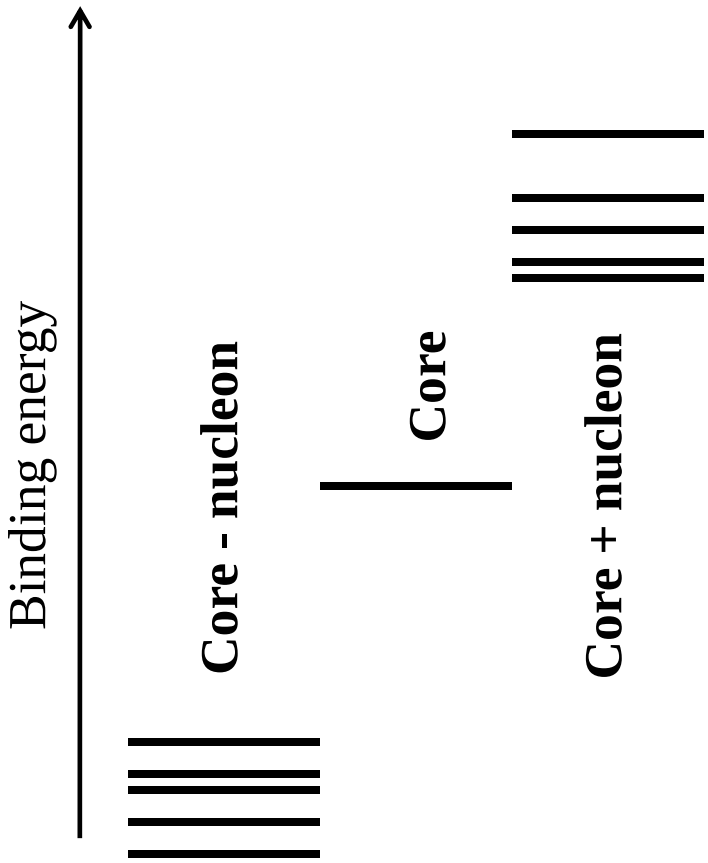
With relativistic particle-vibration coupling calculations

Such an approach allows to see whether

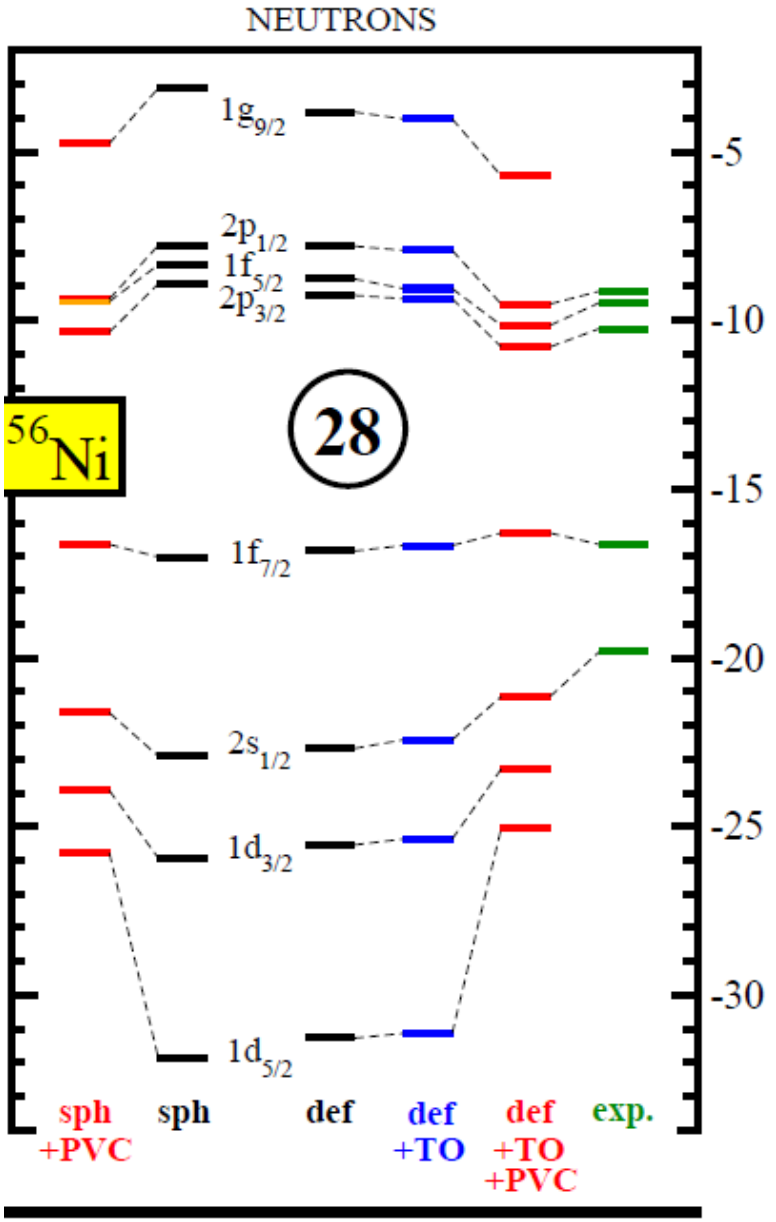
(i) the inclusion of particle-vibration coupling improves the description of specific physical observables and

(ii) the conclusions reached earlier on the mean field level are valid or not.

