



HPCI project field 5
“The origin of matter and the universe”

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Large-scale shell-model calculations of nuclei around $N=80$



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NUCLEAR STUDY

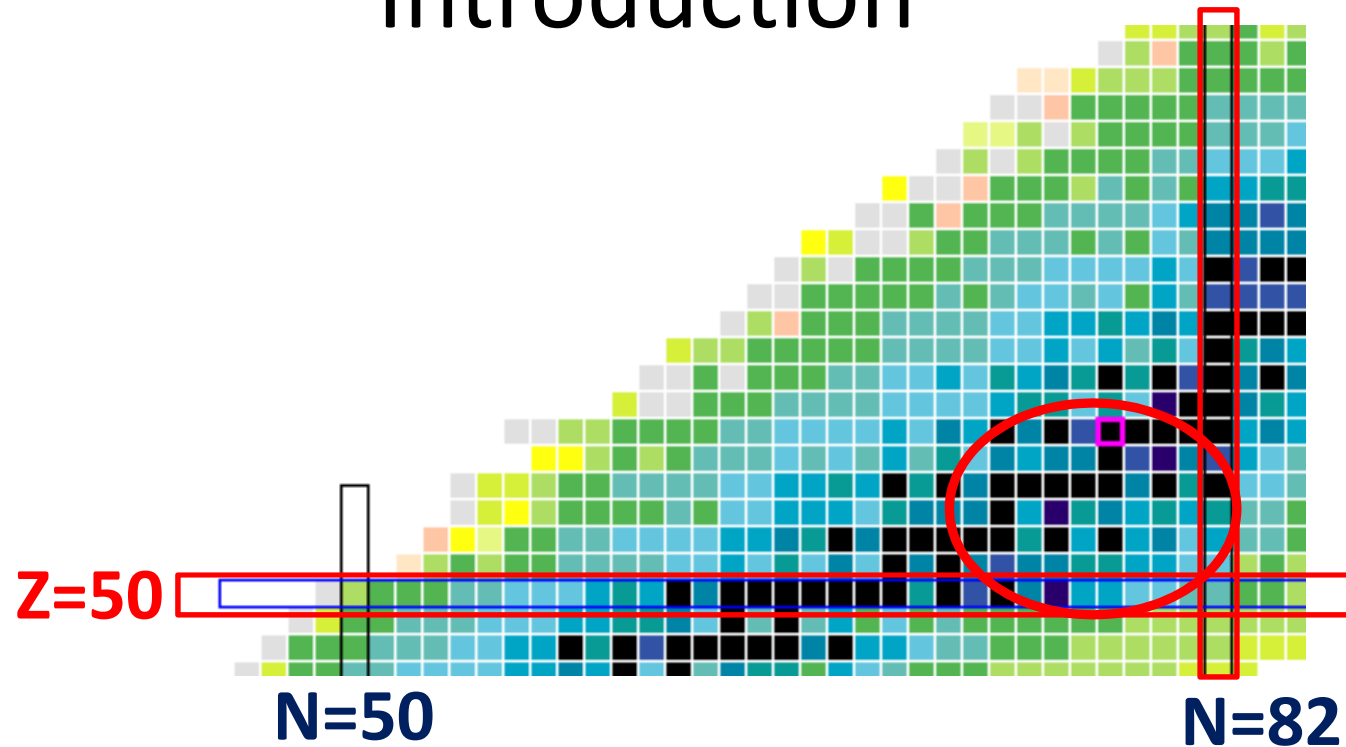
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Introduction



- Quadrupole collectivity, triaxial deformation, mixed symmetry state, E(5) critical point symmetry, scissors mode, isomers, ...
- Shell-model study is a challenge in this region due to huge configuration space
 - E. Teruya *et al.*, PRC 92, 034320 (2015), C. Qi *et al.*, PRC 86 044323 (2014), C. Bianco *et al.*, PRC 85, 034332 (2012), K. Sieja *et al.* PRC 80, 054311 (2009), B. A. Brown *et al.*, PRC 71, 044317 (2005) ...

Two tools for shell-model calculations

3×10^{14} M-scheme dim. for ^{140}Ho

- Large-scale shell model calculations (LSSM)
 - conventional Lanczos method in parallel computation
 - Max: $\sim O(10^{10})$ M-scheme dimension
- advanced Monte Carlo shell model (MCSM)
 - a tool to go beyond Lanczos limit
 - variation after superposition of J -projected Slater determinants
 - extrapolation utilizing energy variance

$$|\Psi^{IM\pi}(N_b)\rangle = \sum_{d=1}^{N_b} f^{(d)} \sum_{K=-I}^I g_K^{(d)} \hat{P}^\pi \hat{P}_{MK}^I |\varphi(D^{(d)})\rangle$$

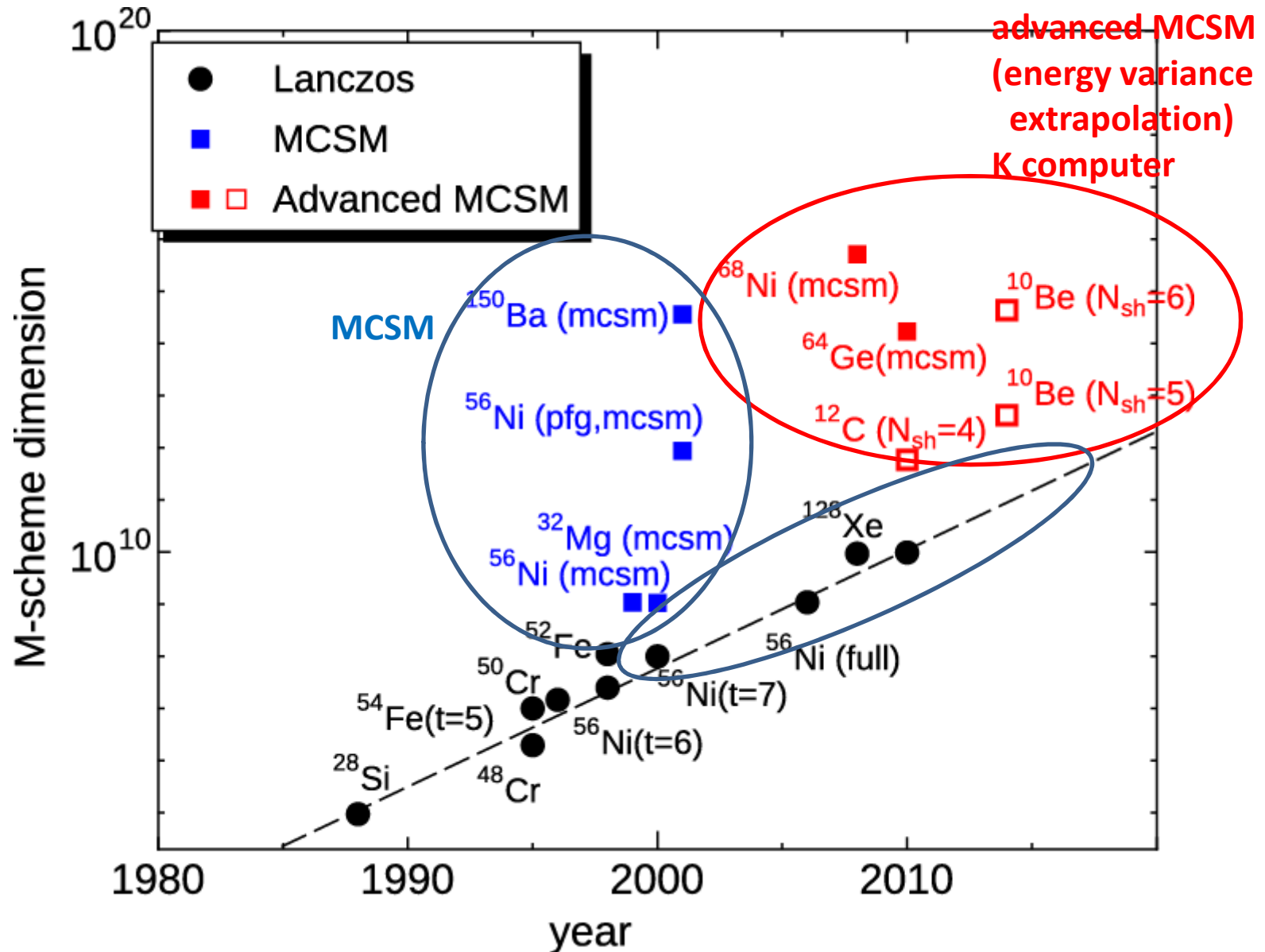
MCSM basis dimension ≈ 100

The diagram illustrates the components of the MCSM basis dimension. A blue bracket under the equation groups the terms into three parts:

- superposition**: Corresponds to the sum over d from 1 to N_b .
- projection onto good quantum numbers**: Corresponds to the sum over K from $-I$ to I .
- optimized Slater determinant**: Corresponds to the Slater determinant $|\varphi(D^{(d)})\rangle$.

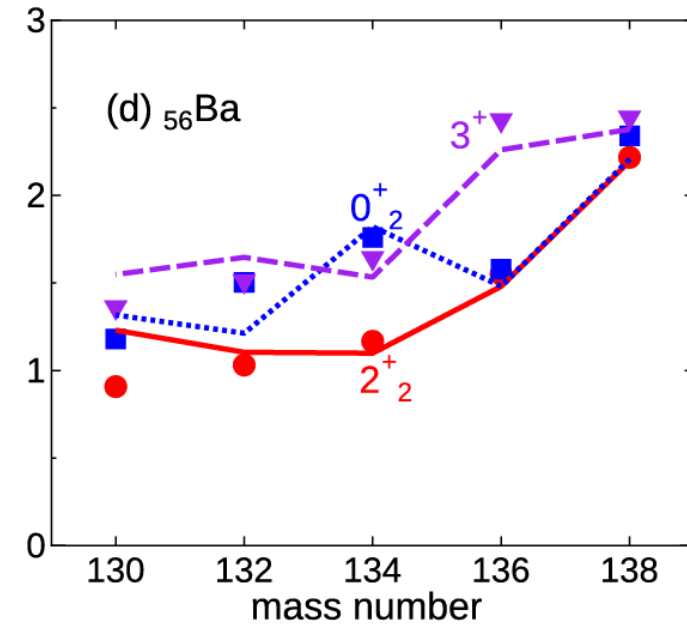
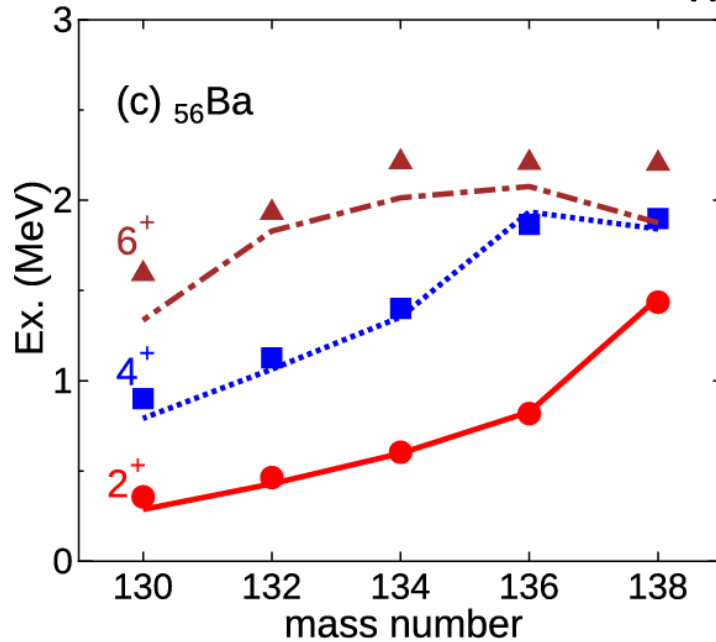
 A blue arrow points from the text 'MCSM basis dimension ≈ 100 ' to the N_b term in the equation.

