Effectively-truncated large-scale shell-model calculations and nuclei around ^{100}Sn

Angela Gargano, INFN Napoli

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L. Coraggio, A. Covello, A. G., N. Itaco, T.T.S. Kuo, Phys. Rev. C **91**, 041301(R) (2015)
L. Coraggio, A. G, and N. Itaco, Phys. Rev. C **93**, 064328 (2016)

Few words on shell model

The nuclear SM is likely the most widely used framework to describe the structure of atomic nuclei

The idea behind this approach is that each nucleon inside the nucleus moves independently from the others in a spherically mean field including a strong spin-orbit force. Then

- the nucleons arrange themselves into groups of levels, the **“shells”**, well separated from each other;
- the nucleus may be considered as an “inert core”, made up by filled shells, plus a certain number of external nucleons, the **“valence”** nucleons, interacting in a truncated **model space** through a **“residual” interaction**.

Shell-model Hamiltonian

***H$_{\text{eff}}$* is defined for *N*-valence nucleons in the chosen model space**

Mean field

$$H_{\text{eff}} = \sum_i U_i + \sum_{i<j} V_{ij}$$

Residual interaction

empirical **microscopic**

should account for the degrees of freedom not considered explicitly

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The usage of shell model is **limited by numerical complexity**, especially for medium- and heavy-mass nuclei when large model space and/or many valence nucleons are involved

- Full space diagonalization is only feasible for all nuclei up to *fp* shell
- Actually the non-public version of the ANTOINE code allows to treat m-scheme dimensions of ~10^{10}

LSSM calculations

The need of LSSM calculations is strongly emphasized by recent data on medium- and heavy-mass exotic nuclei

Novel features are emerging when going towards unbalanced neutron-proton systems **whose description requires model spaces with a large capacity**

A notable example:

Shell Evolution: Changes in the shell structure

→

- Onset of collectivity
- Island of inversion
- Shape coexistence in the same nucleus

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The case of light Sn isotopes

Light Sn isotopes with realistic SM calculations

Only neutron degrees of the freedom: ^{100}Sn core + neutrons in the 50-82 shell

SP space				
$0g_{7/2}$	$1d_{5/2}$	$1d_{3/2}$	$2s_{1/2}$	$0h_{11/2}$

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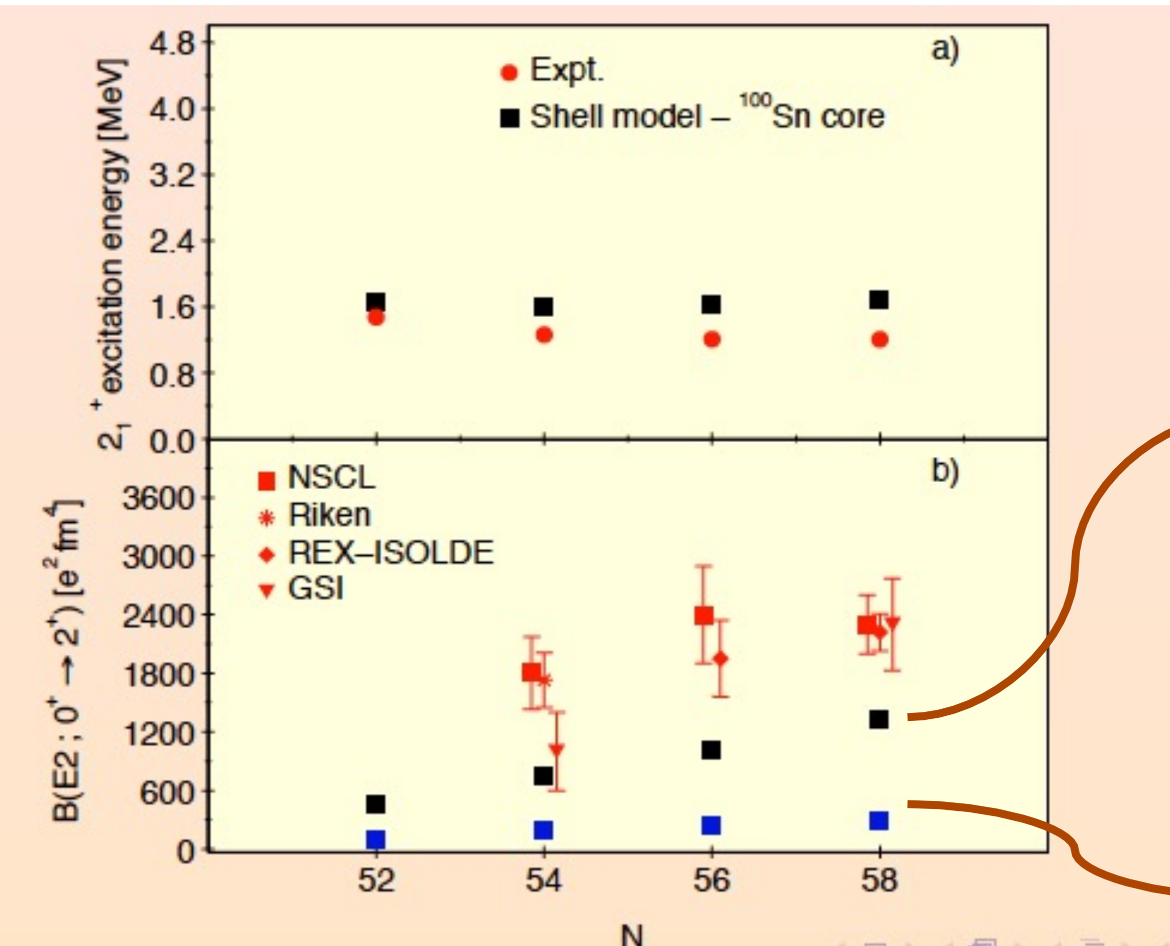

Microscopic neutron charge

a	b	$\langle a \vert e_n \vert b \rangle$ (in e)
$0g_{7/2}$	$0g_{7/2}$	1.20
$0g_{7/2}$	$1d_{5/2}$	1.27
$0g_{7/2}$	$1d_{3/2}$	1.19
$1d_{5/2}$	$1d_{5/2}$	0.81
$1d_{5/2}$	$1d_{3/2}$	0.83
$1d_{5/2}$	$2s_{1/2}$	0.79
$1d_{3/2}$	$1d_{3/2}$	0.87
$1d_{3/2}$	$2s_{1/2}$	0.85
$0h_{11/2}$	$0h_{11/2}$	0.78

▪ empirical neutron charge: 0.5 e

Light Sn isotopes with realistic SM calculations

When using only neutron degrees of freedom

- Large renormalization of the theoretical effective electric-quadrupole operator
- B(E2) values still too small with respect to the experiment

→ need of degrees of freedom outside the chosen model space: proton excitations across the Z=50 shell

^{88}Sr core: neutron and proton degrees of the freedom

proton SP space	neutron SP space
$1p_{1/2}$	
$0g_{9/2}$	
$0g_{7/2}$	$0g_{7/2}$
$1d_{5/2}$	$1d_{5/2}$
$1d_{3/2}$	$1d_{3/2}$
$2s_{1/2}$	$2s_{1/2}$
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↓