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)

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

1. The Dirac equation for fermions

$$\hat{h}_D = \boldsymbol{\alpha}(-i\boldsymbol{\nabla} - \boldsymbol{V}(\boldsymbol{r})) \; + \; V_0(\boldsymbol{r}) \; + \; \beta(m + S(\boldsymbol{r}))$$

Magnetic potential

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

⇨ Time-odd mean fields

Klein-Gordon equations for mesons

$$\begin{aligned}
\left\{-\Delta + m_\sigma^2\right\} \sigma(\boldsymbol{r}) &= -g_\sigma[\rho_s^n(\boldsymbol{r}) + \rho_s^p(\boldsymbol{r})] \\
&\quad -g_2\sigma^2(\boldsymbol{r}) - g_3\sigma^3(\boldsymbol{r}) \\
\left\{-\Delta + m_\omega^2\right\} \omega_0(\boldsymbol{r}) &= g_\omega[\rho_v^n(\boldsymbol{r}) + \rho_v^p(\boldsymbol{r})], \\
\left\{-\Delta + m_\omega^2\right\} \boldsymbol{\omega}(\boldsymbol{r}) &= g_\omega[\boldsymbol{j}^n(\boldsymbol{r}) + \boldsymbol{j}^p(\boldsymbol{r})]
\end{aligned}$$

2. Relativistic particle-vibration coupling (PVC) model

The equation of the one-nucleon motion has the form (in single-particle Green functions)

$$\left(\varepsilon - h^D - \beta\,\Sigma_s^e(\varepsilon) - \Sigma_0^e(\varepsilon)\right) G(\varepsilon) = 1$$

$$\sum_l \left\{(\varepsilon - \varepsilon_k)\delta_{kl} - \Sigma_{kl}^e(\varepsilon)\right\} G_{lk'}(\varepsilon) = \delta_{kk'}$$

particle-phonon coupling model:

energy-dependent part of the mass operator is a convolution of the particle-phonon coupling amplitude Γ and the exact single-particle Green's function

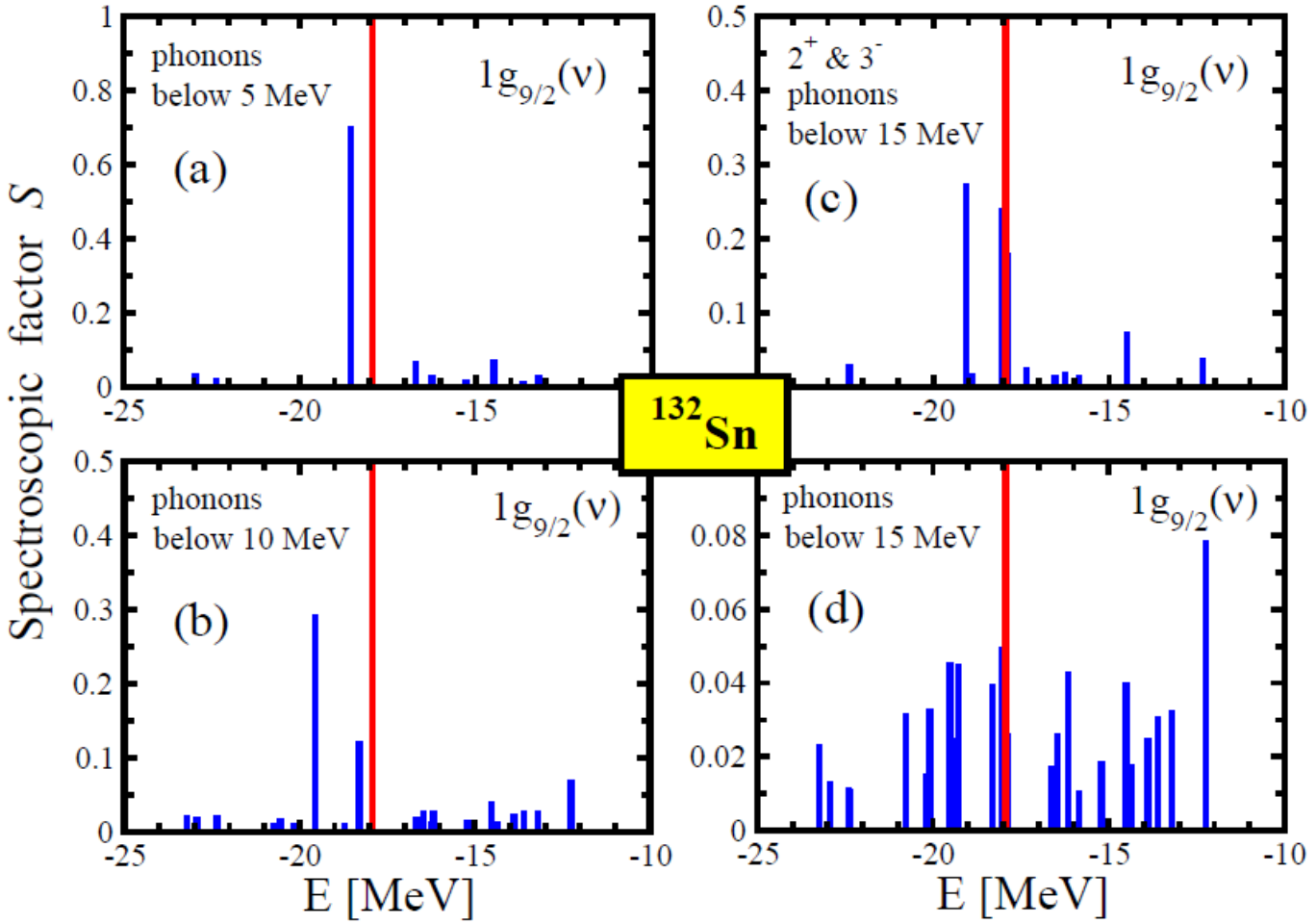
$$\Sigma_{kl}^e(\varepsilon) = \sum_{k'l'} \int_{-\infty}^{+\infty} \frac{d\omega}{2\pi i} \Gamma_{kl'lk'}(\omega) G_{k'l'}(\varepsilon + \omega)$$