M-scheme dimension vs. year

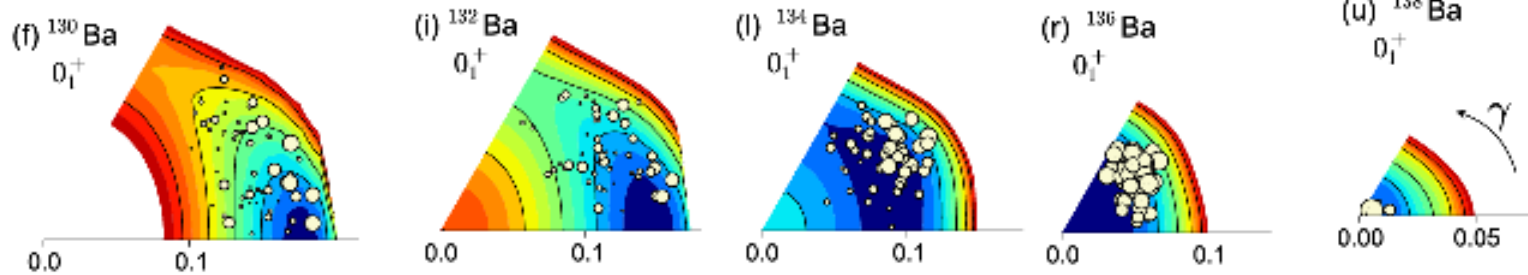


symbol: exp.
line : theory

Shape evolution of Ba isotopes with Monte Carlo Shell Model and P+QQ int.



model space:
 $50 < N, Z < 82$



Monte Carlo Shell Model wave function

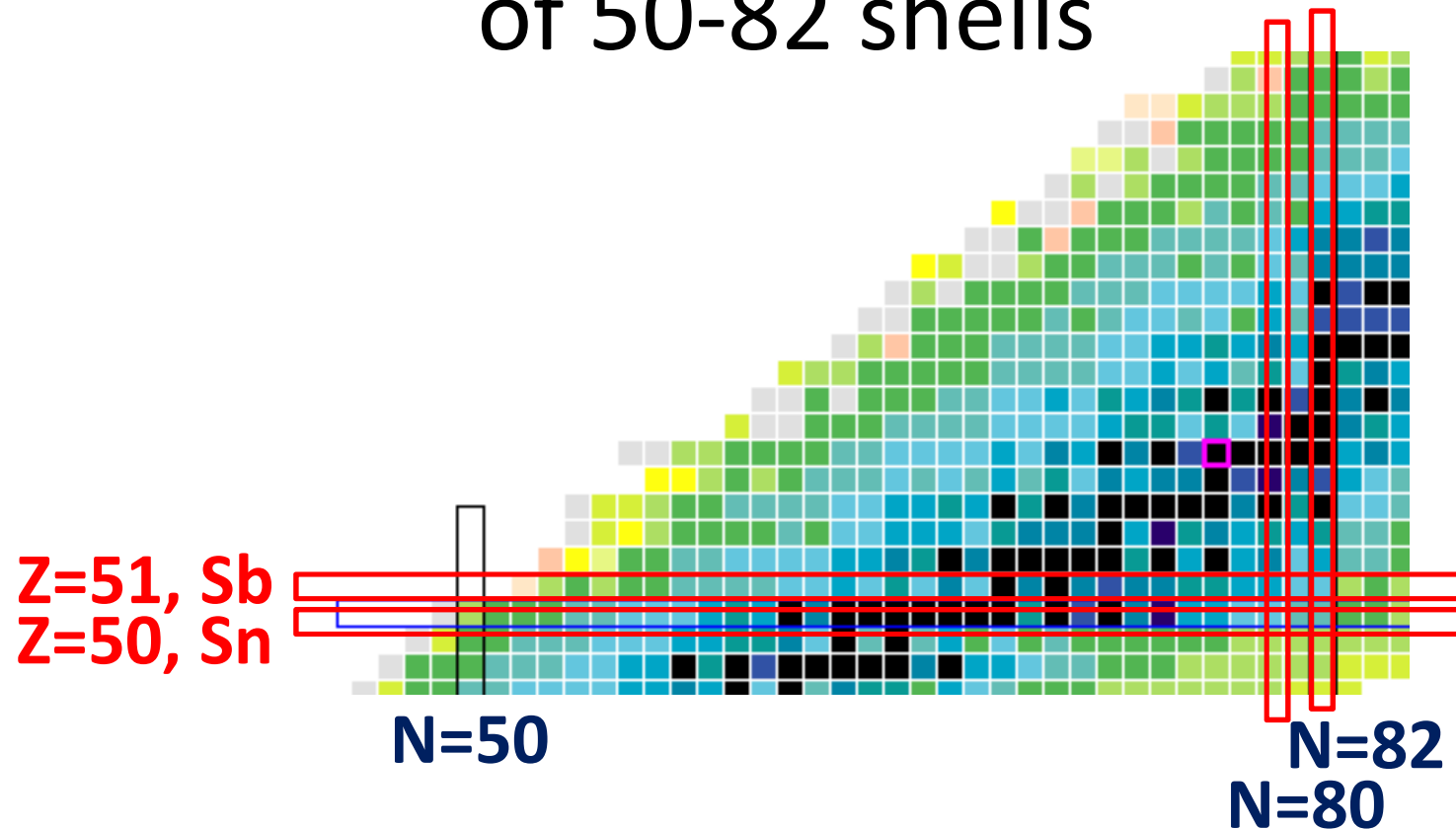
$$|\Psi\rangle = \sum_{k=1}^{N_{MCSM} \sim 100} f_k P^{J,\pi} |\phi_k\rangle$$

PES is calculated by Q-constraint HFB calc.

Location of circle : quadrupole deformation of $|\phi_k\rangle$

Area of circle : overlap probability $\frac{1}{N_k} |\langle \Psi | P^{J,\pi} | \phi_k \rangle|^2$

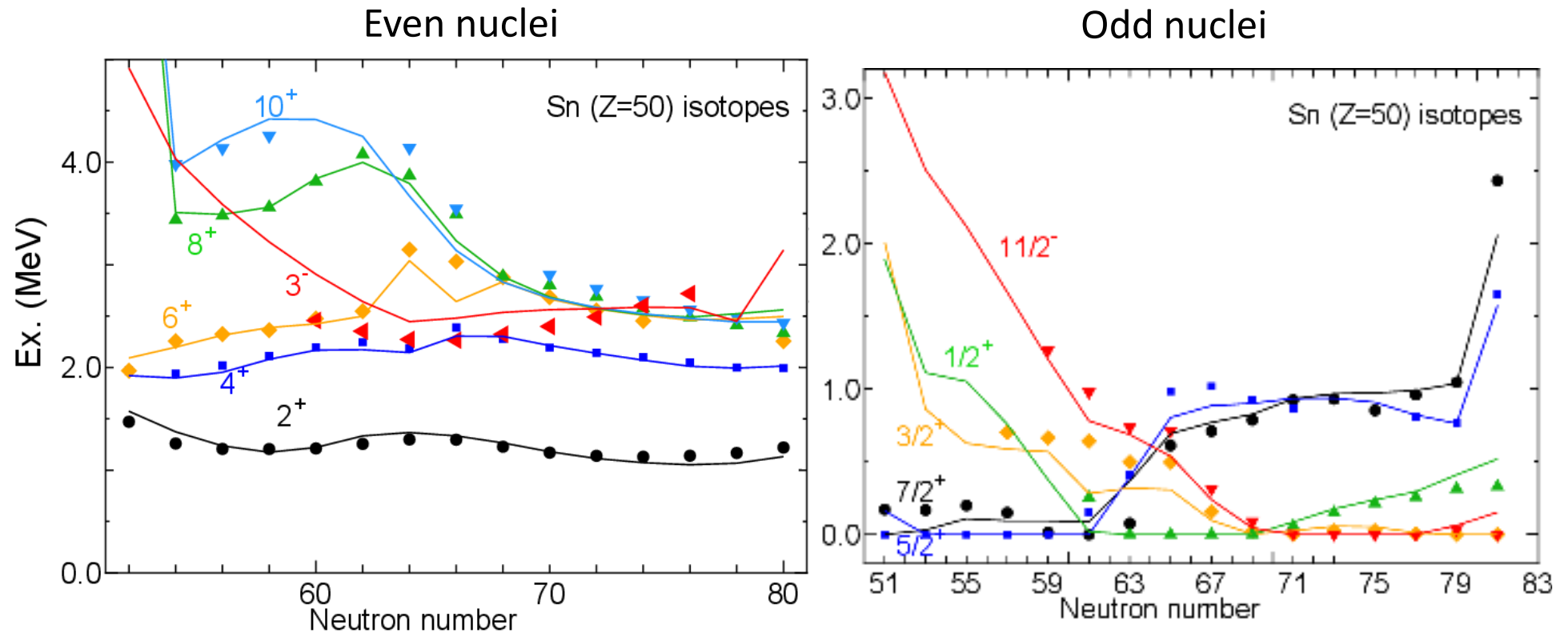
Investigate realistic effective interaction Towards unified description of 50-82 shells



SNBG3 interaction

Realistic interaction for $50 < N < 82$ Sn isotopes

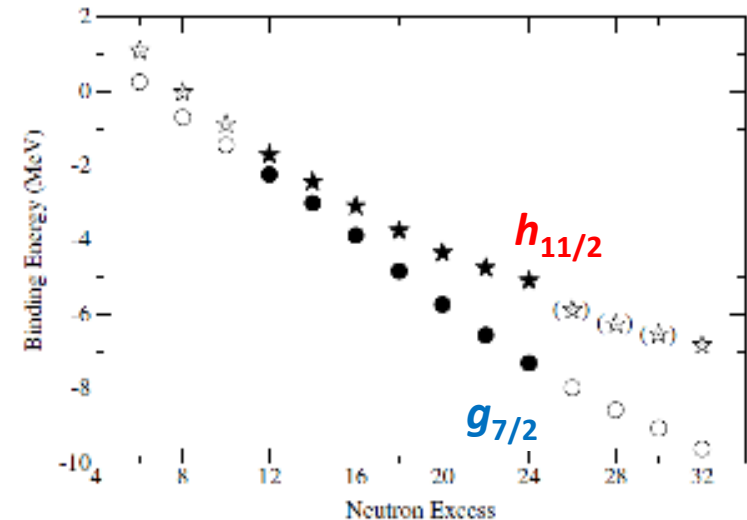
- start with N3LO + G-matrix
- chi-square fit with linear-combination method for ~ 300 experimental data including 3^- states



Shell evolution in Sb isotopes

- Shell evolution
 - Important not only in single-particle energy levels but also in collectivity
- How to deduce?
 - Follow the change of “single-particle energies” along a long isotope chain.
- Purity of single-particle (SP) states
 - Controversial levels in Sb ($Z=51$) isotopes
 - SP (Schiffer et al., 2004) or coupling to collective (Sorlin and Porquet, 2008)
 - Absolute values of C^2S : ambiguous

Many-body calculations with a suitable shell-evolution mechanism are needed.