One has to find a way to reduce the dimensions of the matrices to be diagonalized and make the shell-model calculations feasible

Usually truncations are performed by allowing up to limited number of protons excitations across the Z=50 shell [see for instance PRC **72**, 061305 (2005)]

Double-step truncation procedure

aimed at preserving as much as possible the role of the rejected degrees of freedom in an effective approach

1. Derivation of the realistic shell-model Hamiltonian in a large model space: "mother" Hamiltonian

2. Evolution of the ESPE as a function of neutron and/or proton number to identify the most relevant degrees of freedom to be taken into account in the construction of a truncated shell-model Hamiltonian, namely the single-particle orbitals that will constitute a new truncated model space

3. Construction of a new shell-model Hamiltonian in the truncated model space by a unitary transformation of the original Hamiltonian
→ the new Hamitonian accounts effectively for the excluded single-particle orbitals

Step 1 – Derivation of H^{75} (spe & TBME)

[75] model space	proton SP space	neutron SP space
	$1p_{1/2}$	
	$0g_{9/2}$	
	$0g_{7/2}$	$0g_{7/2}$
	$1d_{5/2}$	$1d_{5/2}$
	$1d_{3/2}$	$1d_{3/2}$
	$2s_{1/2}$	$2s_{1/2}$
	$0h_{11/2}$	$0h_{11/2}$

H_{eff} in the [75] model space → H^{75}

a) V_{NN} high-precision CD-Bonn

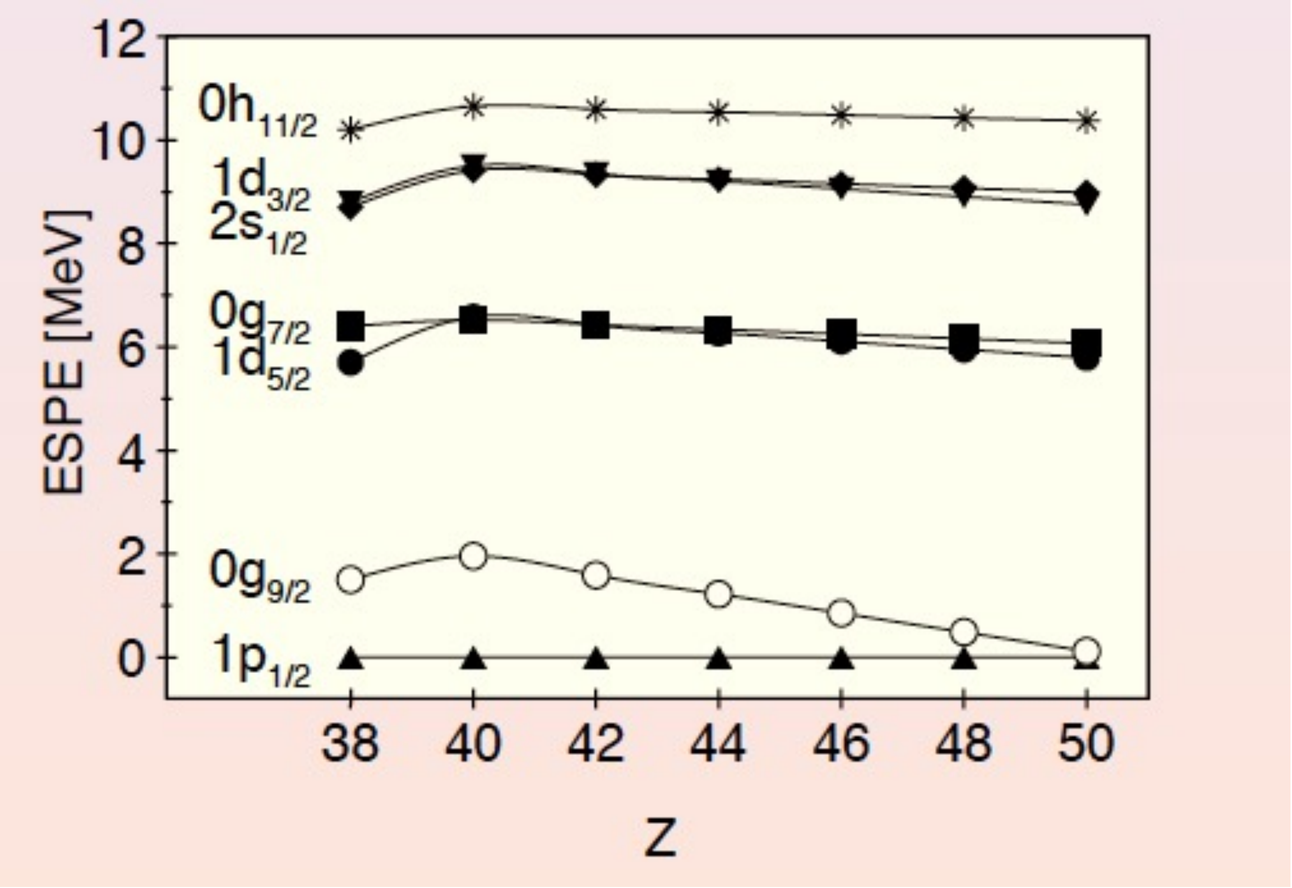
b) Renormalization of V_{NN} by means of the V_{low-k} approach with a cutoff momentum Λ=2.6 fm^{-1}

c) Derivation of H^{75} using the perturbative $\hat{Q}$-box folded diagrams approach, the $\hat{Q}$-box being composed of **1- and 2-body diagrams up to third order**

- L. Coraggio, A. Covello, A. G., N. Itaco, and T. T. S. Kuo, Prog. Part. Nucl. Phys. **62,** 135 (2009)
- L. Coraggio, A. Covello, A. G., N. Itaco, and T. T. S. Kuo. Annals of Phys. **327,** 2061 (2012)

