A new double-step procedure for the derivation of effective shell-model hamiltonians

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L.C., A. Covello, A. Gargano, N. Itaco, and T. T. S. Kuo, Phys. Rev. C **91**, 041301 (2015).

Motivations

- Large-scale shell-model calculations are, at present, a consolidated tool to investigate nuclear properties.
- The new physics coming from RIBs facilities provides a challenging ground, since they are approaching the nuclear driplines.
- Shell-model practitioners experience often the need to truncate the number of configurations of shell-model basis to overcome the computational complexity.

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Full pf shell model study of A=48 nuclei

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(Received 16 December 1993)

Exact diagonalizations with a minimally modified realistic force lead to detailed agreement with measured level schemes and electromagnetic transitions in ^{48}Ca, ^{48}Sc, ^{48}Ti, ^{48}V, ^{48}Cr, and ^{48}Mn. Gamow-Teller strength functions are systematically calculated and reproduce the data to within the standard quenching factor. Their fine structure indicates that fragmentation makes much strength unobservable. As a by-product, the calculations suggest a microscopic description of the onset of rotational motion. The spectroscopic quality of the results provides strong arguments in favor of the general validity of monopole corrected realistic forces, which is discussed.

PACS number(s): 21.10.−k, 27.40.+z, 21.60.Cs, 23.40.−s

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Nuclear Shell Model by the Quantum Monte Carlo Diagonalization Method

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(Received 29 April 1996)

The feasibility of shell-model calculations is radically extended by the quantum Monte Carlo diagonalization method with various essential improvements. The major improvements are made in the sampling for the generation of shell-model basis vectors, and in the restoration of symmetries such as angular momentum and isospin. Consequently the level structure of low-lying states can be studied with realistic interactions. After testing this method on ^{24}Mg, we present first results for energy levels and $E2$ properties of ^{64}Ge, indicating its large and γ-soft deformation. [S0031-9007(96)01252-5]