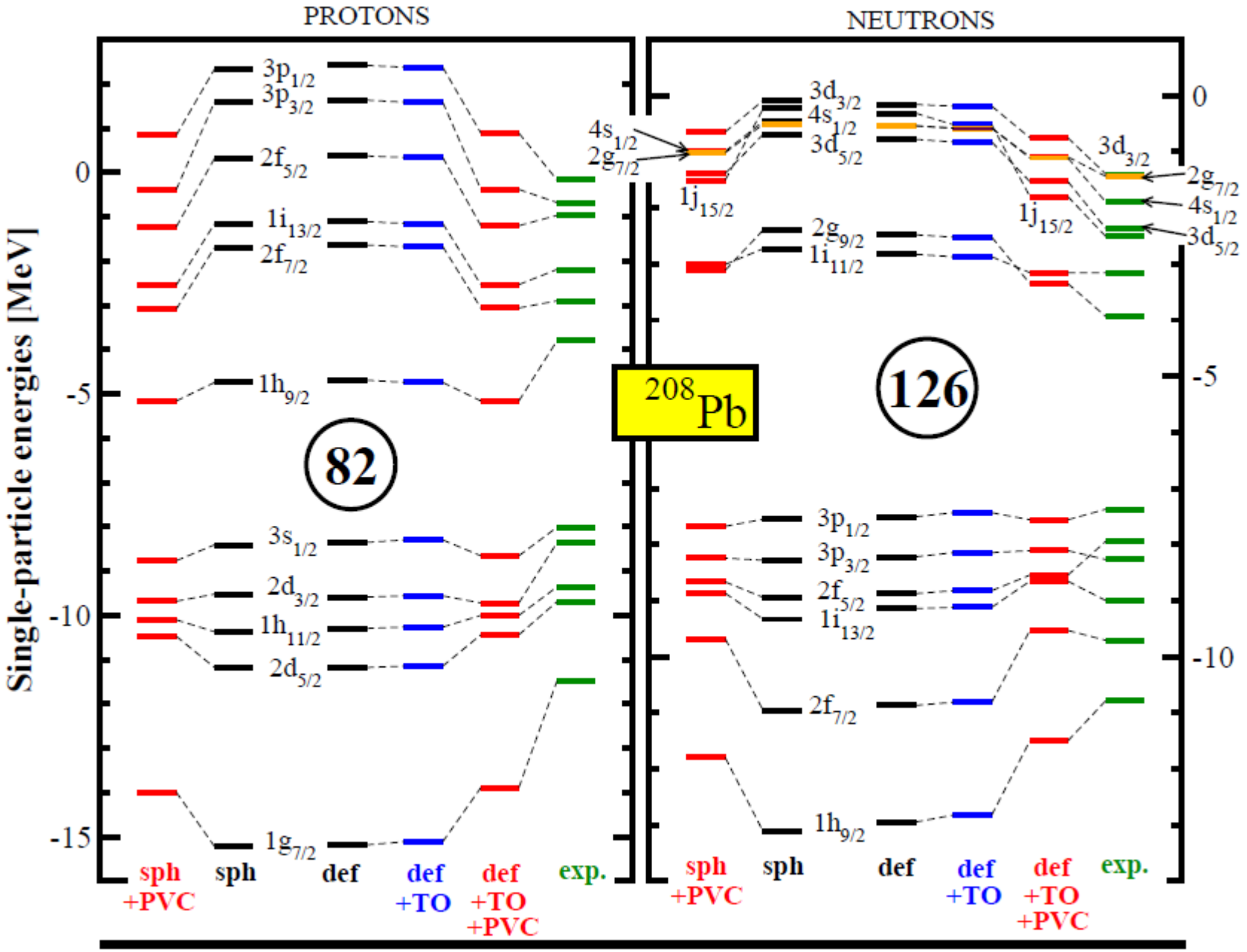
depends on phonon vertexes $\gamma_{kl}^{\mu} = \sum_{k'l'} V_{kl'lk'}\,\delta\rho_{k'l'}^{\mu}$

$V_{kl'lk'}$ - the relativistic matrix element of the residual interaction and $\delta\rho$ is the transition density. We use the linearized version of the model which assumes that $\delta\rho$ is not influenced by the particle-phonon coupling and can be computed within relativistic RPA.