Step 2 – Analysis of the ESFE: proton case

Proton ESPE as a function of the proton valence number



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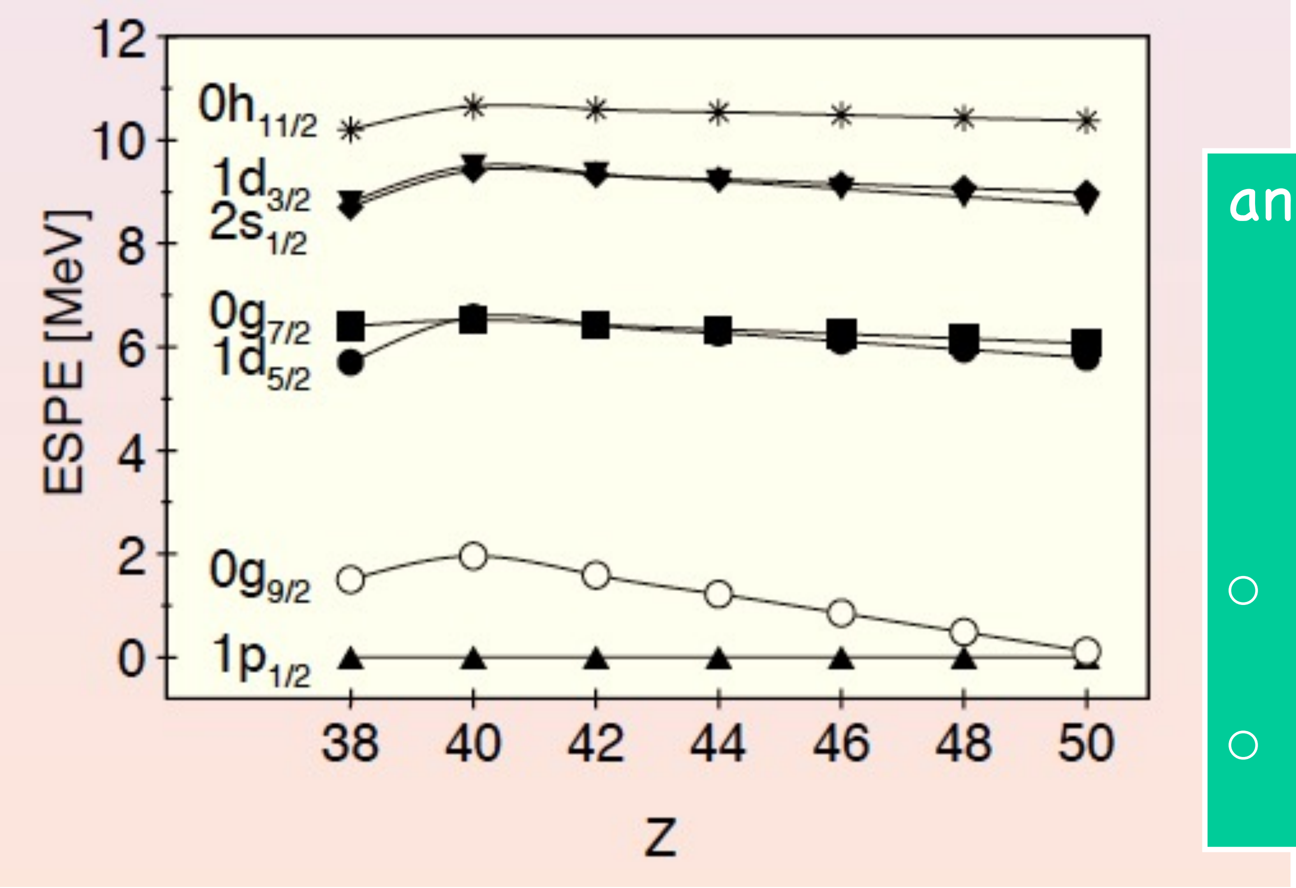

an almost constant gap of ~3 MeV separates the two proton subspaces:

- $1p_{1/2}$ $0g_{9/2}$ $1d_{5/2}$ $0g_{7/2}$
- $2s_{1/2}$ $2d_{3/2}$ $0h_{11/2}$

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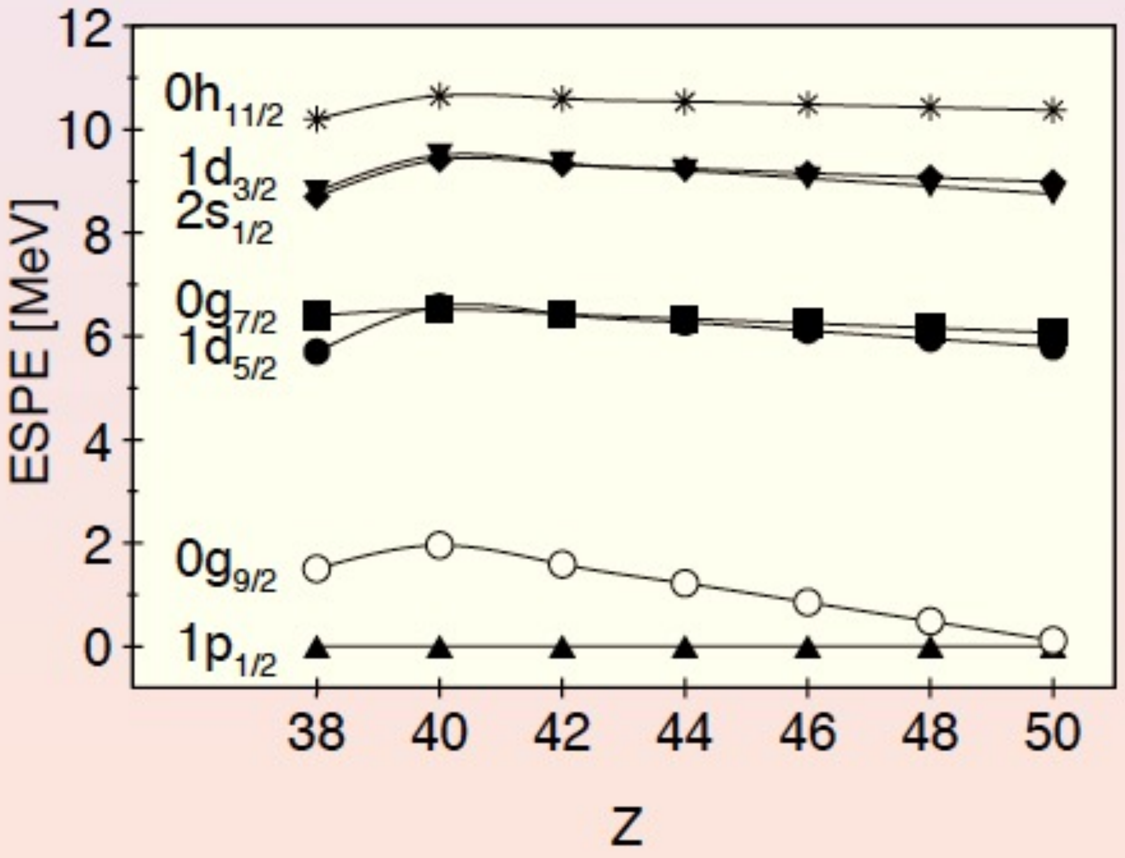