PACS numbers: 21.60.Ka, 21.60.Cs, 24.10.Cn, 27.50.+e

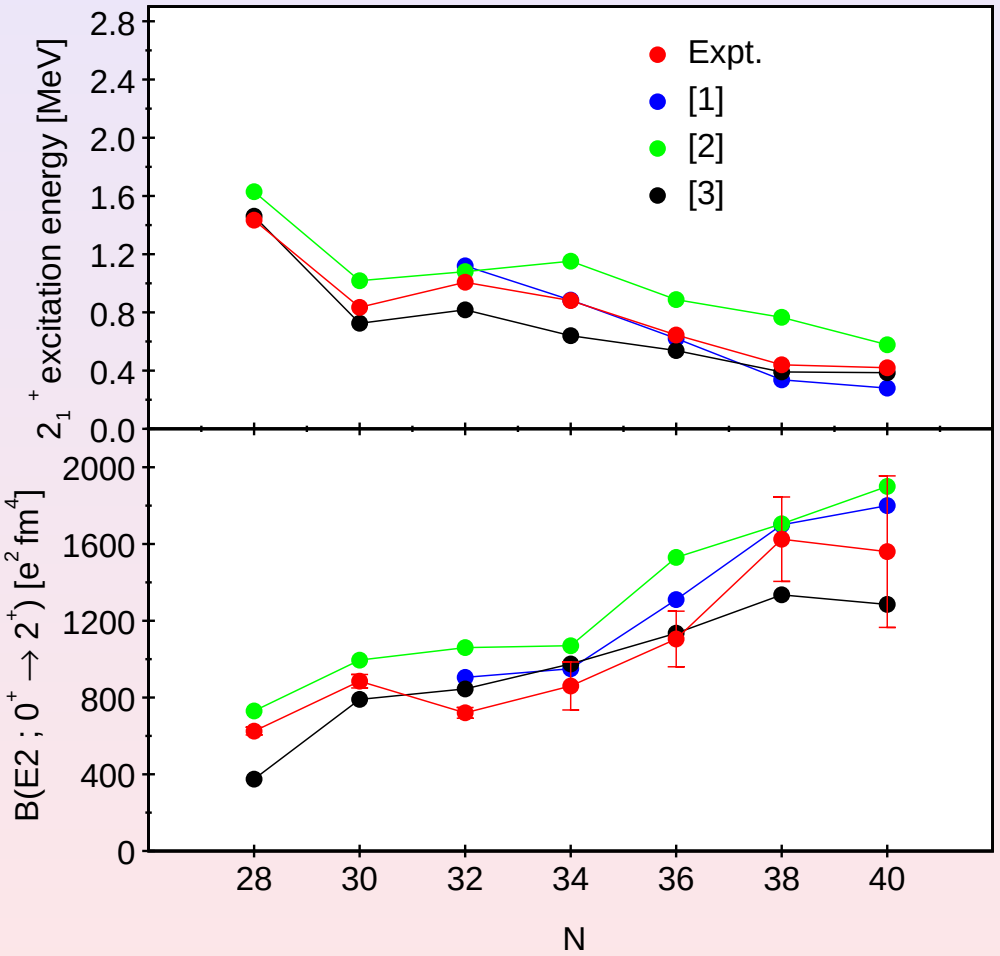
Large-scale shell model

Large-scale shell model: shell model calculations performed within a model space made up by a number of orbitals larger than usual.

An extended model space enables to study exotic (for shell model) properties: collective motion, deformation, clustering, etc.

Dealing with many valence nucleons makes the diagonalization of the shell-model eigenvalue problem quite demanding.

An example: quadrupole collectivity in Cr isotopes



The onset of collectivity in Cr isotopes at $N = 40$ can be explained at least within neutron model space $1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$

1. H. L. Crawford *et al.*, Phys. Rev. Lett. **110**, 242701 (2013).
2. N. Shimizu *et al.*, Prog. Theor. Exp. Phys. **2012**, 01A205 (2012).
3. L. Coraggio *et al.*, Phys. Rev. C **89**, 024319 (2014).

An example: quadrupole collectivity in Cr isotopes

- In calculations [1] both proton model space is spanned by the four orbitals $0f_{7/2}, 1p_{3/2}, 1p_{1/2}, 0f_{5/2}$ and the five neutron ones $1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$ outside ^{48}Ca core, and the shell model basis is truncated so to retain up to $14p-14h$ excitations across the $Z=28$ and $N=40$ gaps.
- In calculations [2] both proton and neutron model spaces are spanned by the six orbitals $0f_{7/2}, 1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$ outside ^{40}Ca core, and the reduction of the matrices to be diagonalized is provided by the importance sampling of the shell-model basis performed within the Monte Carlo Shell Model (MCSM) approach.
- In calculations [3] a realistic shell-model interaction has been derived so to be effective in a reduced proton model space spanned by the $0f_{7/2}, 1p_{3/2}$ orbitals and the five neutron $1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$ ones outside ^{48}Ca.

Calculations with a large number of valence nucleons need to employ reduction/truncation schemes.

Those schemes need to be under control, convergence properties and theoretical error estimates are an important tool to understand the reliability of the shell-model calculations.

A modest proposal

A "Poor Man's Approach" to lighten the computational complexity of diagonalizing a "mother hamiltonian" defined in a large shell-model space:

- First step: analyze the evolution of the effective single-particle energies (ESPE) of the "mother hamiltonian", so to locate the relevant degrees of freedom (single-particle orbitals) that characterize the physical system.
- Second step: perform a unitary transformation of the "mother hamiltonian" into a reduced model space, so to obtain an effective hamiltonian that is more manageable from the computational point of view.

Valence-nuclei outside ^{88}Sr

As a physical case, let us consider nuclei with valence nucleons outside ^{88}Sr.

Our interest: to study quadrupole collectivity around doubly closed ^{100}Sn, considering explicitly $Z = 50$ cross-shell excitations.