Cut-off of phonon basis in the RRPA calculations

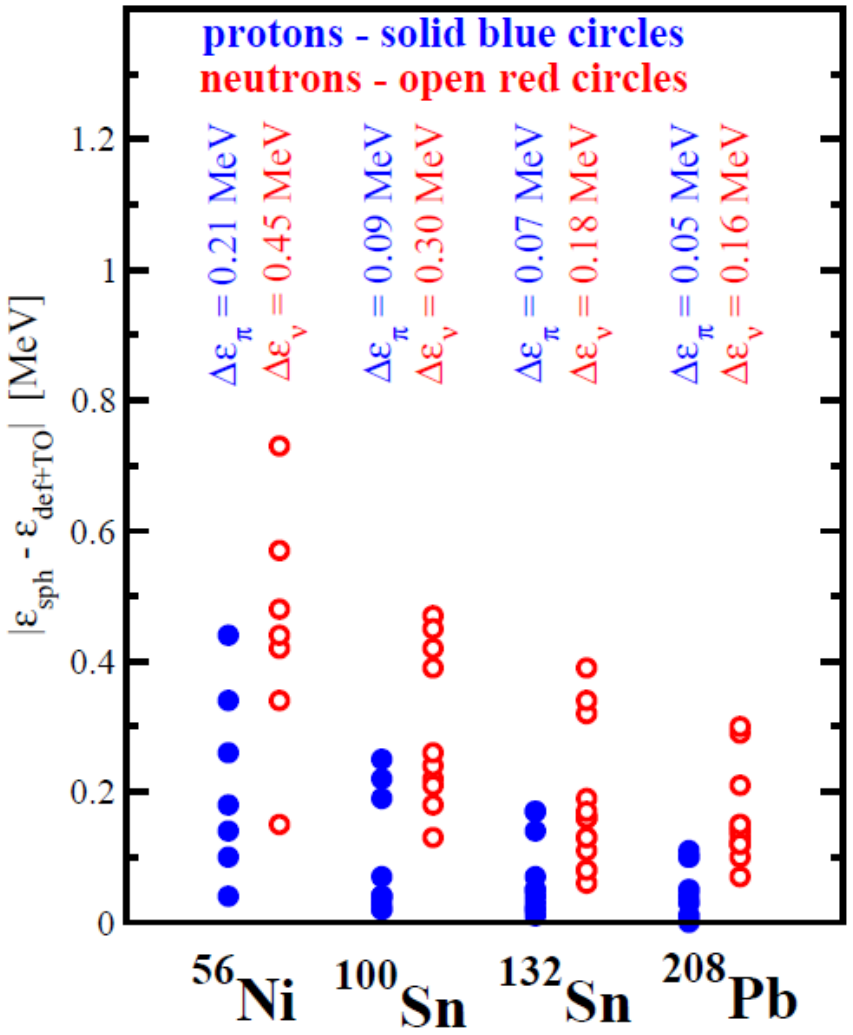
Phonons of the multipolarities 2^+, 3^-, 4^+, 5^-, 6^+ with energies below 15 MeV are included in the model space of the PVC calculations. The addition of phonon modes with energies above 15 MeV does not affect the results. The phonon energies and their coupling vertices have been computed within the self-consistent RRPA.





Detailed calculations are also performed for ^{100,132}Sn and ^{56}Ni

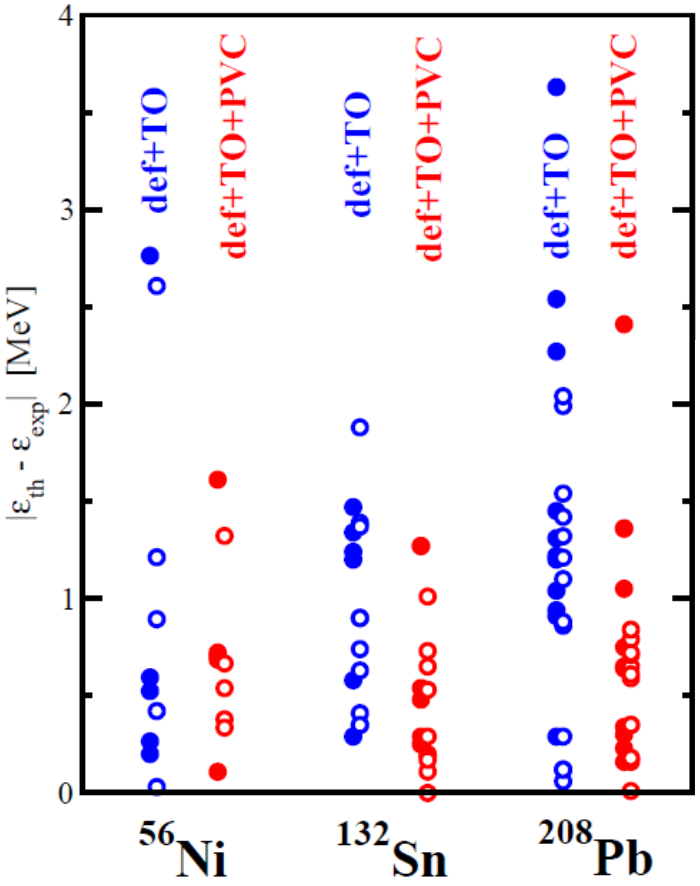
Combined polarization effects due to deformation and time-odd mean fields



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.