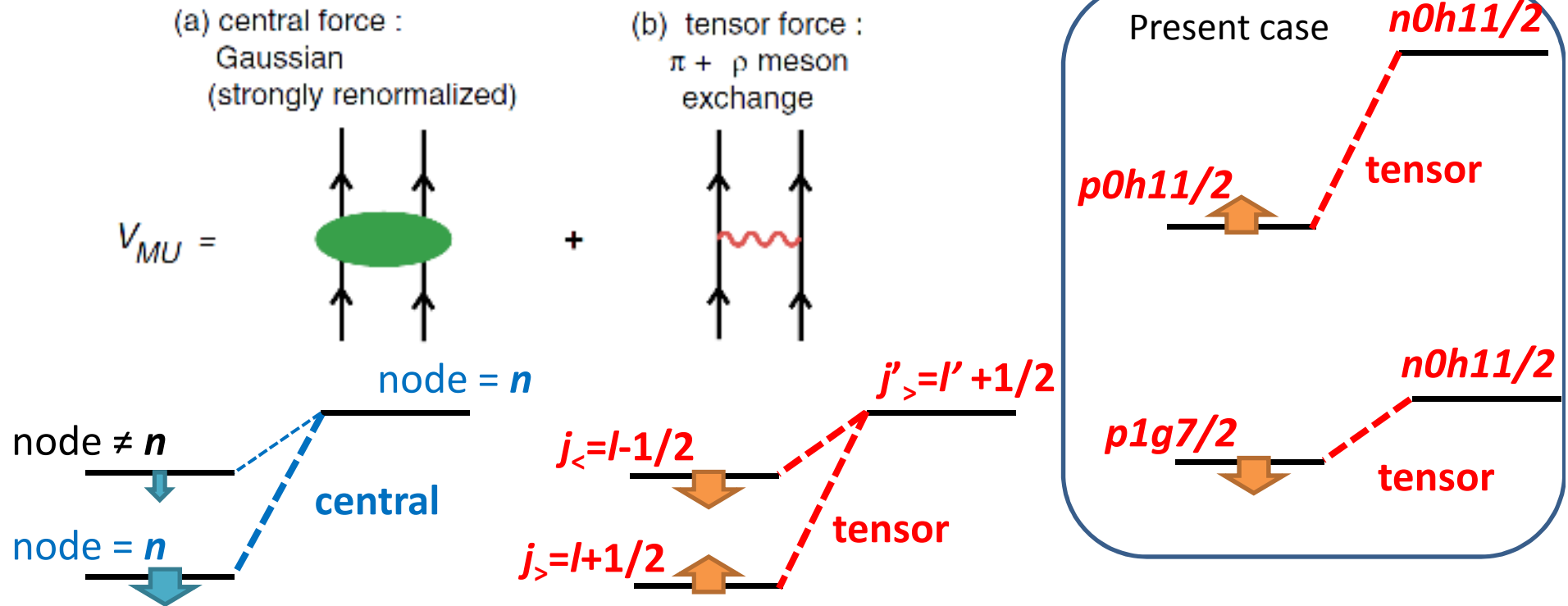


J. P. Schiffer et al., Phys. Rev. Lett. 92, 162501 (2004).

Two major sources of evolution in p - n channel

For a review of shell-evolution mechanism, see T. Otsuka, Phys. Scr. T152, 014007 (2013).

- Central and tensor forces



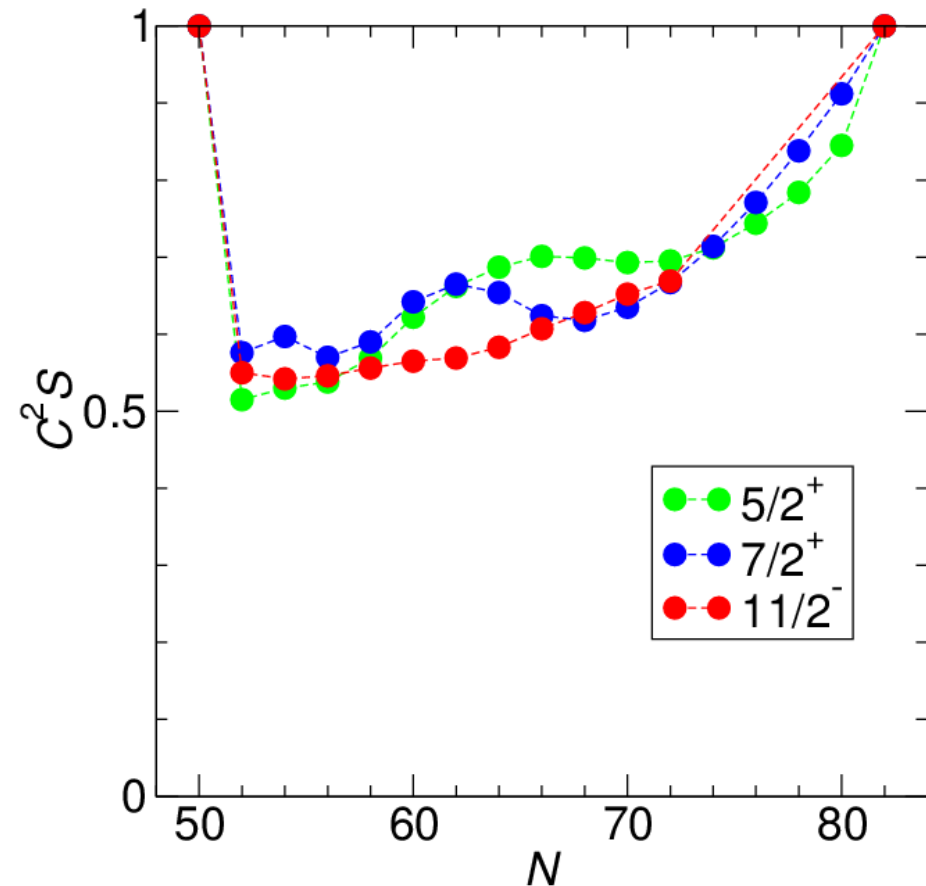
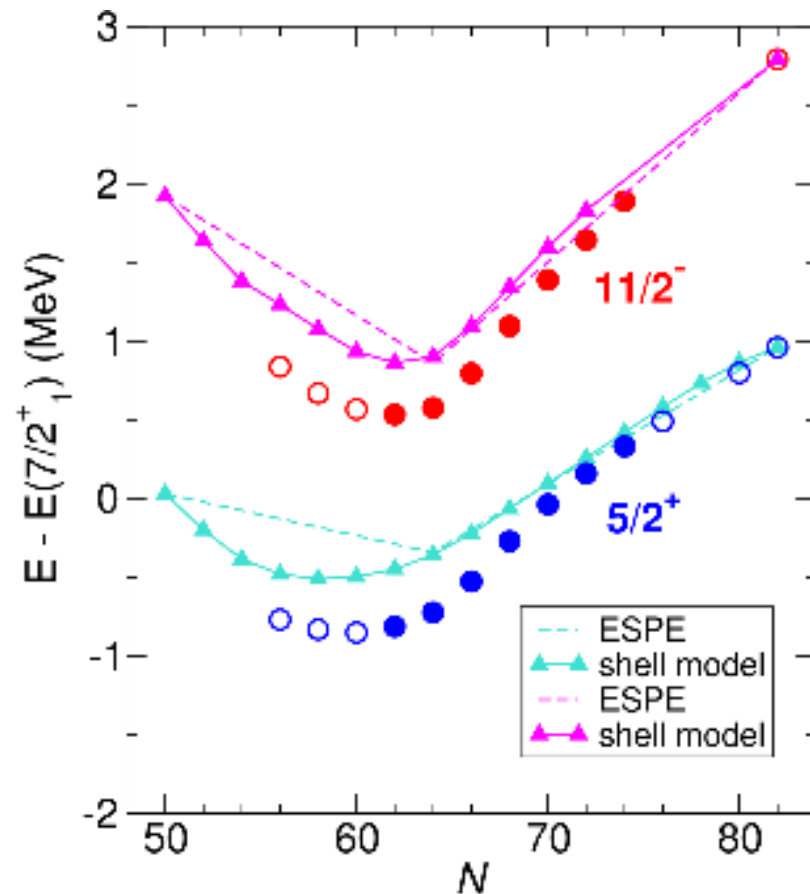
known for several decades

known for a decade: Otsuka mechanism (2005)

- Monopole-based universal interaction V_{MU} (Otsuka et al., 2010)
 - Quantitative implementation of this concept on a microscopic basis of “Renormalization Persistency” (N. Tsunoda et al., 2011)

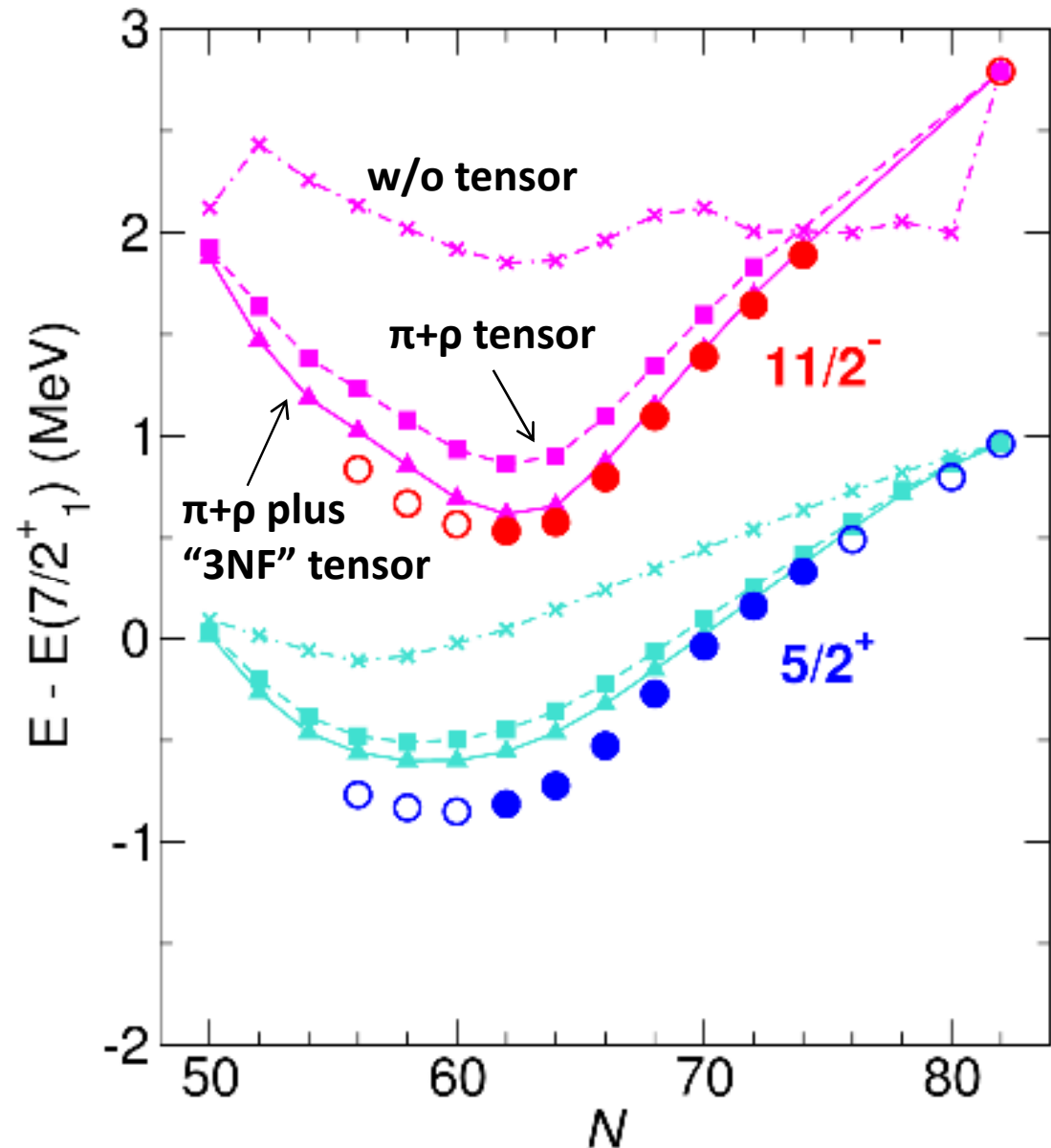
Sb ($Z=51$) isotopes

- Shell-model calculation in the $50 \leq N(Z) \leq 82$ space
 - n - n interaction: semi-empirical SNBG3 by Honma *et al.* (good fit including 3^-)
 - p - n interaction: V_{MU} with a scaling factor 0.84 for the central (binding energy)