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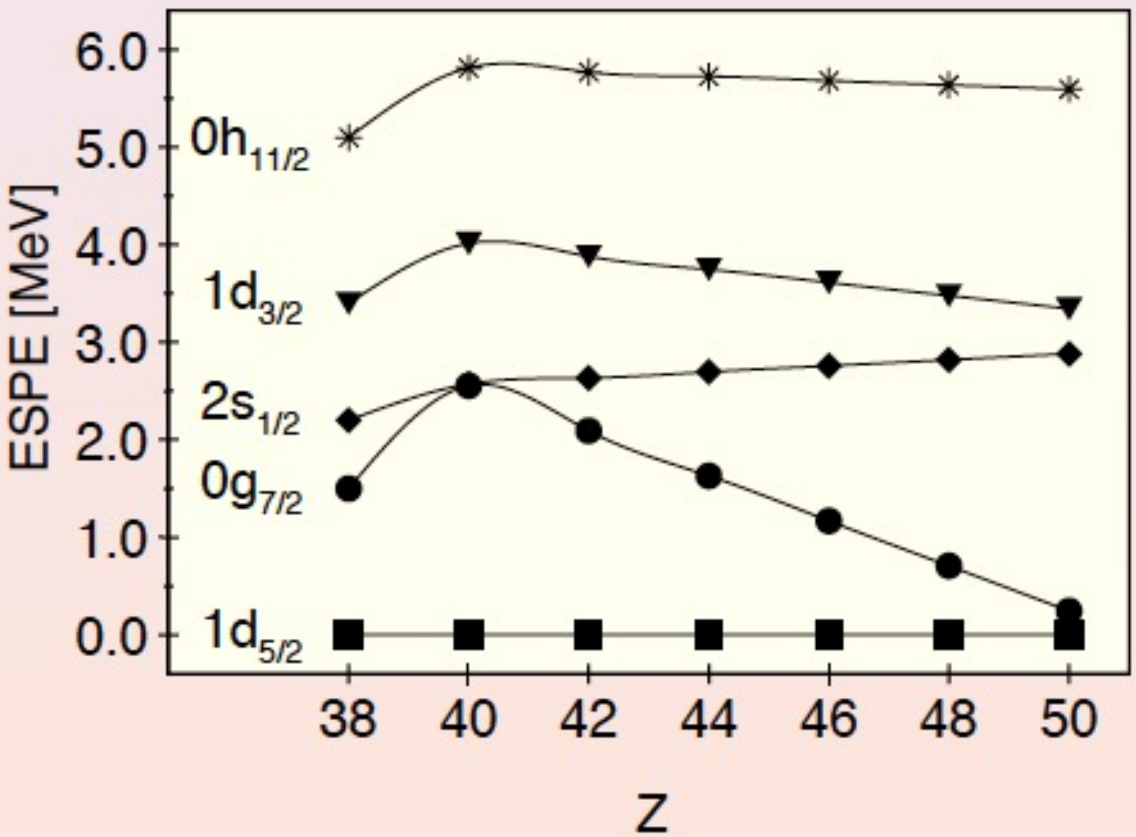
Step 2 – Analysis of the ESFE: neutron case

Neutron ESPE as a function of the proton valence number



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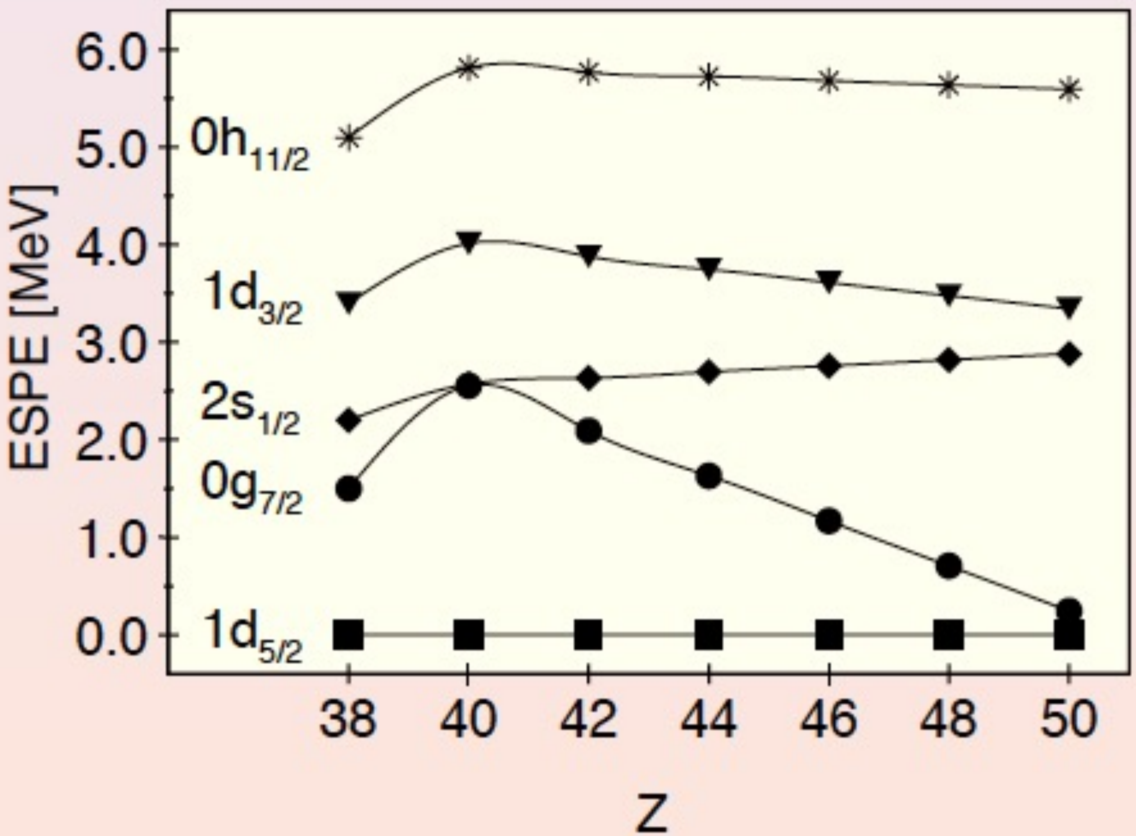
Neutron ESPE as a function of the proton valence number



✓ No signficant gap for low Z values

The filling of the proton $0g_{9/2}$ induces a relevant gap (~2.5 MeV) between the two neutron subspaces:

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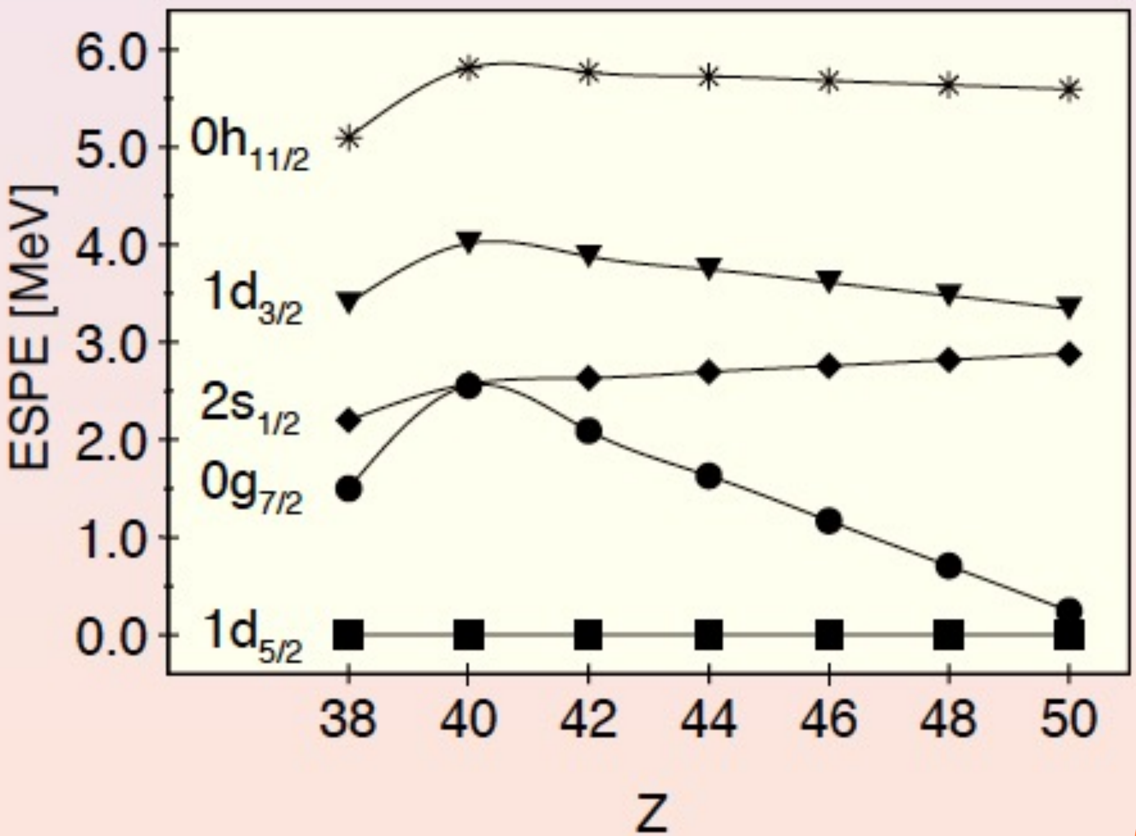