Model space of the "mother hamiltonian":

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

The shell-model effective hamiltonian

The effective hamiltonian H^{75} is derived from a $V_{\mathrm{low-k}}$ by way of the time-dependent perturbative approach as developed by Kuo and his co-workers in the 1970s (see *T. T. S. Kuo and E. Osnes, Lecture Notes in Physics vol. 364 (1990)*)

In this approach the effective hamiltonian H_{eff} is expressed as

$$H_{\mathrm{eff}} = \hat{Q} - \hat{Q}' \int \hat{Q} + \hat{Q}' \int \hat{Q} \int \hat{Q} - \hat{Q}' \int \hat{Q} \int \hat{Q} \int \hat{Q} \cdots ,$$

- The so-called $\hat{Q}$-box is a collection of irreducible valence-linked diagrams
- The integral sign represents a generalized folding operation

- Input V_{NN}: $V_{\mathrm{low-k}}$ derived from the high-precision *NN* CD-Bonn potential with a cutoff: $\Lambda = 2.6$ fm^{-1}.
- H_{eff} obtained calculating the Q-box up to the 3rd order in $V_{\mathrm{low-k}}$.
- Single-particle energies and effective state-dependent charges are taken from the theory

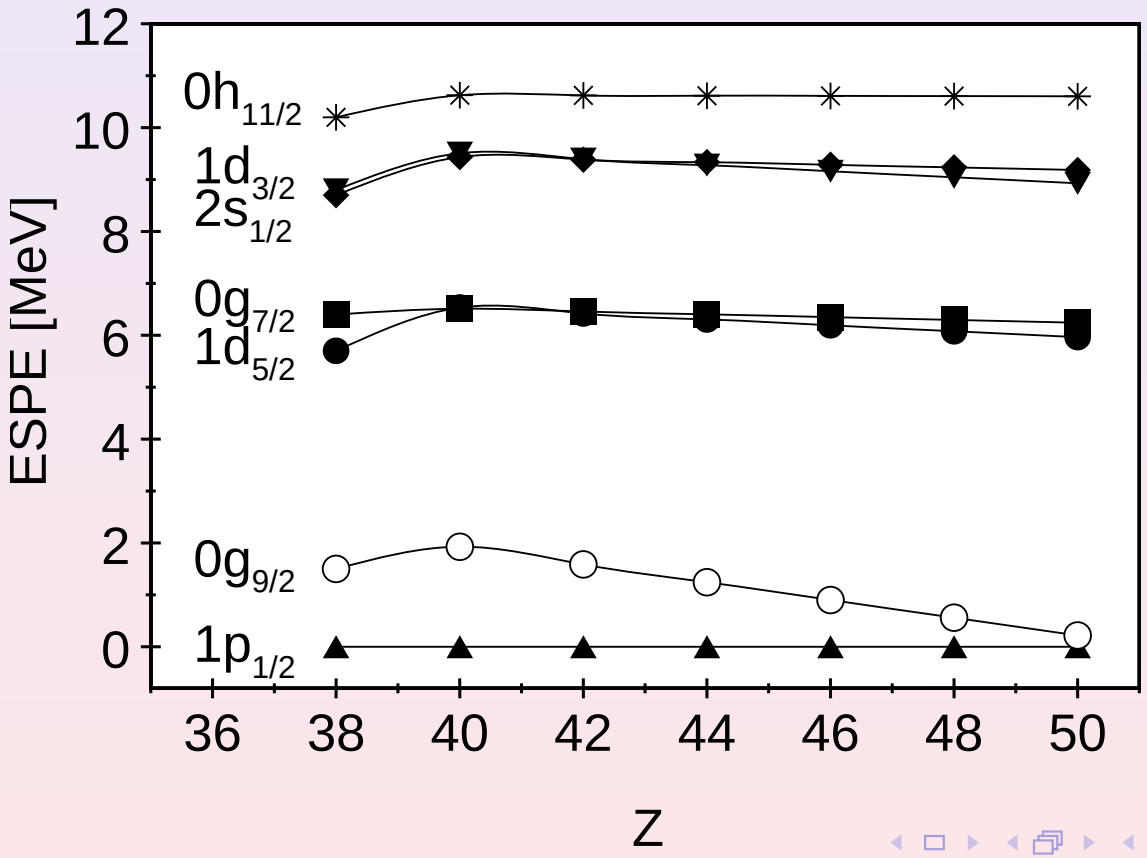
Single-particle properties with H^{75}

orbital	proton s.p.e.
$1p_{1/2}$	0.0
$0g_{9/2}$	1.5
$0g_{7/2}$	5.7
$1d_{5/2}$	6.4
$1d_{3/2}$	8.8
$2s_{1/2}$	8.7
$0h_{11/2}$	10.2
orbital	neutron s.p.e.
$1d_{5/2}$	0.0
$0g_{7/2}$	1.5
$2s_{1/2}$	2.2
$1d_{3/2}$	3.4
$0h_{11/2}$	5.1

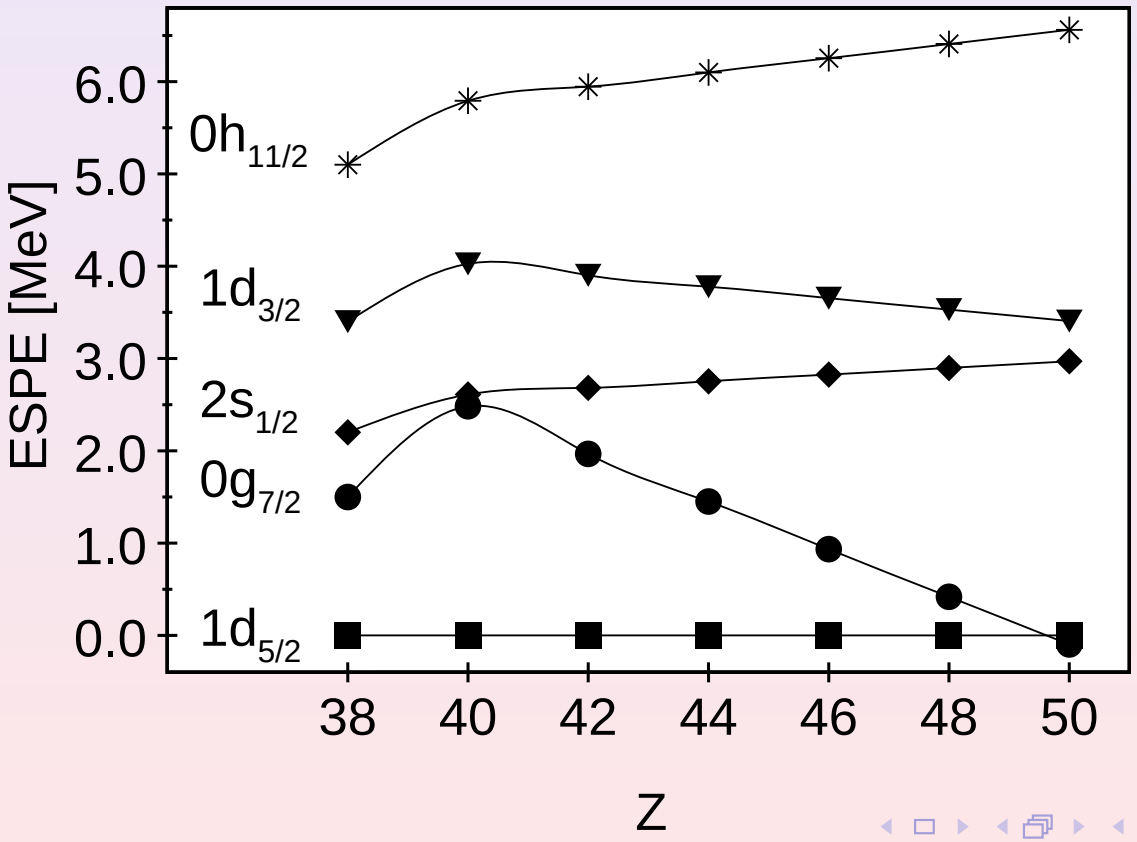
$n_a l_a j_a \; n_b l_b j_b$	$\langle a\|e_p\|b\rangle$
$0g_{9/2}\; 0g_{9/2}$	1.62
$0g_{9/2}\; 0g_{7/2}$	1.67
$0g_{9/2}\; 1d_{5/2}$	1.60
$0g_{7/2}\; 0g_{7/2}$	1.73
$0g_{7/2}\; 1d_{5/2}$	1.74
$0g_{7/2}\; 1d_{3/2}$	1.76
$1d_{5/2}\; 1d_{5/2}$	1.73
$1d_{5/2}\; 1d_{3/2}$	1.72
$1d_{5/2}\; 2s_{1/2}$	1.76
$1d_{3/2}\; 1d_{3/2}$	1.74
$1d_{3/2}\; 2s_{1/2}$	1.76
$0h_{11/2}\; 0h_{11/2}$	1.72