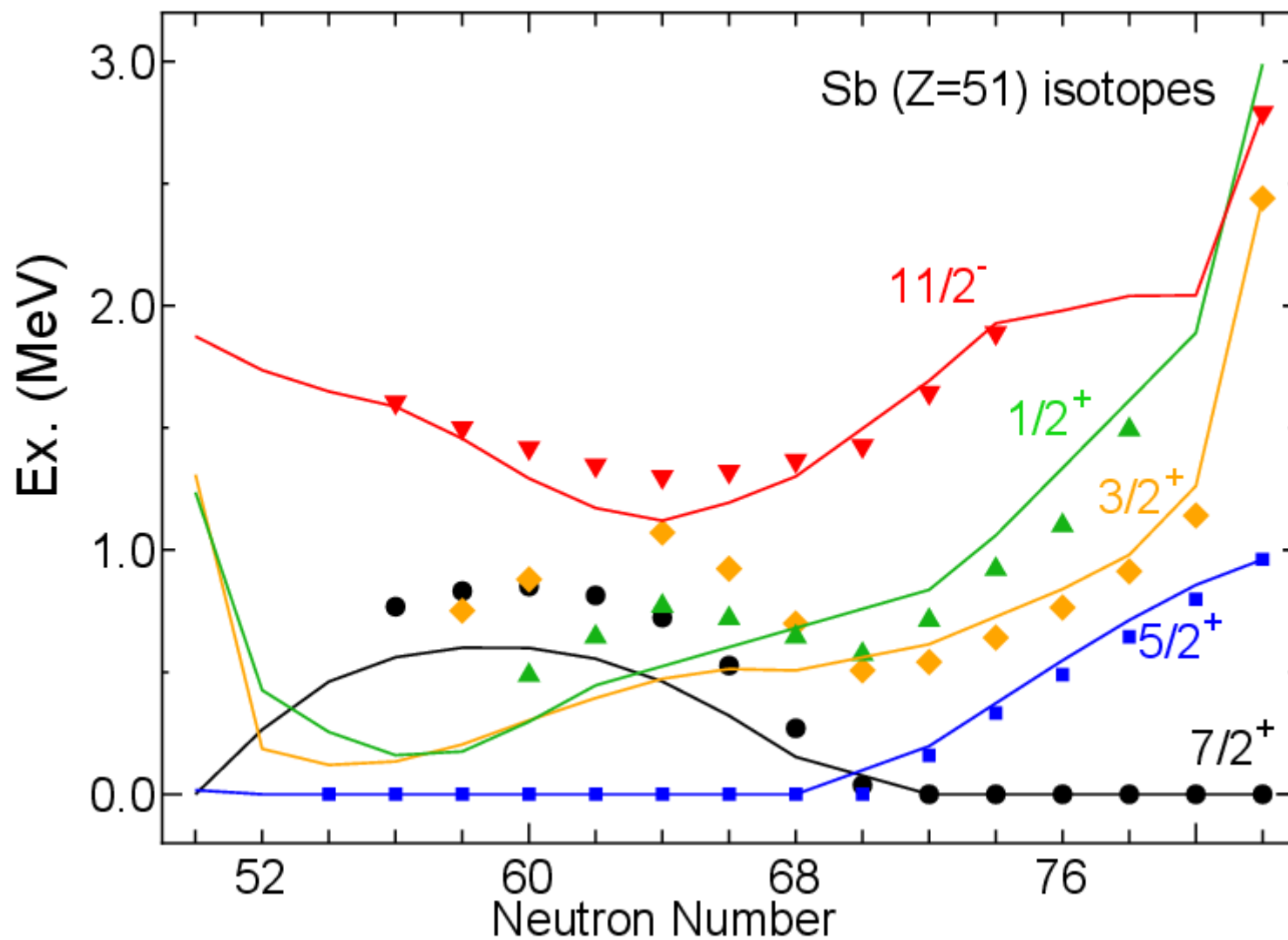
Importance of the tensor force

- Without tensor
 - $11/2^- \approx 2$ MeV
- 3NF effect
 - enhances effective $T=0$ tensor force (Kohno, 2013).
 - Almost perfect agreement with experiment

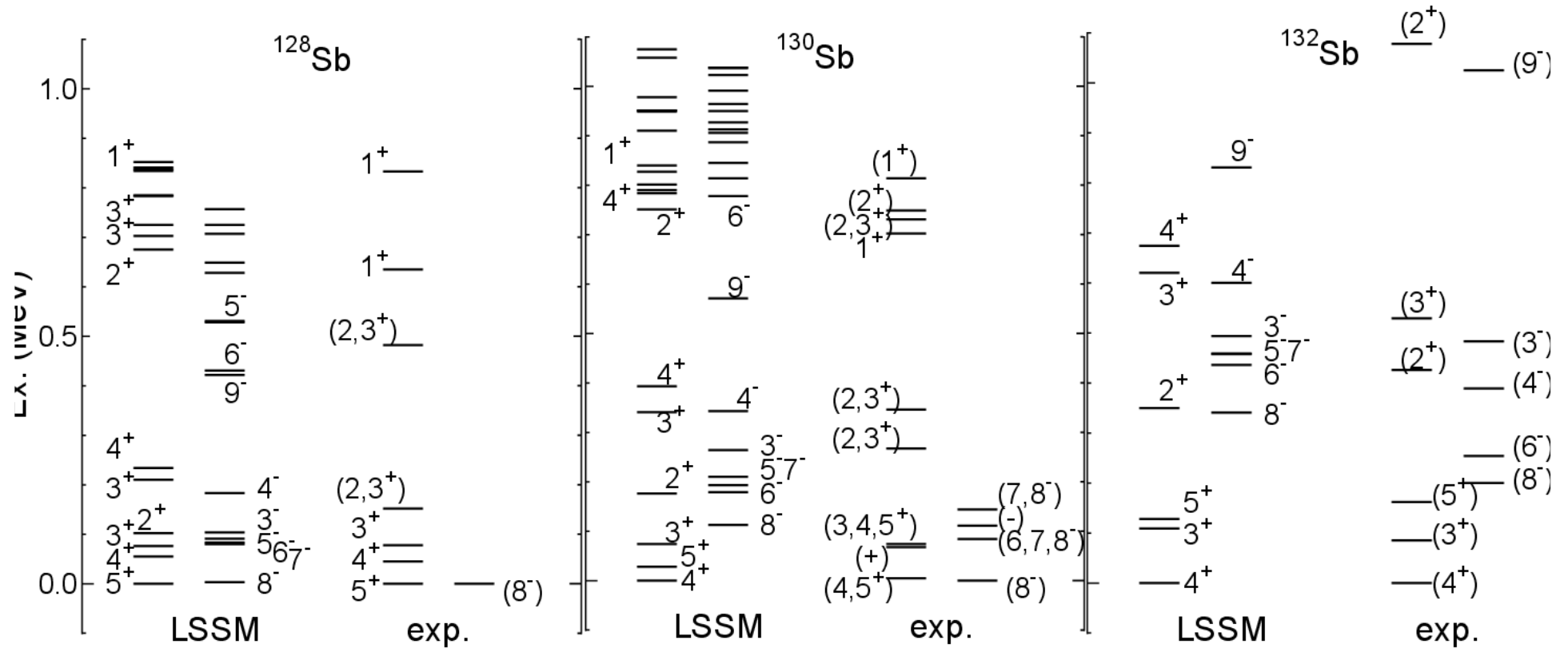


Sb isotopes

Excitation energies



Sb isotopes (odd-odd nuclei)



Reasonable description of low-lying states
 valid proton-neutron interaction (VMU)

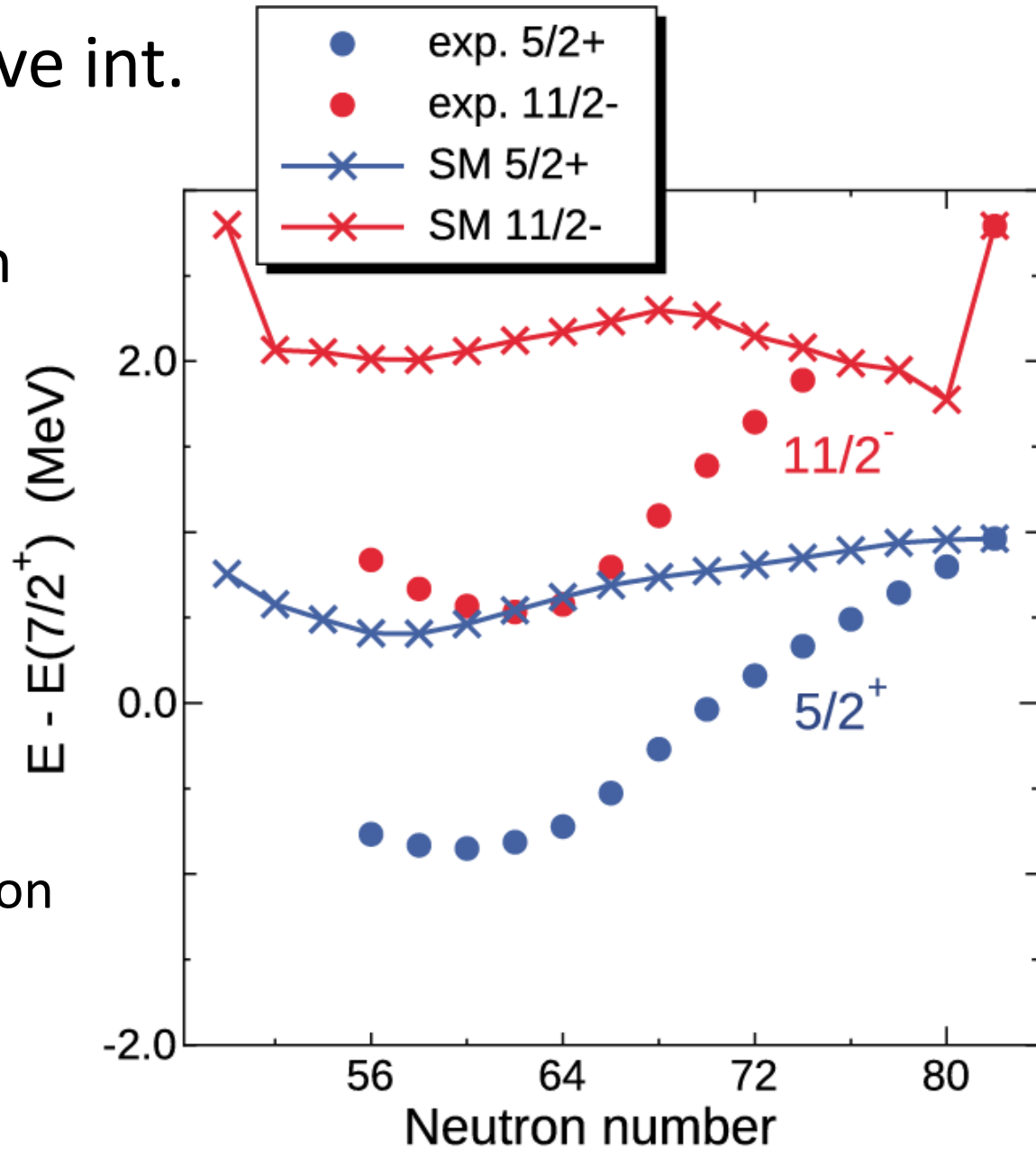
Microscopic effective int.