The deviations of calculated energies of the single-particle states from experimental ones



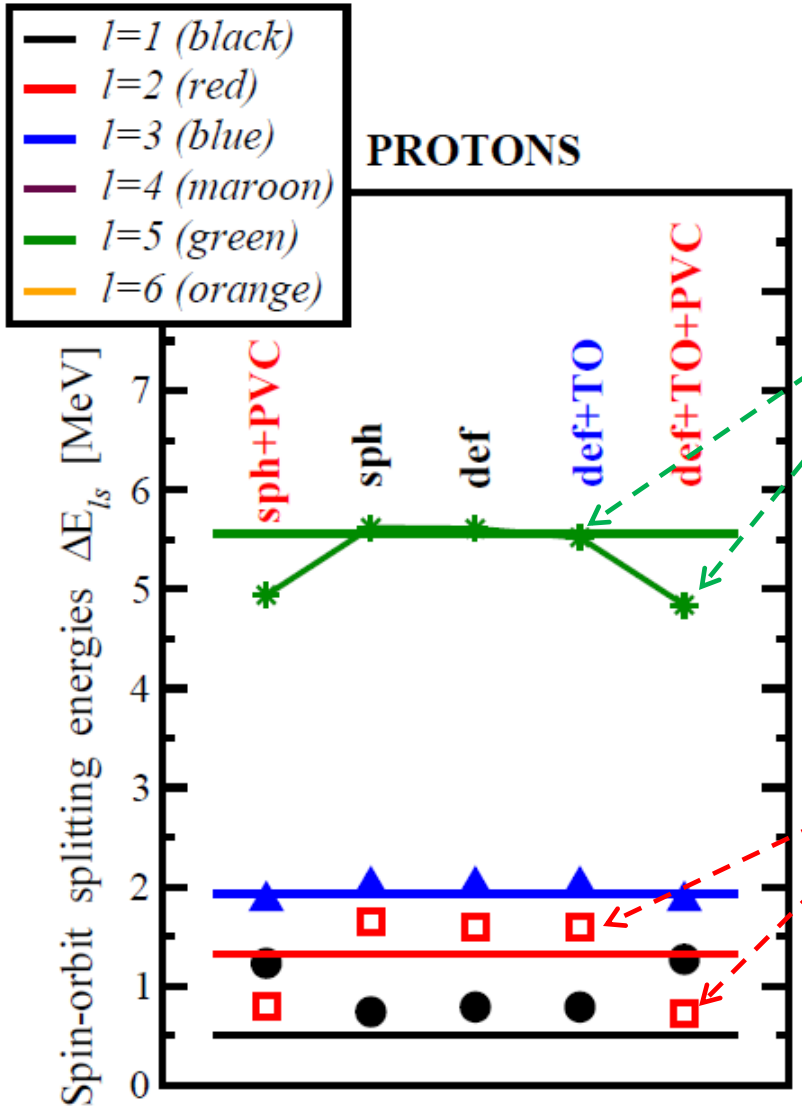
The results for proton and neutron states are given by solid and open circles.

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.

$$\Delta\epsilon = \frac{\sum_{i=1}^{N} |\epsilon_i^{th} - \epsilon_i^{exp}|}{N}$$