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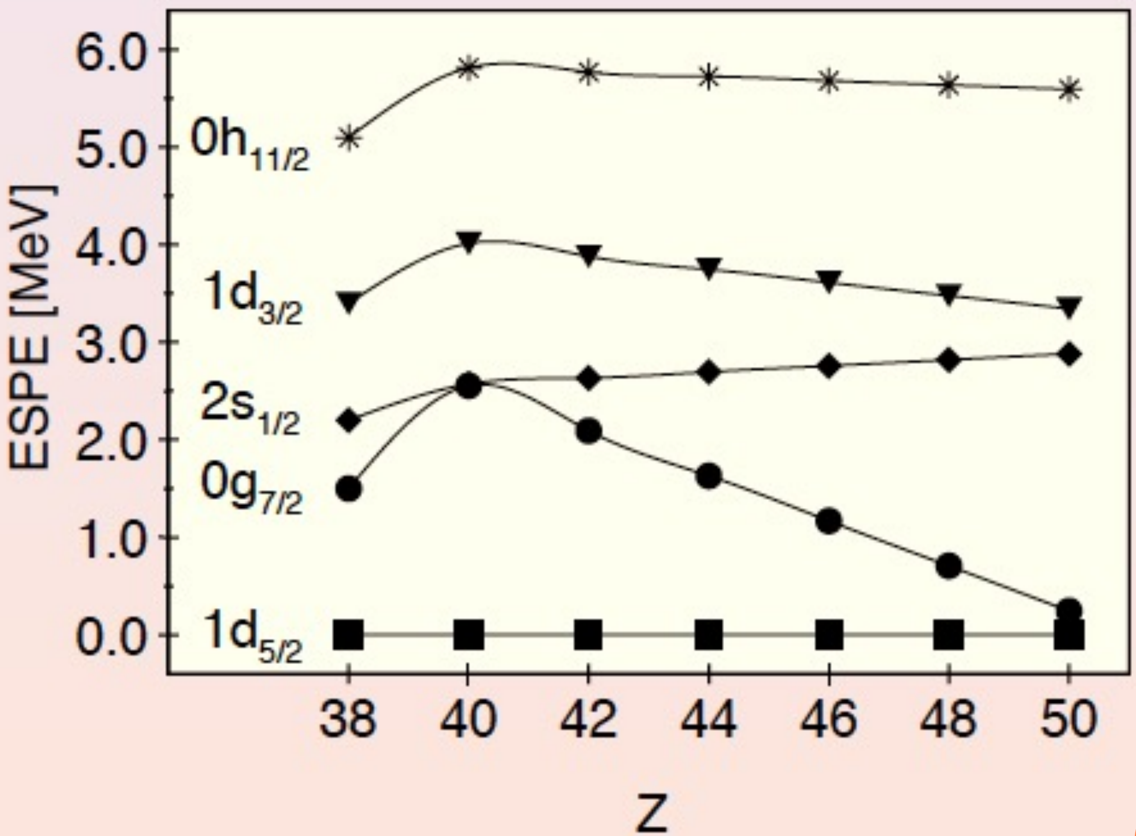

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[45]: $1p_{1/2}$ $0g_{9/2}$ $1d_{5/2}$ $0g_{7/2}$ π
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[42]: $1p_{1/2}$ $0g_{9/2}$ $1d_{5/2}$ $0g_{7/2}$ π
$1d_{5/2}$ $0g_{7/2}$ ν

Step 3 – Construction of H^{pn}

Unitary transformation of the "mother" Hamiltonian H^{75}

$$H^{75}|\psi_K\rangle = (H_0 + V)|\psi_K\rangle = E_K|\psi_K\rangle$$

[75] =

- [pn] → $P = \sum_{i=1}^{d} |i\rangle\langle i|$
- [7-p,5-n] → $Q=[75]-P$

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$$H^{pn} = \sum_{k=1}^{d} E_k\, |\phi_k >< \tilde{\phi}_k|$$