SN100PN interaction

CD-Bonn + G-matrix
+ 3rd order Q-box

successful description
for even-even nuclei
around ^{132}Sn

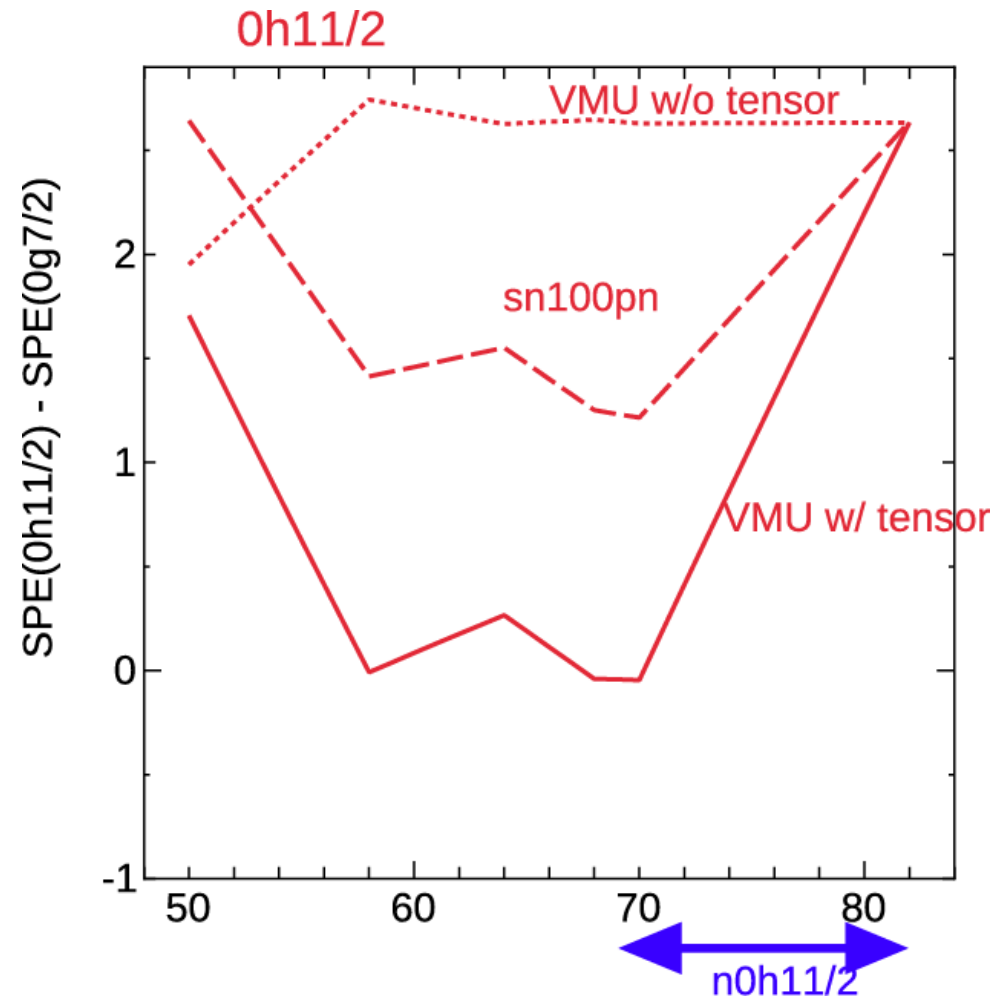
... failed in the description
of Sb isotopes.
What happens?



Effective SPEs of Sb isotopes

- Although SN100PN includes tensor force, the shift of single-particle energy is half of the VMU with bare pi+rho tensor force
- Proton-neutron monopole interaction has a problem

$$H^{(m)} = \sum_{ij} V_{ij}^{(m)} n_i n_j$$



This gradient
 $V(n0h11/2-p0h11/2) - V(n0h11/2-p0g7/2)$

Monopole part of the effective interaction and many-body perturbation theory (MBPT)

	VMU	$V_{\text{low-k}}$	SN100PN (KK 3 rd)	KK 2 nd order	EKK 2 nd order	EKK large space
n0h11/2- p0h11/2	-0.34	-0.27	-0.31	-0.30	-0.08	-0.38
n0h11/2- p0g7/2	-0.58	-0.48	-0.43	-0.48	-0.43	-0.60
diff	0.23	0.21	0.12	0.18	0.35	0.23
	w/o MBPT		w/ MBPT			
	50 < Z, N < 82, 0g9/2 inert core					0g9/2 active

- VMU ... VMU interaction (pi+rho tensor) “renormalization persistency”
- $V_{\text{low-k}}$... N3LO + $V_{\text{low-k}}$ w/o perturbation for *l*-closed core
- SN100PN ... CD-Bonn + KK 3rd order by Brown, Jensen
- KK 2nd order ... $V_{\text{low-k}}$ + Krenciglwa-Kuo (EKK) method 2nd order
- EKK 2nd order ... $V_{\text{low-k}}$ + Extended Krenciglwa-Kuo (EKK) method 2nd order
- EKK large space ... EKK 2nd order in pf+sdg+h11/2+f7/2+p3/2 KK, EKK by N. Tsunoda

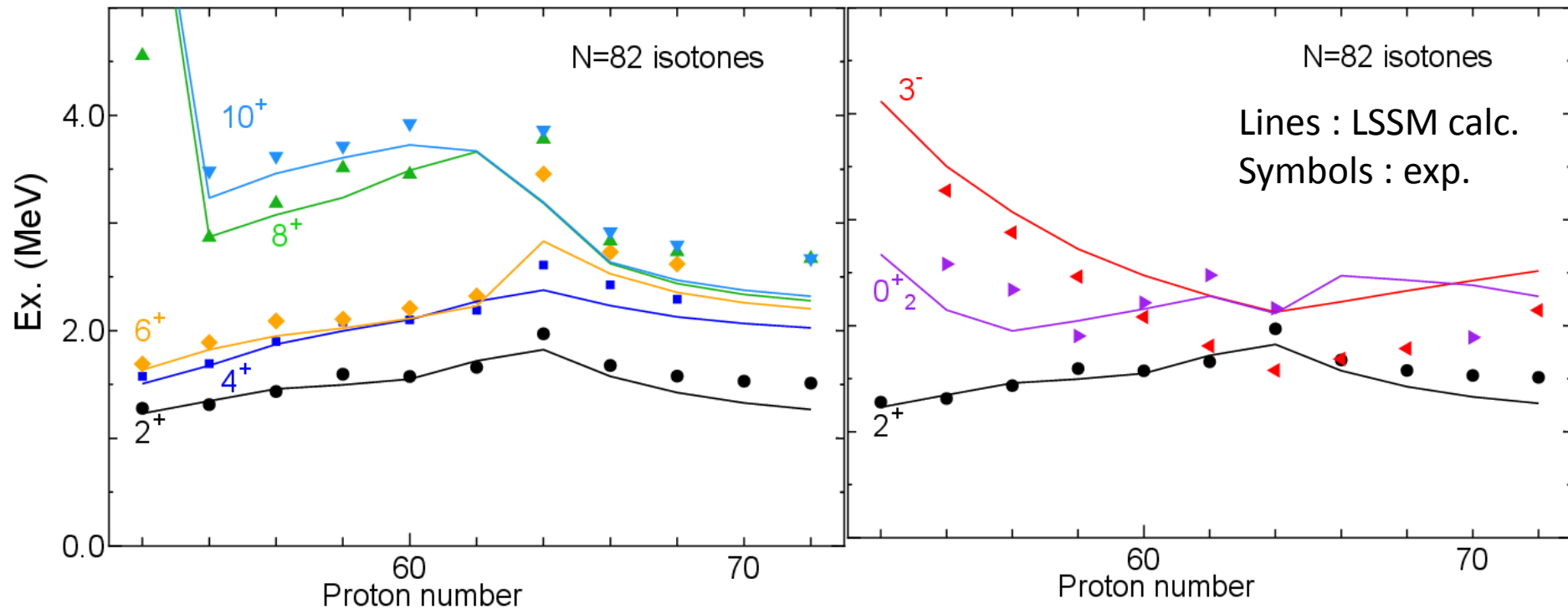
EKK large space is close to VMU with bare tensor force.

2nd order term with *jj*-closed core may deteriorate ?

Further investigation is required. Now, we adopt VMU for p-n interaction.

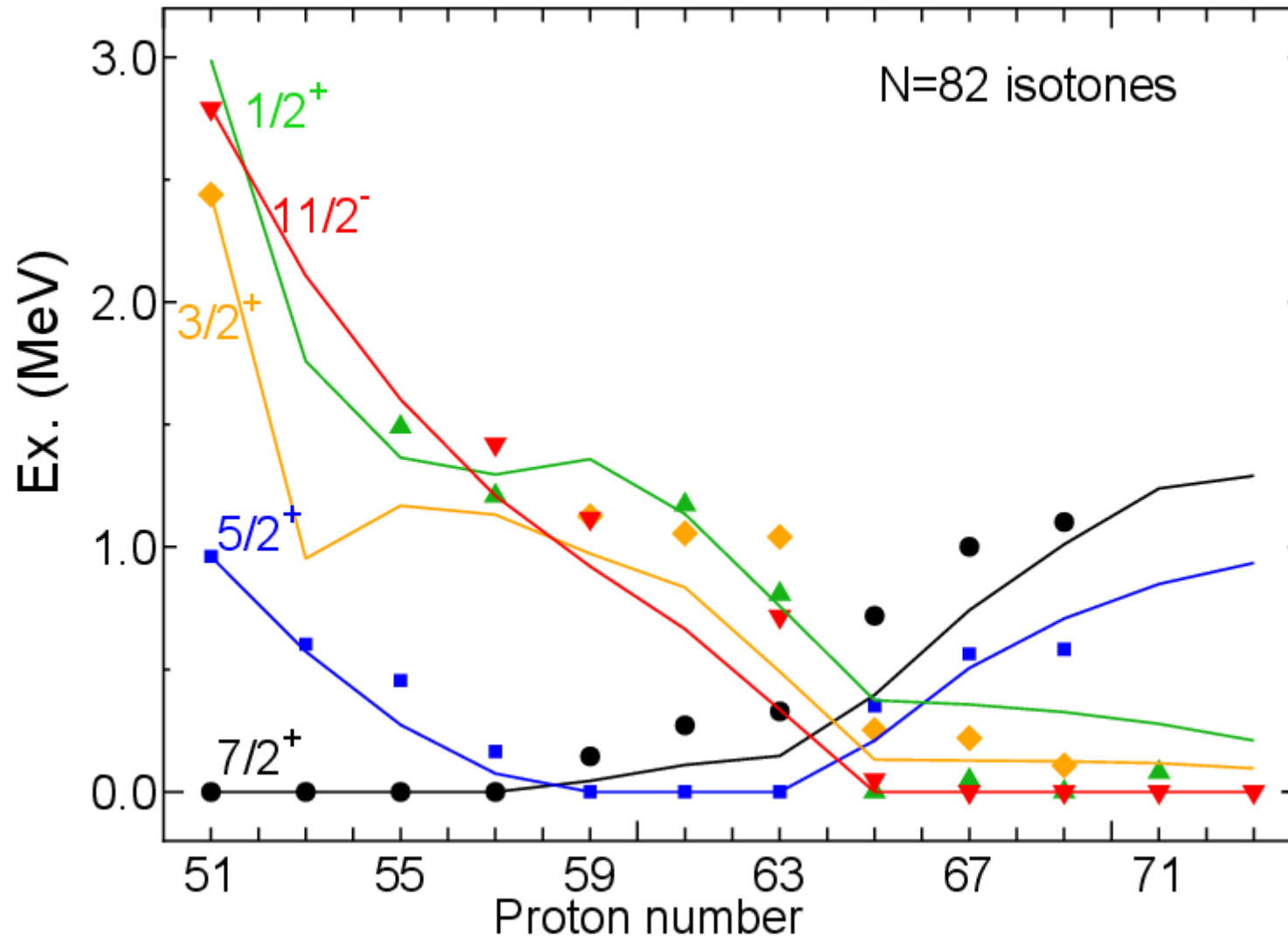
proton-proton int. for N=82 isotones

- SN100PN TBME is used for p-p TBME
 - Mass dependence of TBME, $(A/102)^{-0.3}$ is introduced
 - SN100PN (pp) + SNBG3 (nn) + VMU (pn)