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

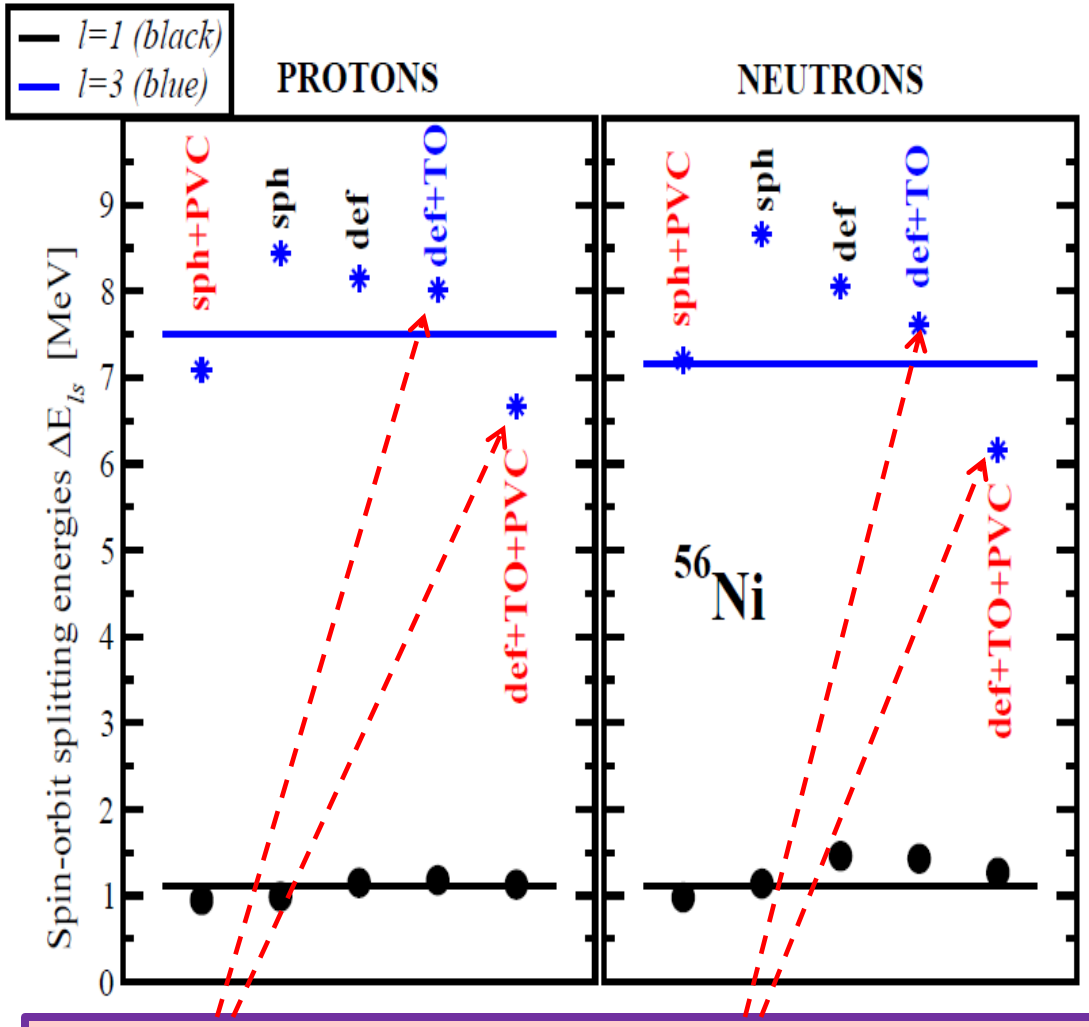
The impact of particle-vibration coupling on spin-orbit splittings.



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 danger of the fit of the model parameters on the DFT level to the single-particle energies

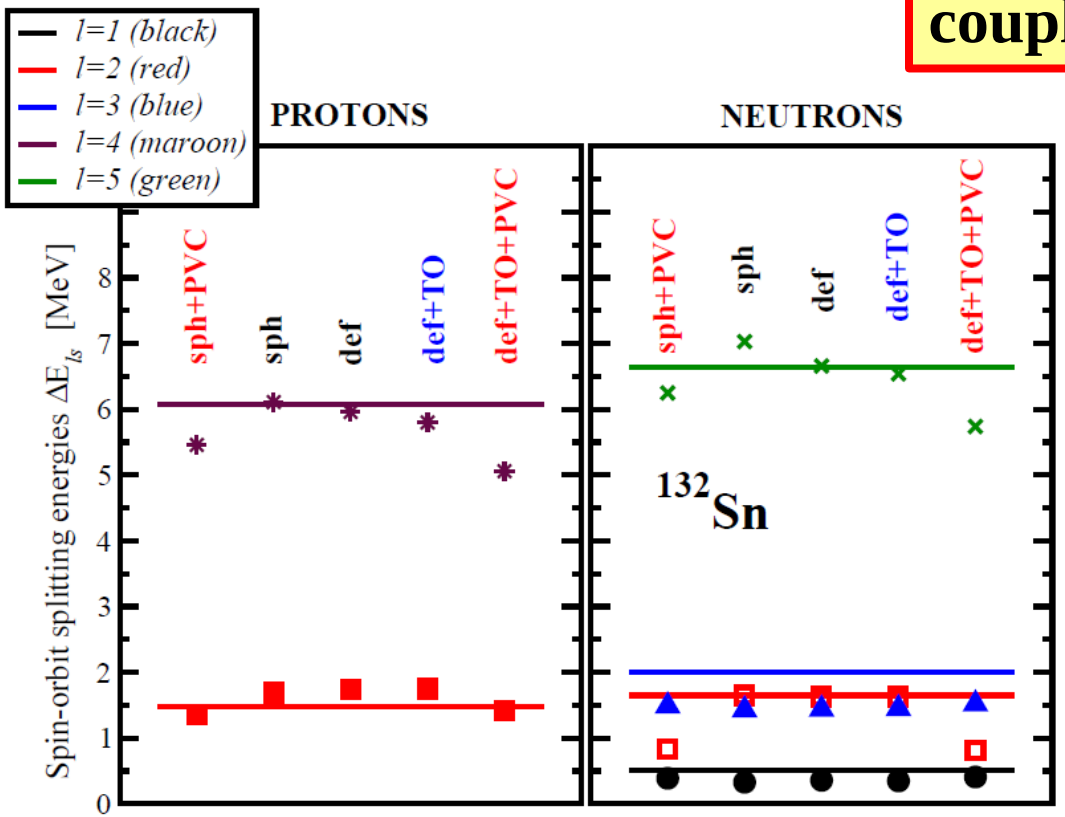


M. Zalewski et al,
PRC 80, 064307 (2009) and
PRC 77, 024316 (2008).
Skyrme DFT

A direct fit of the isoscalar spin-orbit (SO) and both isoscalar and isovector tensor coupling constants to **the *f5/2-f7/2 SO* splittings** in 40Ca, **56Ni**, and 48Ca nuclei requires a drastic reduction of the isoscalar SO strength and strong attractive tensor coupling constants.