$$|\tilde{\phi}_k\rangle\text{: } < \tilde{\phi}_k|\phi_{k'} > = \delta_{kk'}$$

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$E_k ; | \psi_k \rangle$

from the mother Hamiltonian H^{75}

$|\phi_k\rangle = P|\psi_k\rangle$ --> $S_{ik} = <\phi_j|\phi_k>$

$< \tilde{\phi}_j| = \sum_{k=1}^{d} S_{jk}^{-1} < \phi_k|$

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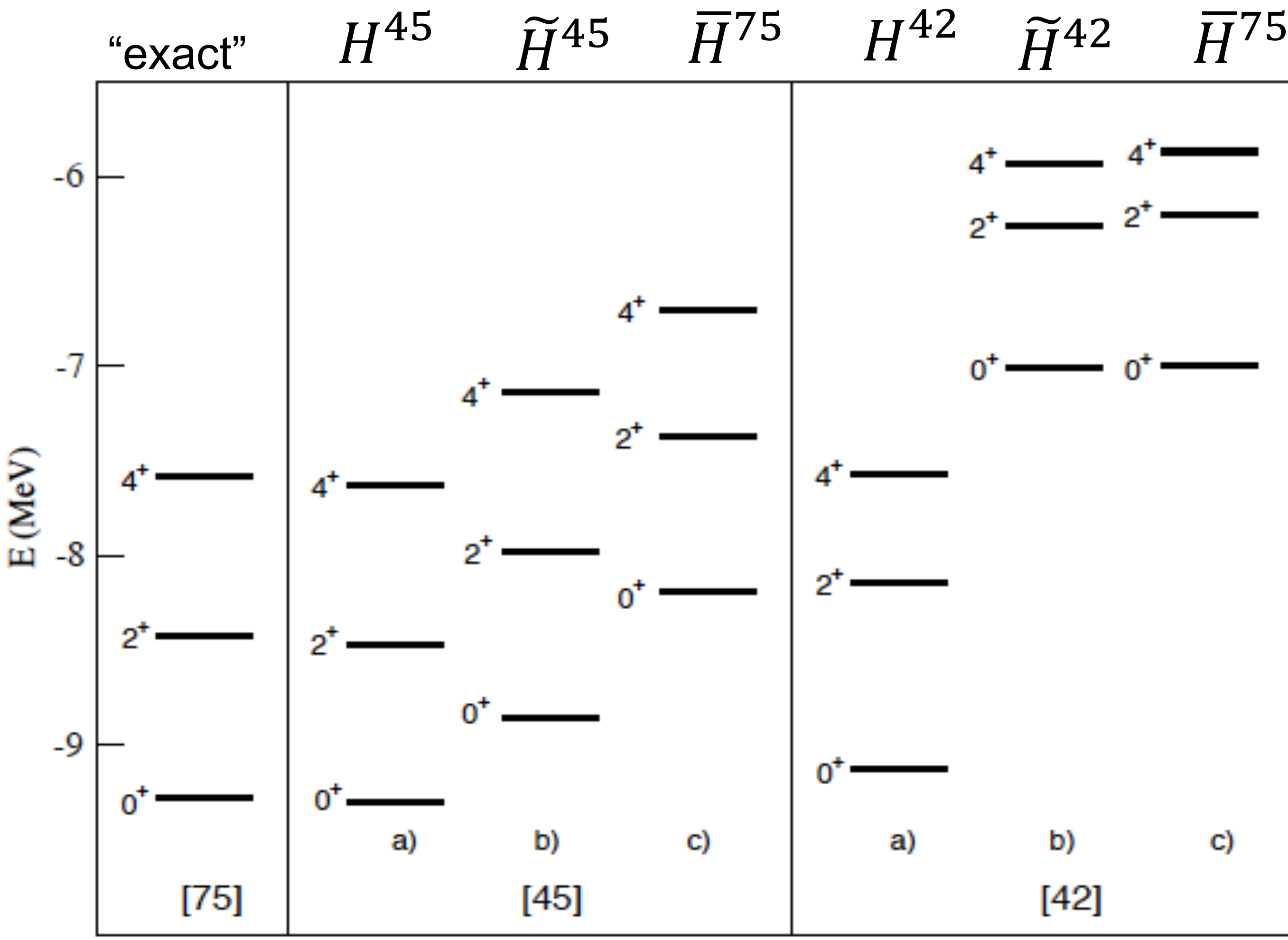
N=2 (^{90}Zr, ^{90}Sr, ^{90}Y) → H^{pn}: 1- + 2-body terms →

for ^{90}Zr, ^{90}Sr, ^{90}Y energy spectra with H^{pn} and H^{75} are "exactly" the same

Test: ^{96}Mo with 4-valence neutrons & 4-valence protons



a) H^{45} and H^{42} from H^{75} by unitary transformations

b) $\widetilde{H}^{45}$ and $\widetilde{H}^{42}$ directly derived from many-body perturbation theory within the model spaces [45] and [42]

c) $\overline{H}^{75}$: H^{75} contrained to the [45] and [42] spaces

Quadrupole properties of even isotopes with Z>38

- excitation energies of the yrast 2^+ states
- $B(E2; 0^+ \rightarrow 2^+)$ transition rates

in Zr, Mo, Ru, Pd, Cd, Sn

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B(E2; $0^+ \rightarrow 2^+$) with E2 effective charges consistent with the "mother" Hamiltonian H^{75}

$n_a l_a j_a$ $n_b l_b j_b$	$\langle a \| e_p \| b \rangle$	$\langle a \| e_n \| b \rangle$
$0g_{9/2}$ $0g_{9/2}$	1.53	
$0g_{9/2}$ $0g_{7/2}$	1.58	
$0g_{9/2}$ $1d_{5/2}$	1.51	
$0g_{7/2}$ $0g_{9/2}$	1.77	
$0g_{7/2}$ $0g_{7/2}$	1.84	1.00
$0g_{7/2}$ $1d_{5/2}$	1.84	0.98
$0g_{7/2}$ $1d_{3/2}$	1.86	0.98
$1d_{5/2}$ $0g_{9/2}$	1.59	
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However within the [45] and [42] spaces one should have used E2 effective operators consistent with H^{45}, H^{42} to account for the further renormalizations induced by neglected degrees of freedom → 2-body E2 effective operator

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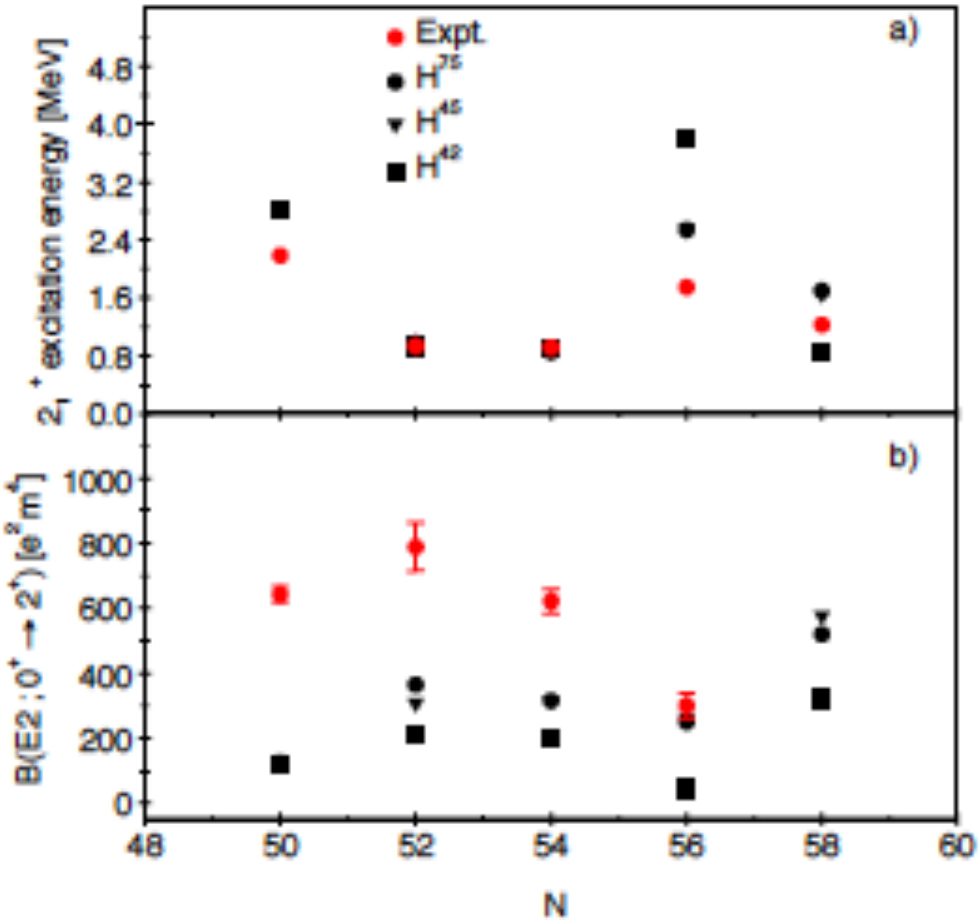
Calculations are performed with the public version of the ANTOINE shell-model code