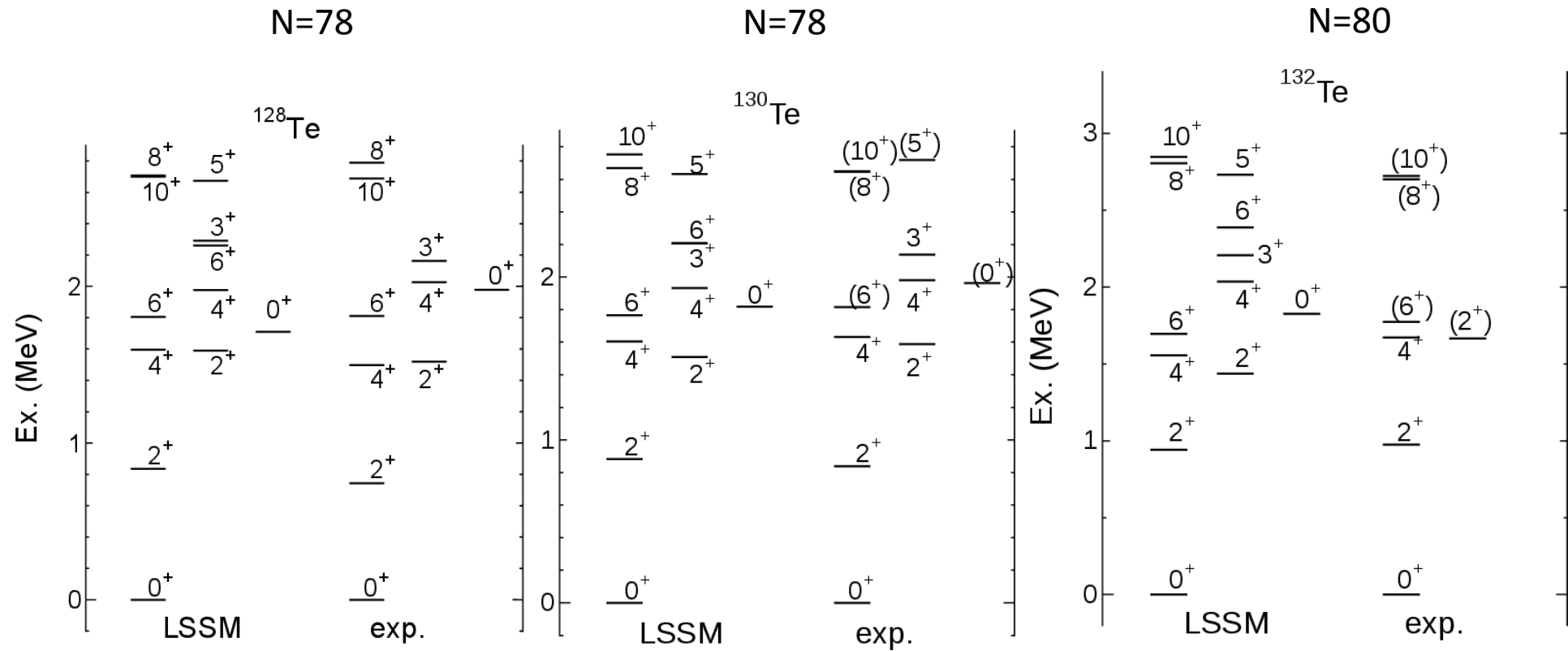


Good agreement at N=64 subshell magic (except for 3- collective states)

N=82 isotone, odd nuclei

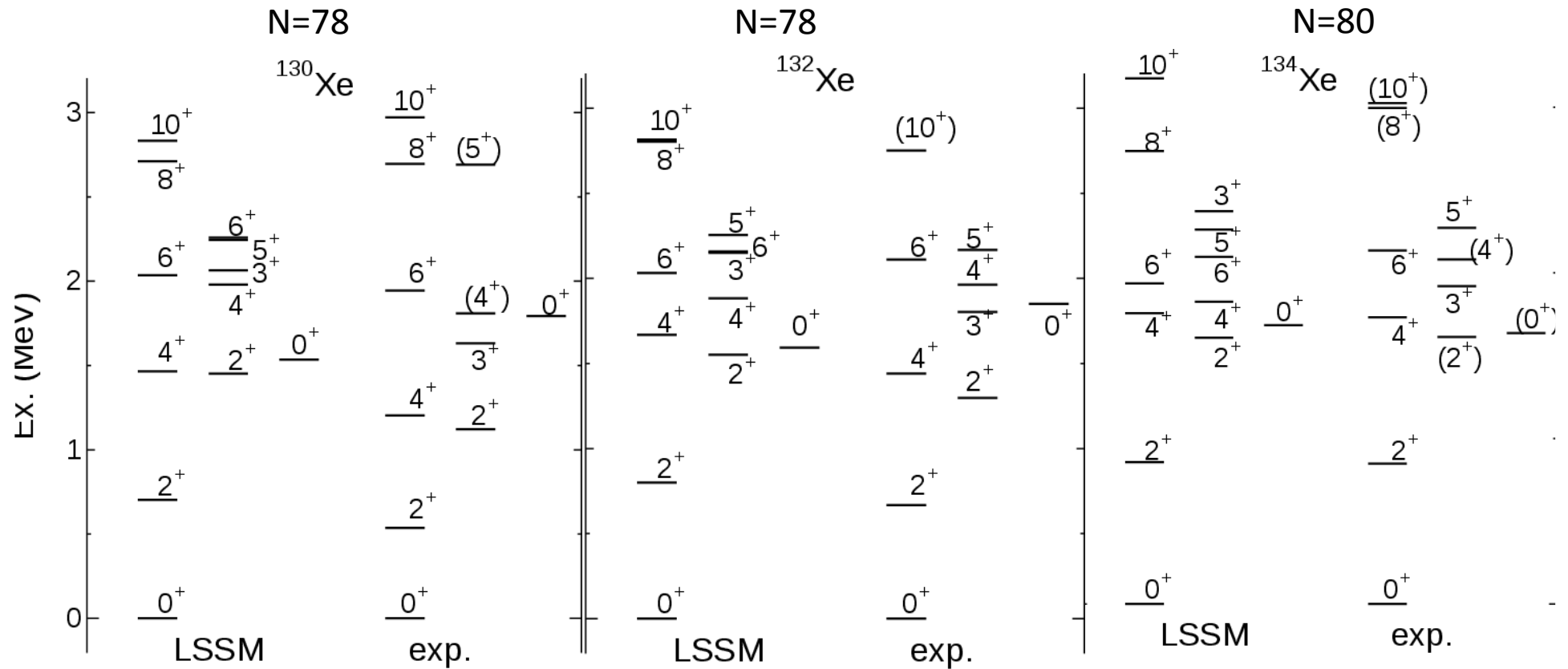


Te isotopes



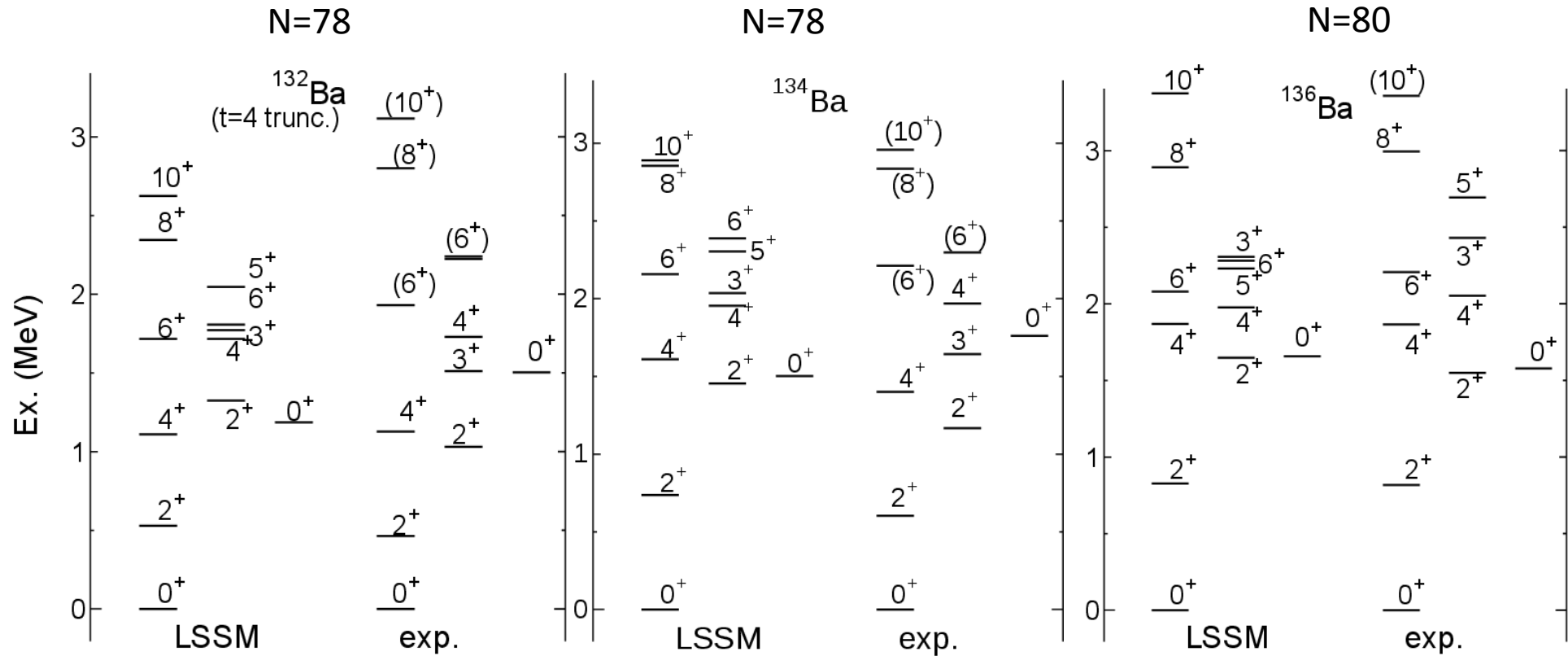
- SN100PN for pp, SNBG3 for nn, VMU for pn interactions
- Good agreements