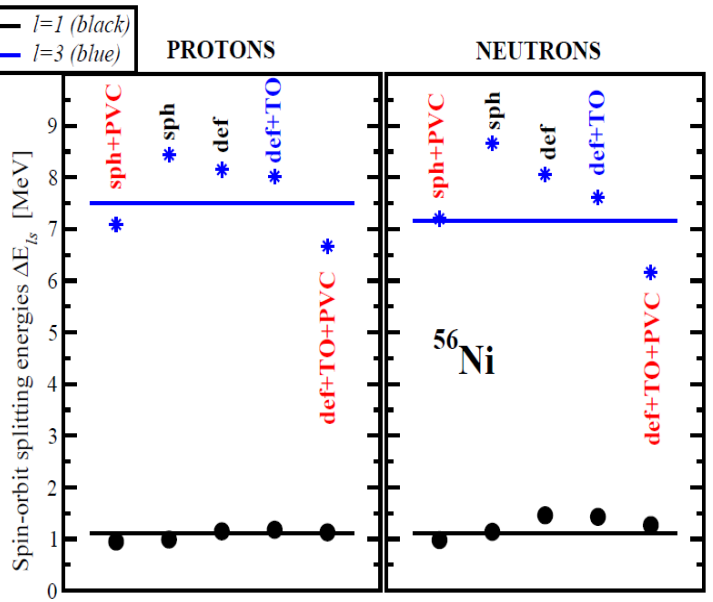
The PVC changes SO splitting in the f5/2-f7/2 doublet by 1.5 MeV

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

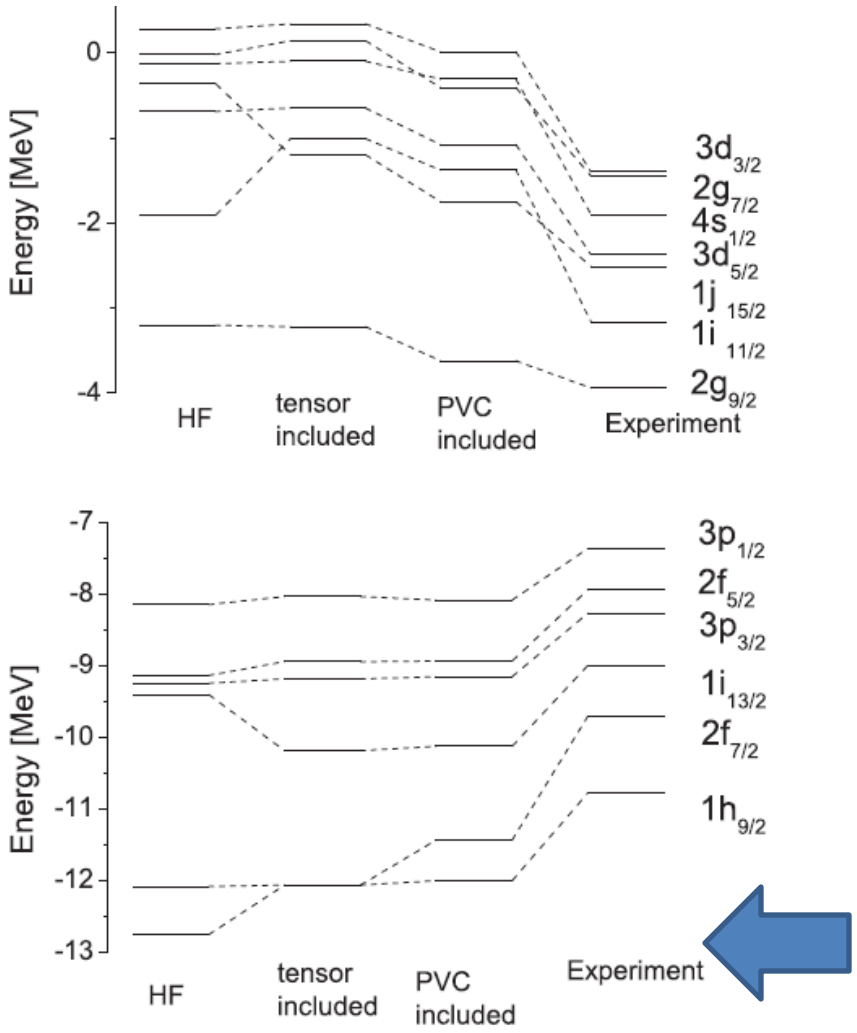


The inclusion of particle-vibration coupling **decreases** the accuracy of the description of spin-orbit splittings.