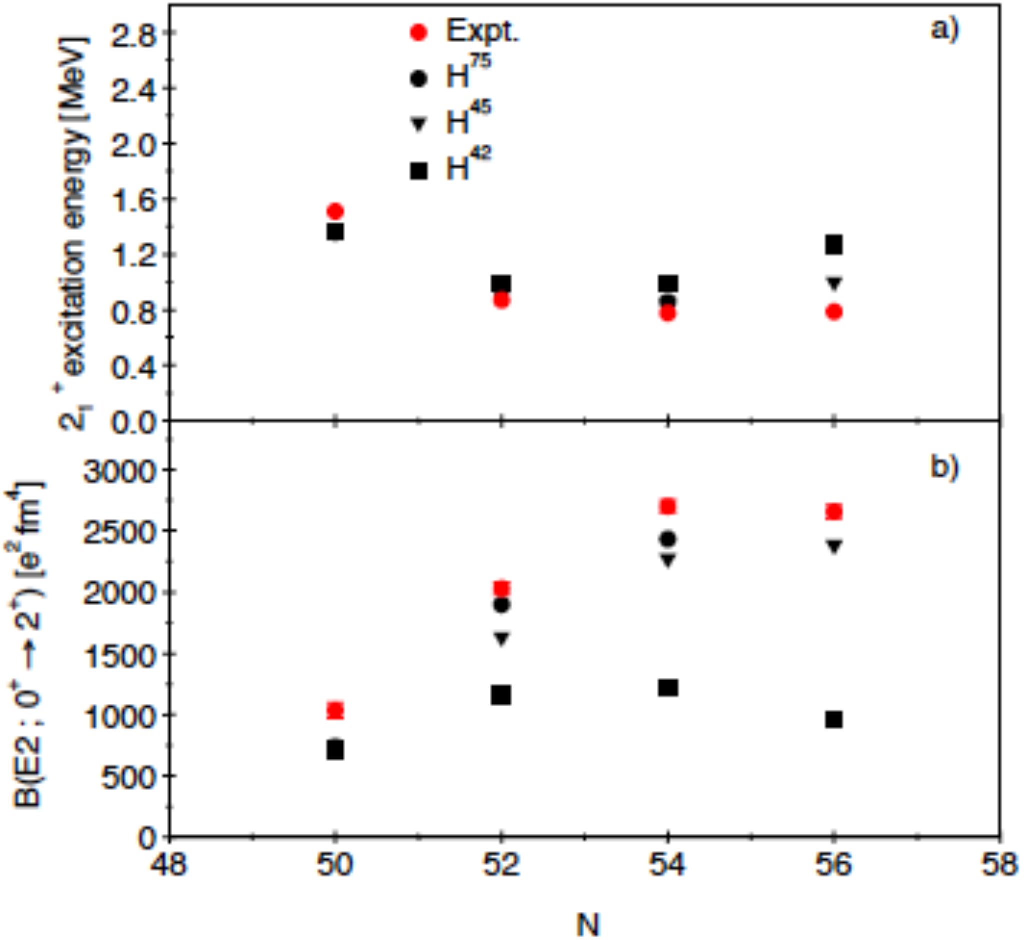
$_{40}$Zr isotopes



- H^{45} and H^{75} results are very close
- H^{42} results are quite different from those obtained with H^{45} and H^{75}
- No agreement with experimental data: B(E2) strongly undersestimated from N=50 to 54

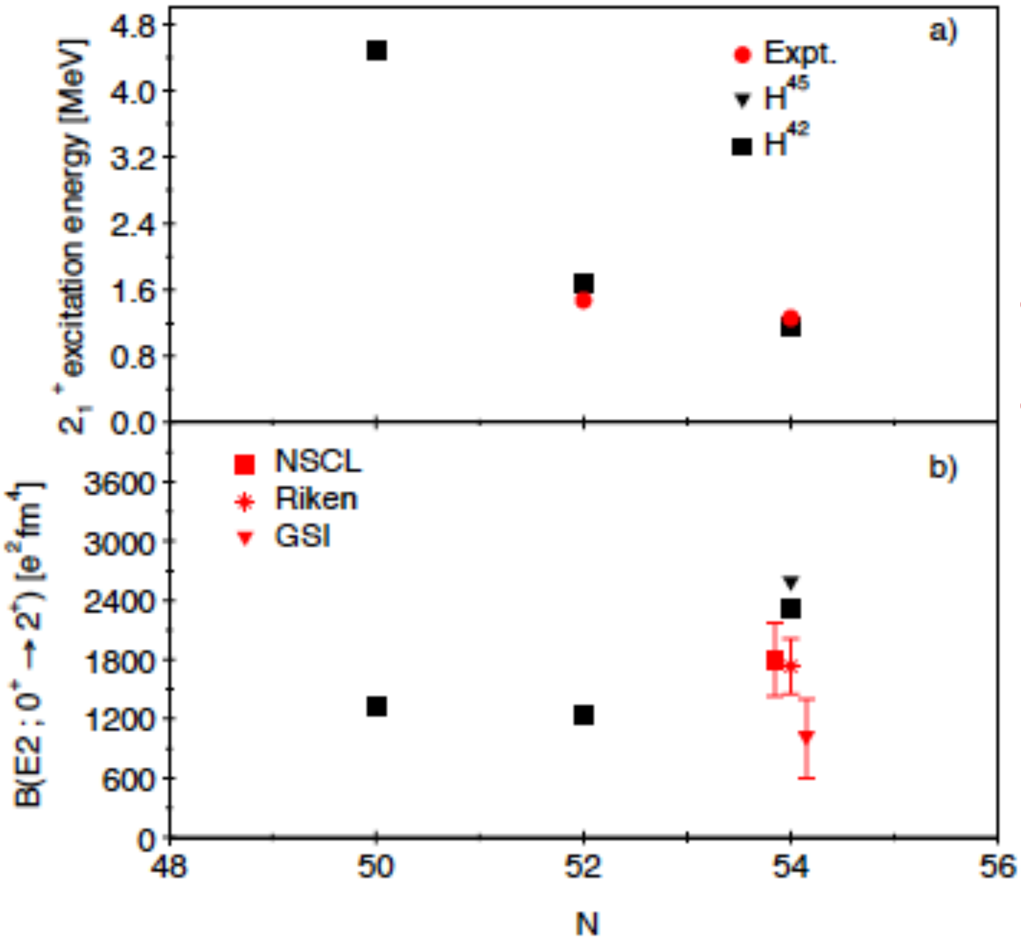
Missing Z = 38 cross shell excitations?