Xe isotopes



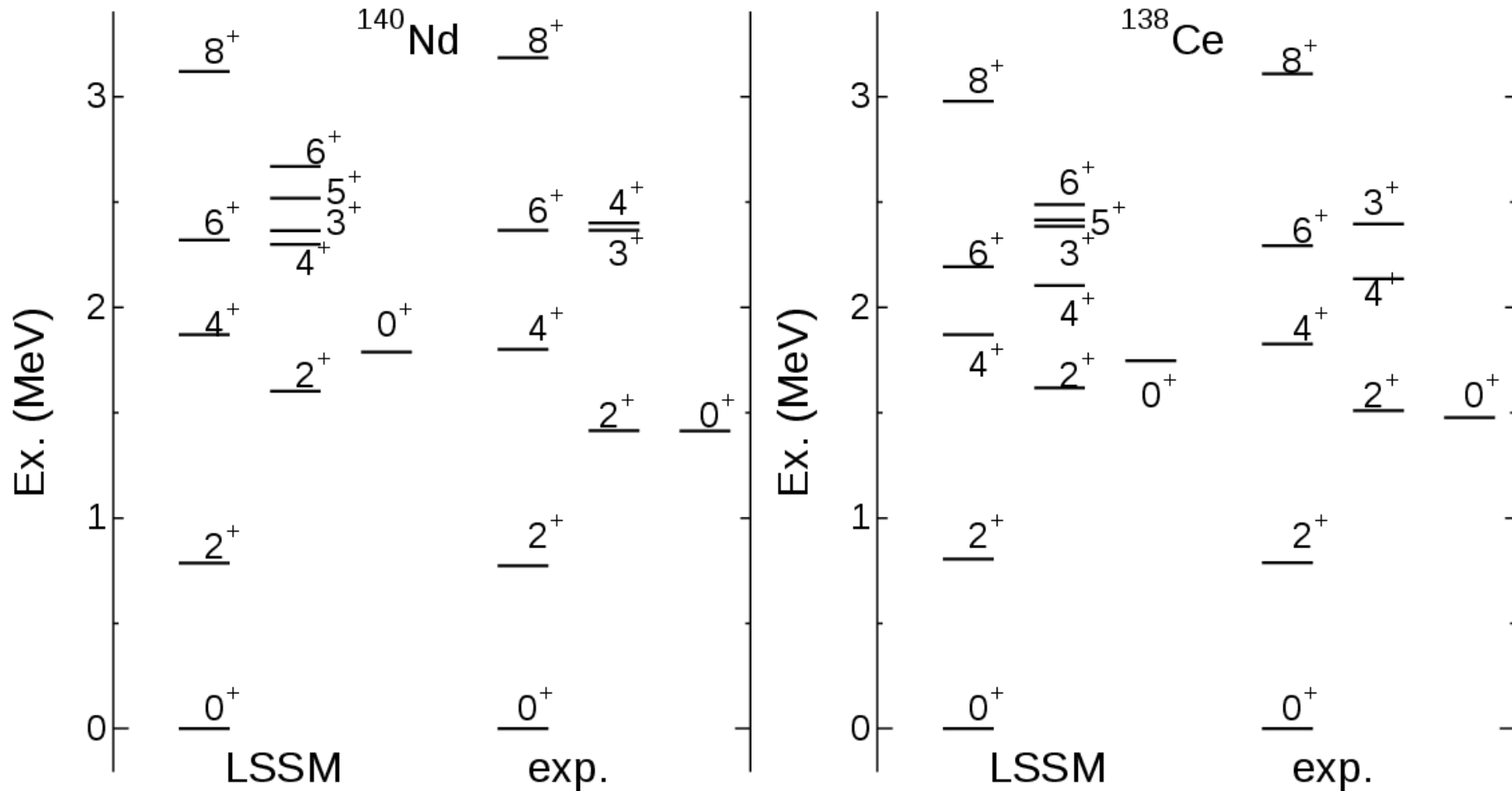
- Good agreements especially for yrast band
- problem in quasi-gamma band

Ba isotopes



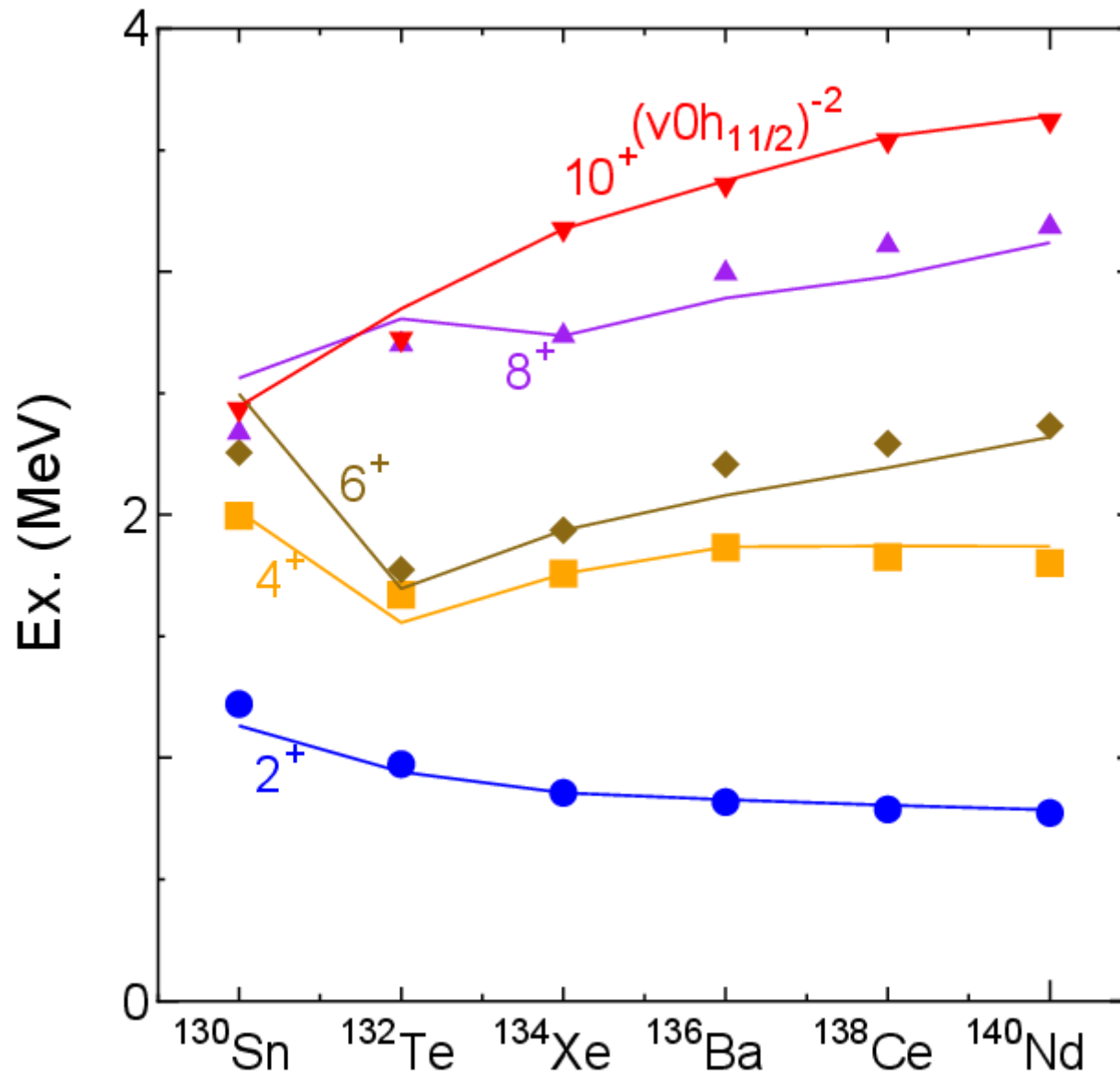
- Good agreements especially for yrast band
- problem in quasi-gamma band

Ce, Nd isotopes (N=80)



- excellent agreement except for N=80 isotones

Yrast levels of N=80 isotones



Mixed symmetry states around N=80 : experiments

$$|2_1^+\rangle \simeq Q_s |0_1^+\rangle = [Q_\pi + Q_\nu] |0_1^+\rangle$$

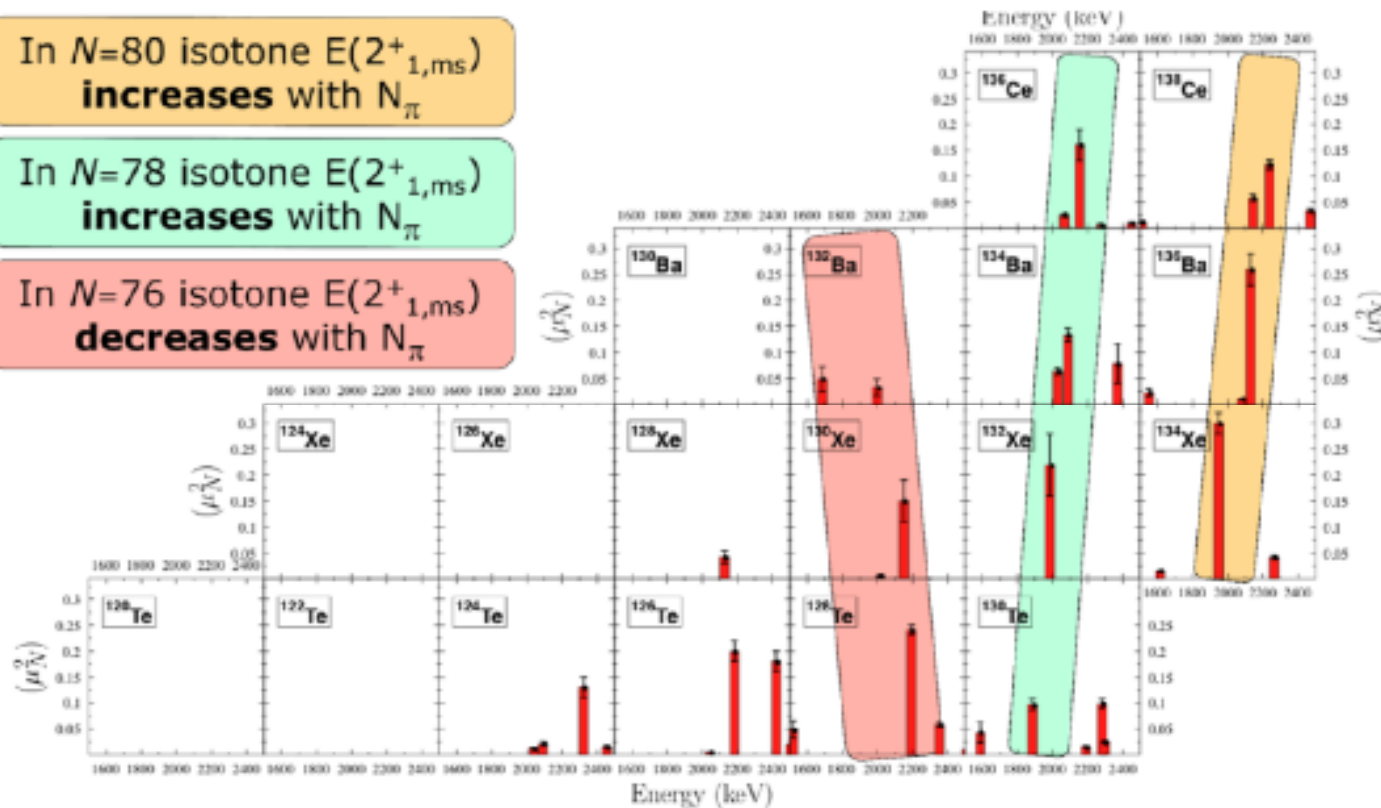
$$|2_{1,ms}^+\rangle \simeq Q_m |0_1^+\rangle = N \left[\frac{Q_\pi}{N_\pi} - \frac{Q_\nu}{N_\nu} \right] |0_1^+\rangle$$