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 spin-orbit splittings: the comparison with Skyrme PVC for neutron subsystem of ^{208}Pb



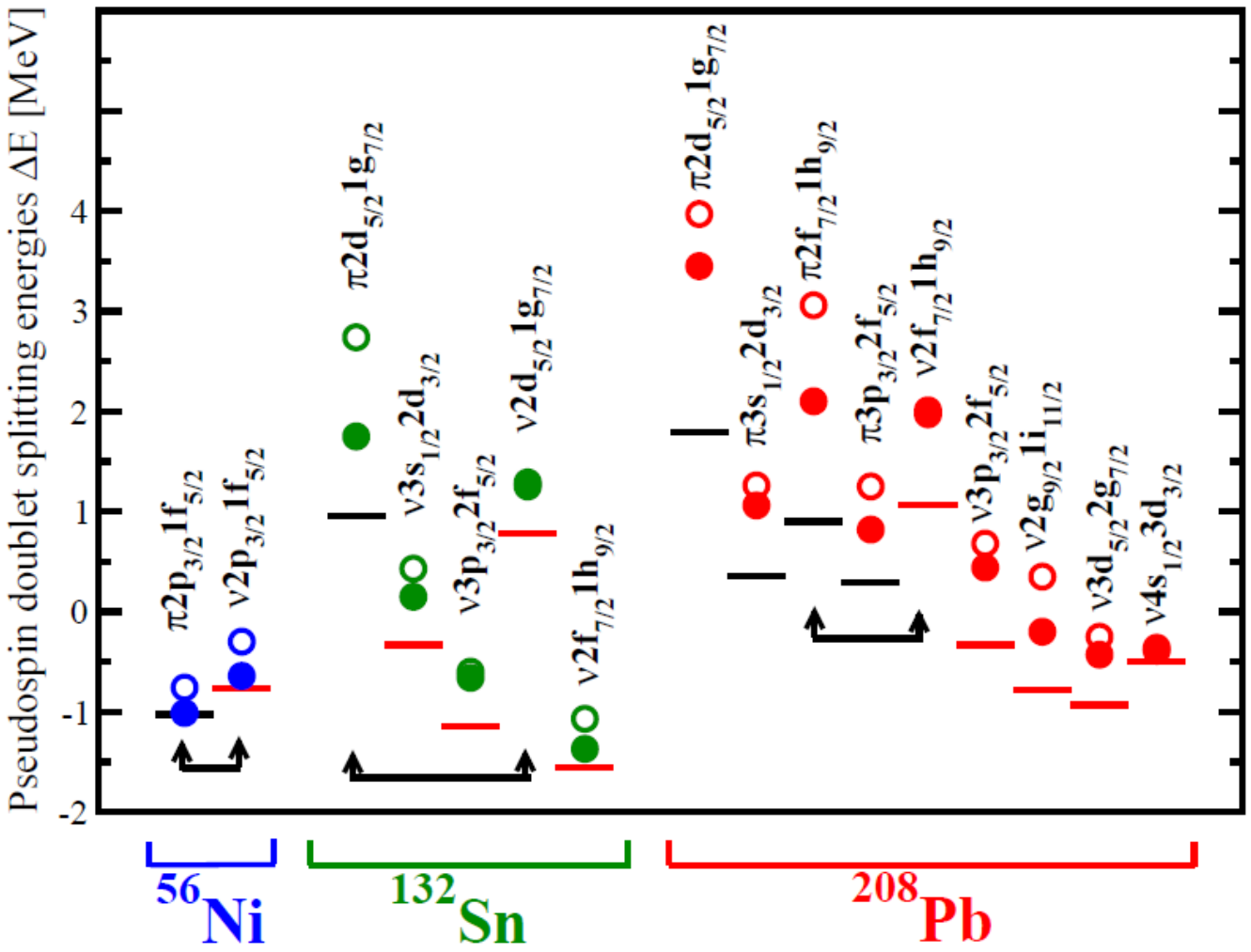
The change of spin-orbit splitting induced by PVC

doublet	Covariant PVC	Skyrme PVC
$3d_{5/2}$-$3d_{3/2}$	+0.14	+0.13
$3p_{3/2}$-$3p_{1/2}$	-0.16	0.00
$2g_{9/2}$-$2g_{7/2}$	+0.32	-0.13
$2f_{7/2}$-$2f_{5/2}$	-1.0	-0.61
$1i_{13/2}$-$1i_{11/2}$	-0.75	-0.40

Skyrme PVC
G.Colo et al, PRC 82, 064307 (2010)

The impact of particle-vibration coupling on pseudospin doublets.

$$\Delta E = E_{n_r,l,j=l+1/2} - E_{(n_r-1),(l+2),j=l+3/2}$$



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 states is insufficient due to low effective mass and wrong relative energies of some subshells at spherical shape.

For example, this will affect the landscapes of flat potential energies surfaces (PES). This can lead to "virtual" results especially in the case of chiral rotation which involves 2-quasiparticle states (the deviation of their energies from experiment can be twice of the ones for 1-qp states) and flat PES characterized by only small barrier (~ 50 keV) between two chiral minima.

3. Particle-vibration coupling (with polarizations accounted)
   - substantially improves the description of the single-particle states in ^{132}Sn and ^{208}Pb.
   - decreases the accuracy of the description of spin-orbit splittings
   - substantially improves the description of splitting energies in pseudospin doublets

Conclusions:

4. **The improvement of spectroscopic properties (single-particle energies) on the DFT level has its own limits.**
It ultimately requires the accounting of particle-vibration coupling.
Ignoring particle-vibration coupling and treating experimental levels as pure single-particle in the fit can lead to wrong conclusions about the energy density functional.

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Statistical analysis of deformed one-quasiparticle states
AA and S.Shawaqfeh, submitted to PLB