$_{42}$Mo isotopes



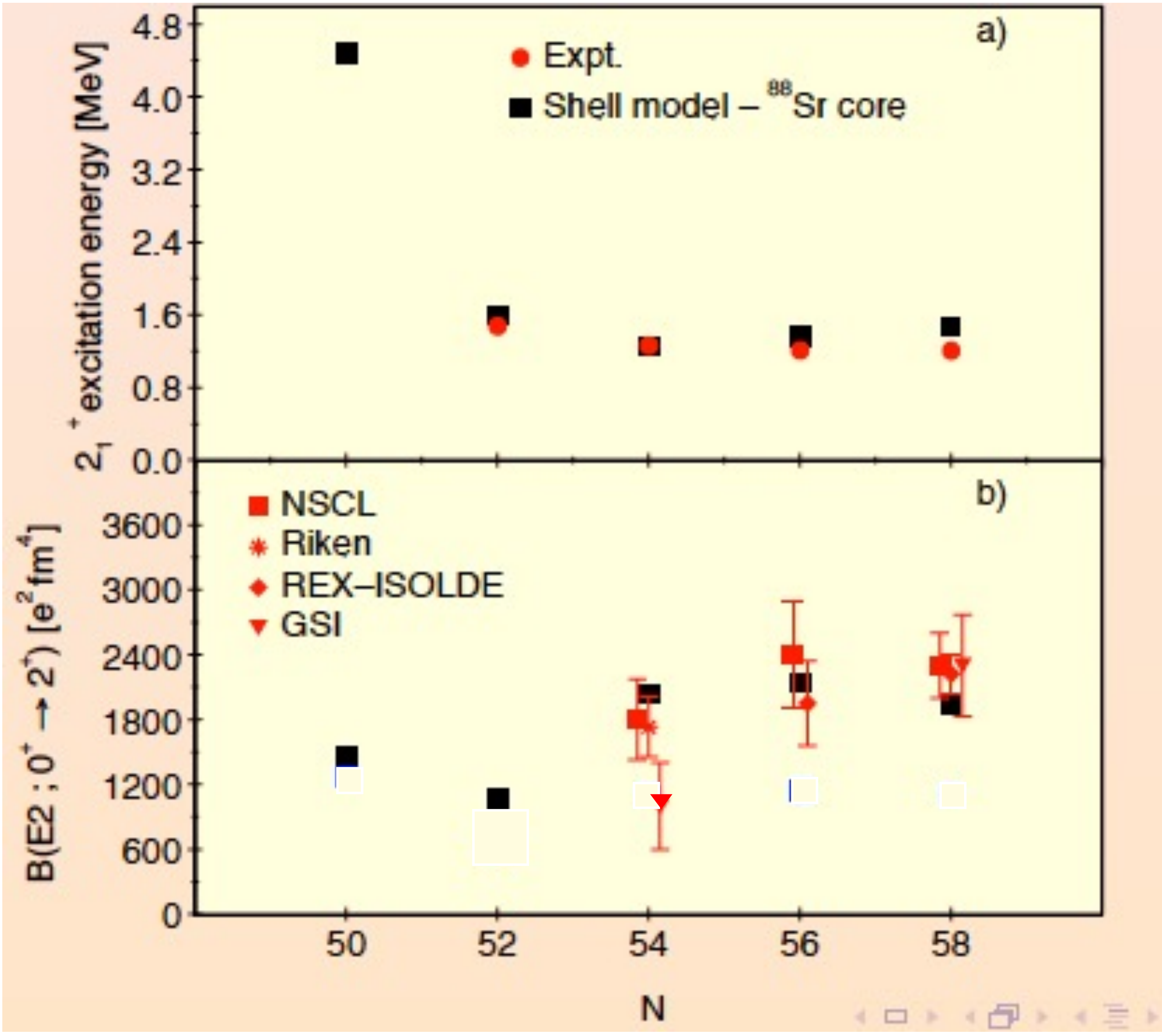
- No H^{75} calculations for N=56
- H^{45} and H^{75} results are very close and in good agreement with experiment. The increase in the number of protons from Zr to Mo is likely to induce a quenching of the Z = 38 cross-shell excitations
- The [42] model space is inadequate, especially for the B(E2)

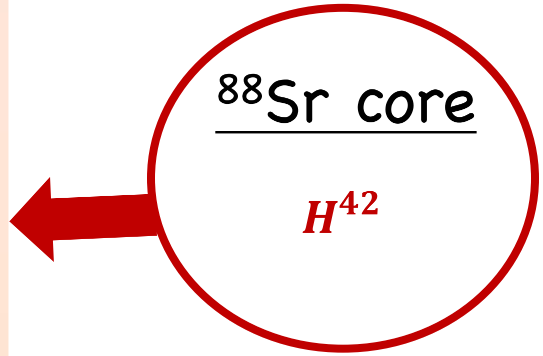
$_{50}$Sn isotopes



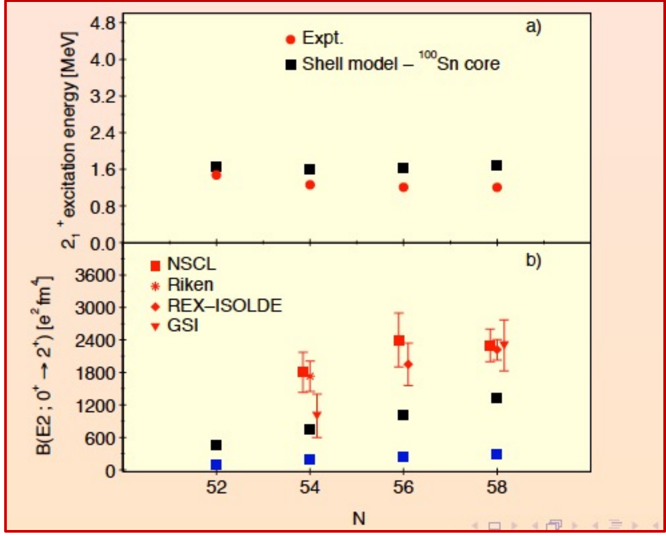
- No H^{75}calculations
- H^{45} and H^{42} results are very close and in good agreement with the availble experimental data

$_{50}$Sn isotopes





Only neutron degrees of freedom



Summary and perspectives

- **Double-step approach** to simplify the computational problem of large-scale shell-model calculations.

  ✓ The core of the method is the study of the ESPE of the large-scale Hamiltonian, so as to identify the most relevant degrees of freedom to be taken into account

  ✓ A unitary transformation is employed to derive new effective shell-model Hamiltonians defined within a reduced set of single-particle orbitals, accordingly to the ESPE analysis.

- Results for nuclei around ^{100}Sn obtained with the effectively truncated Hamiltonians indicates the ability to reproduce energies and electromagnetic transition rates of the original SM Hamiltonian, especially when the ESPE provide a neat separation in energy between the new model subspaces and their complement.

Next steps:

- Extensions to other regions, as for example isotopic and isotonic chains with valence particle outside doubly-magic ^{132}Sn and ^{208}Pb
- Calculations of the effective two-body electromagnetic operators, consistently with the unitary transformation of the Hamiltonian,