$B(M1; 2_1^+ \rightarrow 2_1^+) (\mu_N^2)$

In N=80 isotone $E(2_{1,ms}^+)$ **increases** with N_π

In N=78 isotone $E(2_{1,ms}^+)$ **increases** with N_π

In N=76 isotone $E(2_{1,ms}^+)$ **decreases** with N_π



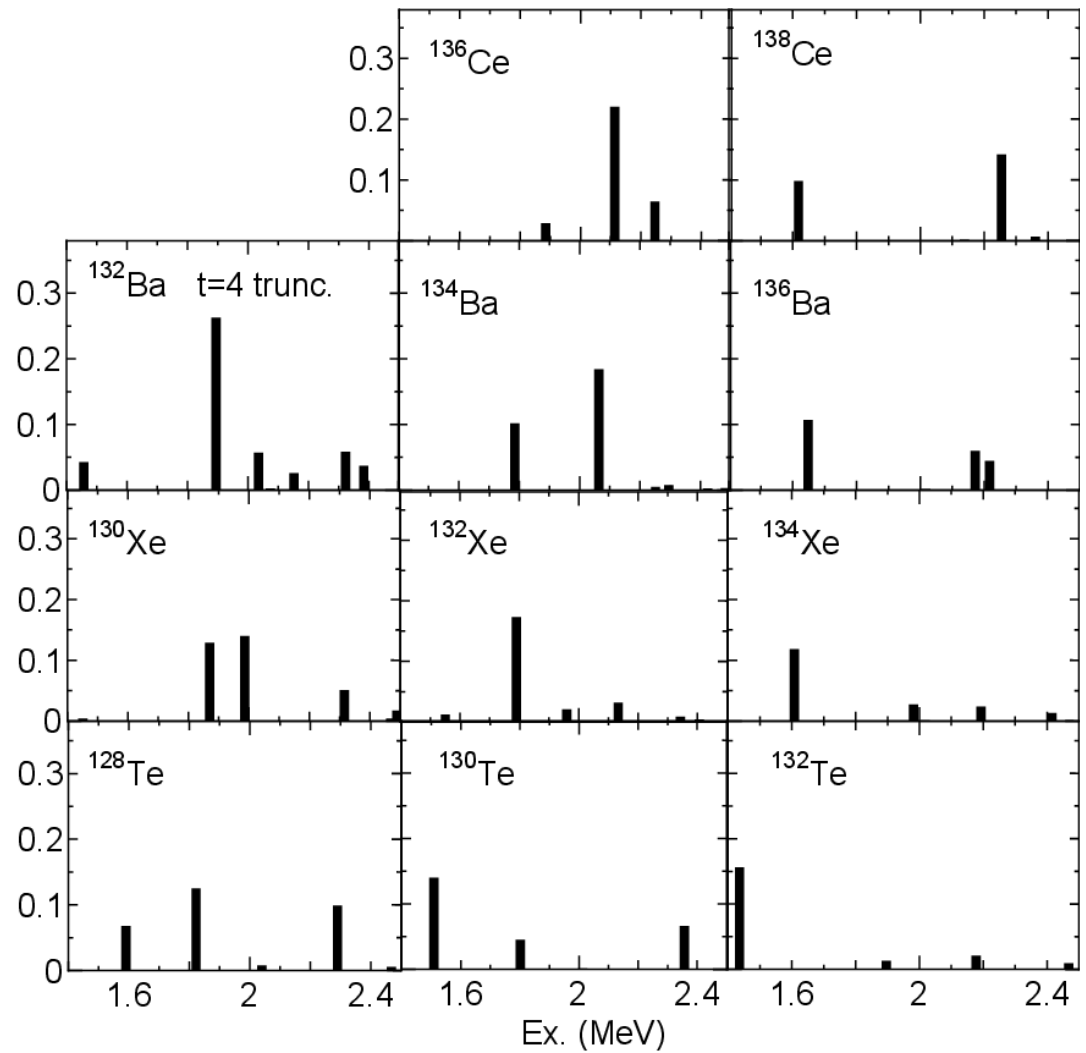
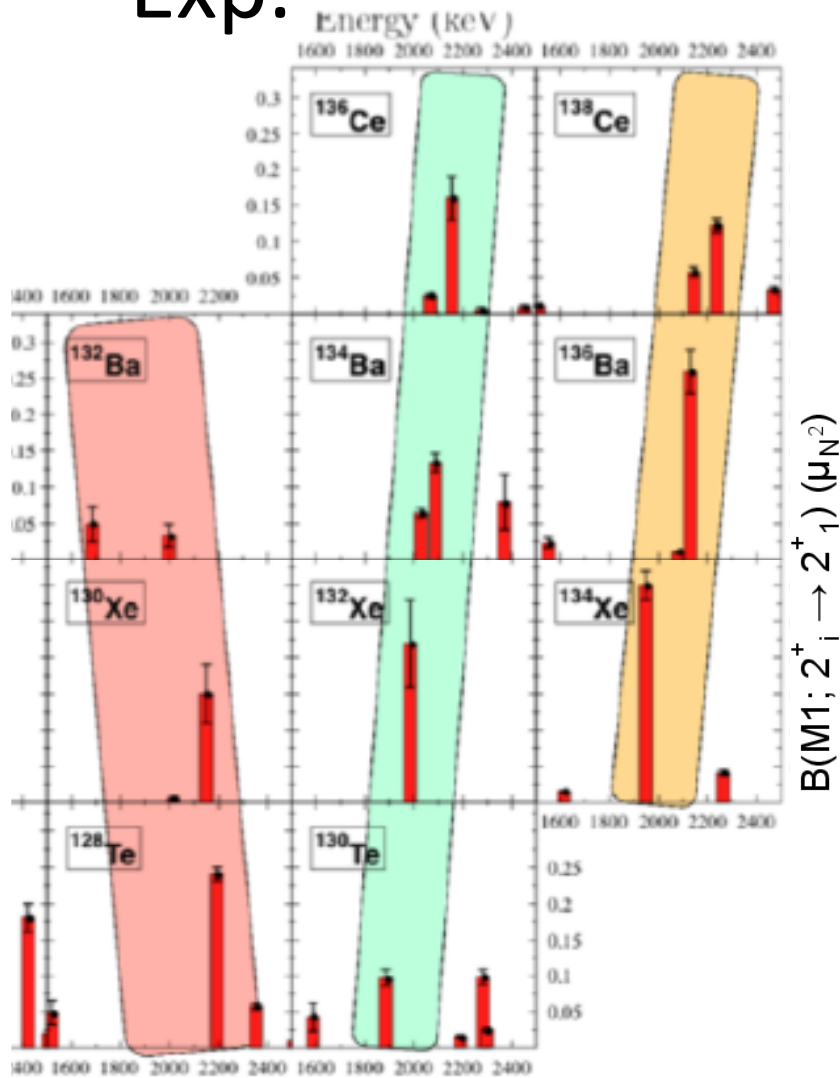
Ref. N. Pietralla *et al.*, J. Phys. Conf. Ser. 445, 012030 (2013)

Mixed symmetry states in N=80 isotones

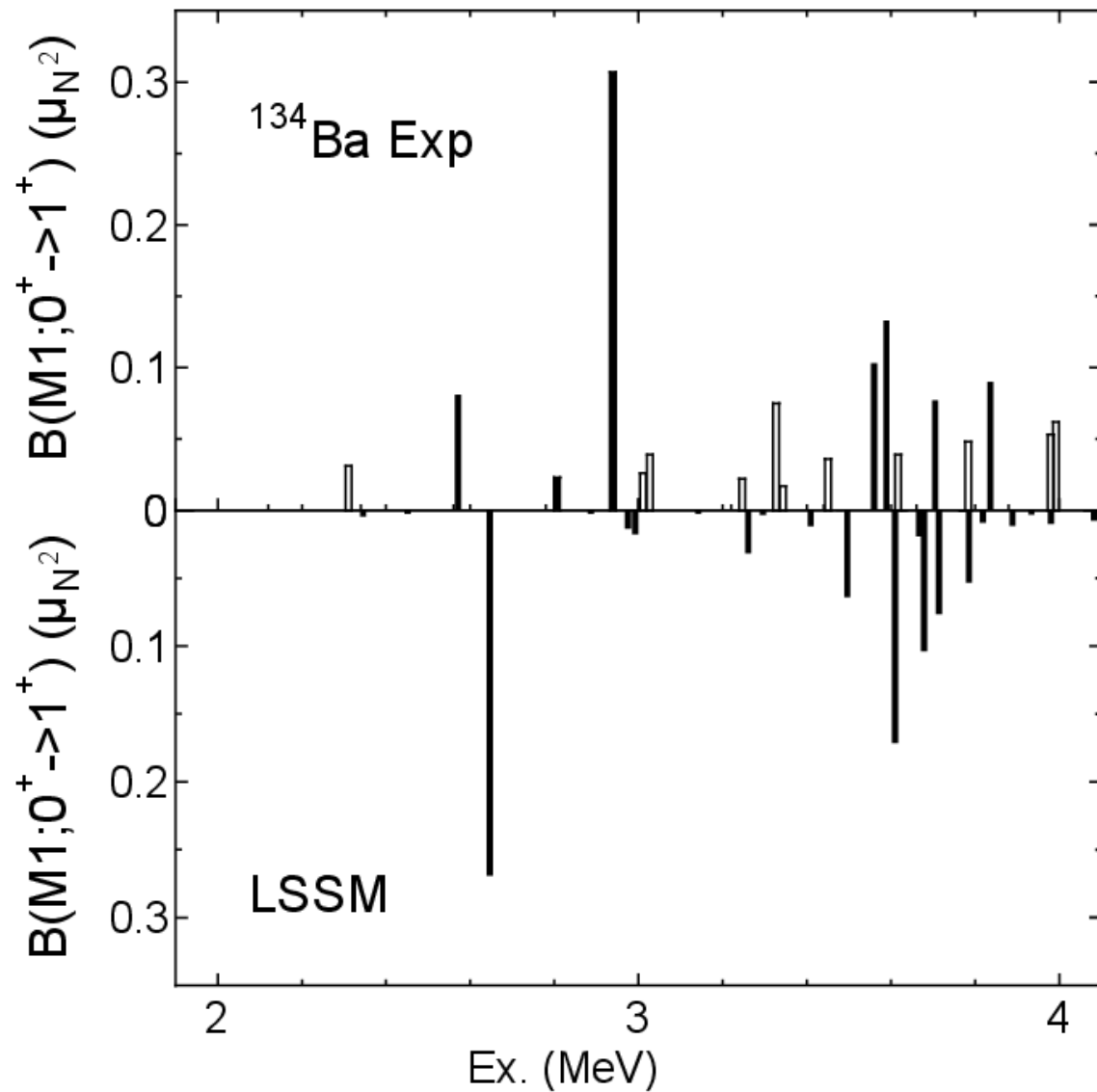
Exp.

LSSM

spin quenching 0.7



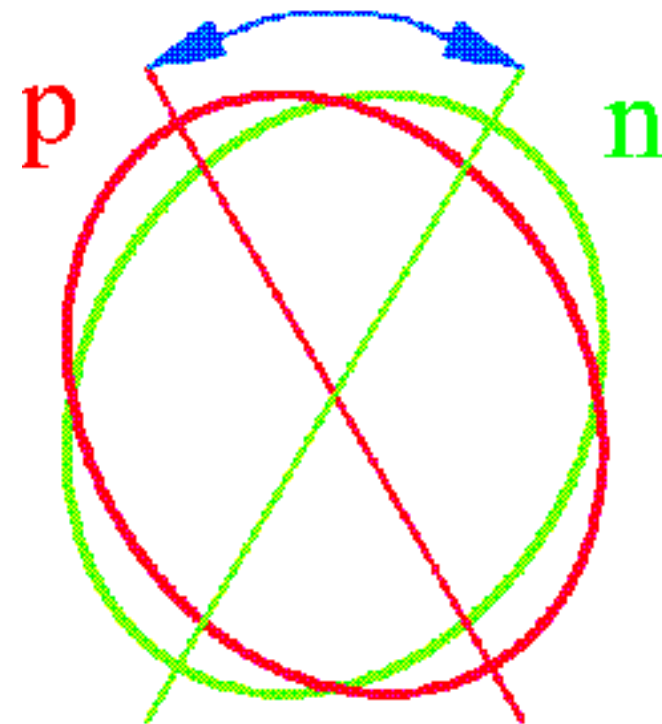
M1 excitation of ^{134}Ba



Solid bar : B(M1)

Open bar : M1/E1 not identified

Scissors mode



Exp. H. Maser et al., PRC 54 2129R (1995)

Summary

- Nuclei around $N=80$ are investigated in LSSM and MCSM
- P+QQ interaction successful for triaxially deformed states
- Construct realistic effective interaction towards unified description of $50 < N, Z < 82$ region
 - Sb isotopes and shell evolution by tensor force
 - discuss mixed symmetry states, scissors mode in LSSM
 - in preparation for MCSM calc.