$n_a l_a j_a \; n_b l_b j_b$	$\langle a\|e_n\|b\rangle$
$0g_{7/2}\; 0g_{7/2}$	0.94
$0g_{7/2}\; 1d_{5/2}$	0.96
$0g_{7/2}\; 1d_{3/2}$	0.95
$1d_{5/2}\; 1d_{5/2}$	0.94
$1d_{5/2}\; 1d_{3/2}$	0.97
$1d_{5/2}\; 2s_{1/2}$	0.79
$1d_{3/2}\; 1d_{3/2}$	0.96
$1d_{3/2}\; 2s_{1/2}$	0.79
$0h_{11/2}\; 0h_{11/2}$	0.87

Proton ESPE


12
10
8
6
4
2
0
ESPE [MeV]
0h11/2
1d3/2
2s1/2
0g7/2
1d5/2
0g9/2
1p1/2
36
38
40
42
44
46
48
50
Z

Neutron ESPE



Truncating the model space

- The evolution of proton and neutron ESPE suggests a possible reduction of both model spaces.
- By way of a unitary transformation we can derive a $H_{\rm eff}^{4n}$ defined in a reduced proton model space spanned only by 4 orbitals $1p_{1/2}, 0g_{9/2}, 0g_{7/2}, 1d_{5/2}$ and a neutron one spanned by both the 5 original orbitals or by only 2 orbitals $0g_{7/2}, 1d_{5/2}$.
- The physics of two valence-nucleon systems is exactly preserved.

The unitary transformation

Let us sketch out the derivation of H^{4n}.

The eigenvalue problem for H^{75} is:

$$H^{75}|\psi_k\rangle = E_k|\psi_k\rangle \qquad k = 1, ..., N$$

H^{75} is the sum of the unperturbed single-particle hamiltonian H_0 and the residual two-body potential V

$$H^{75} = H_0 + V \ .$$

The model space is splitted up in two subspaces P^{4n} and $Q^{3,5-n}$. Since H_0 is diagonal:

$$H_0 = PH_0P + QH_0Q \ .$$

The unitary transformation

The P-space eigenvalue problem is:

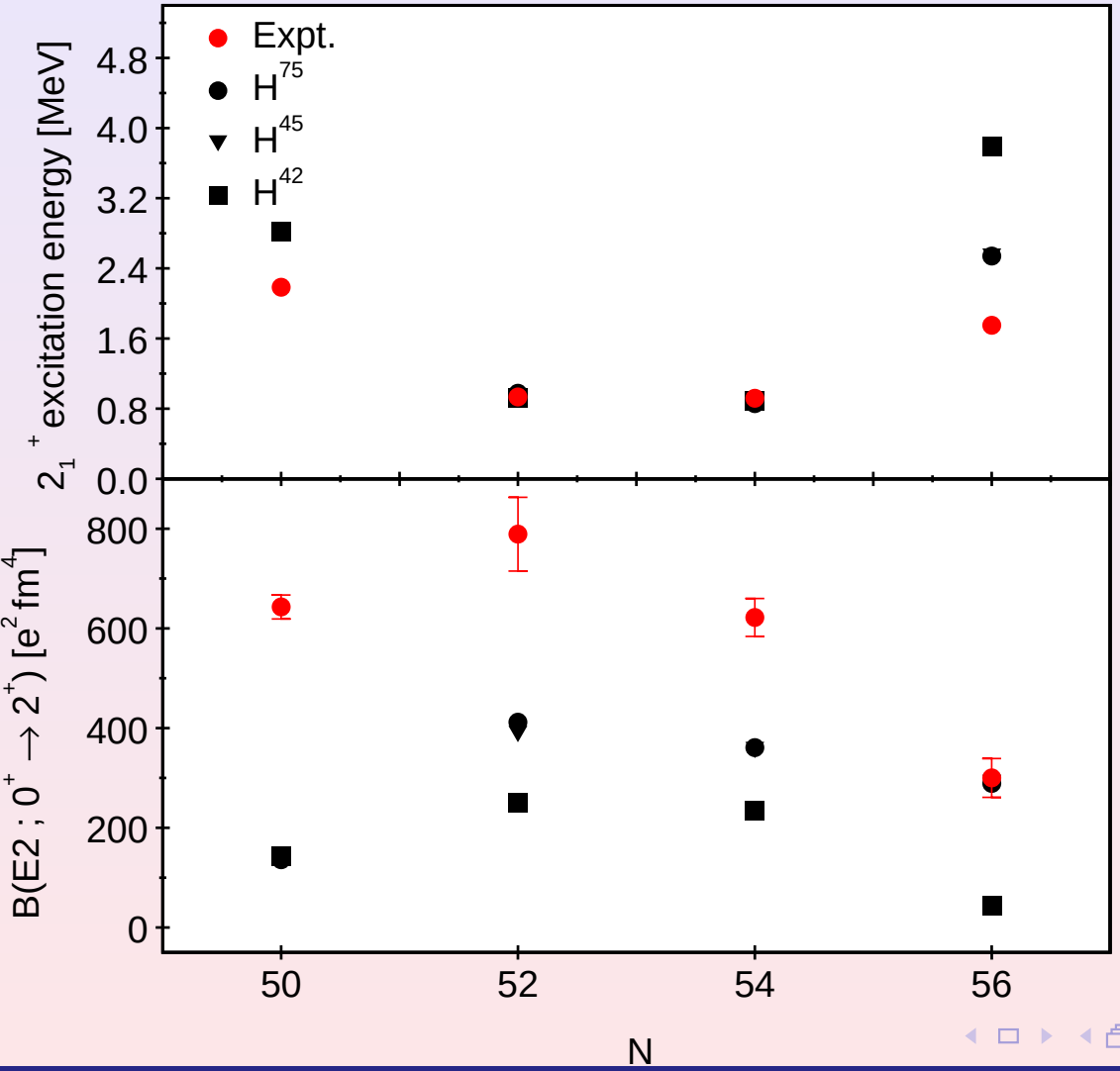
$$H^{4n}|\phi_k\rangle = \left(PH_oP + V^{4n}\right)|\phi_k\rangle = E_k|\phi_k\rangle \quad k = 1, ..., d$$

where $|\phi_k\rangle = P|\psi_k\rangle$.
The eigenvalue problem for H^{75} can be easily solved for the two valence-nucleon systems (^{90}Zr,^{90}Sr,^{90}Y), and consequently providing the E_k, ψ_k.
The solutions of the equation for the effective residual interaction $V^{4,n}$ are given by:

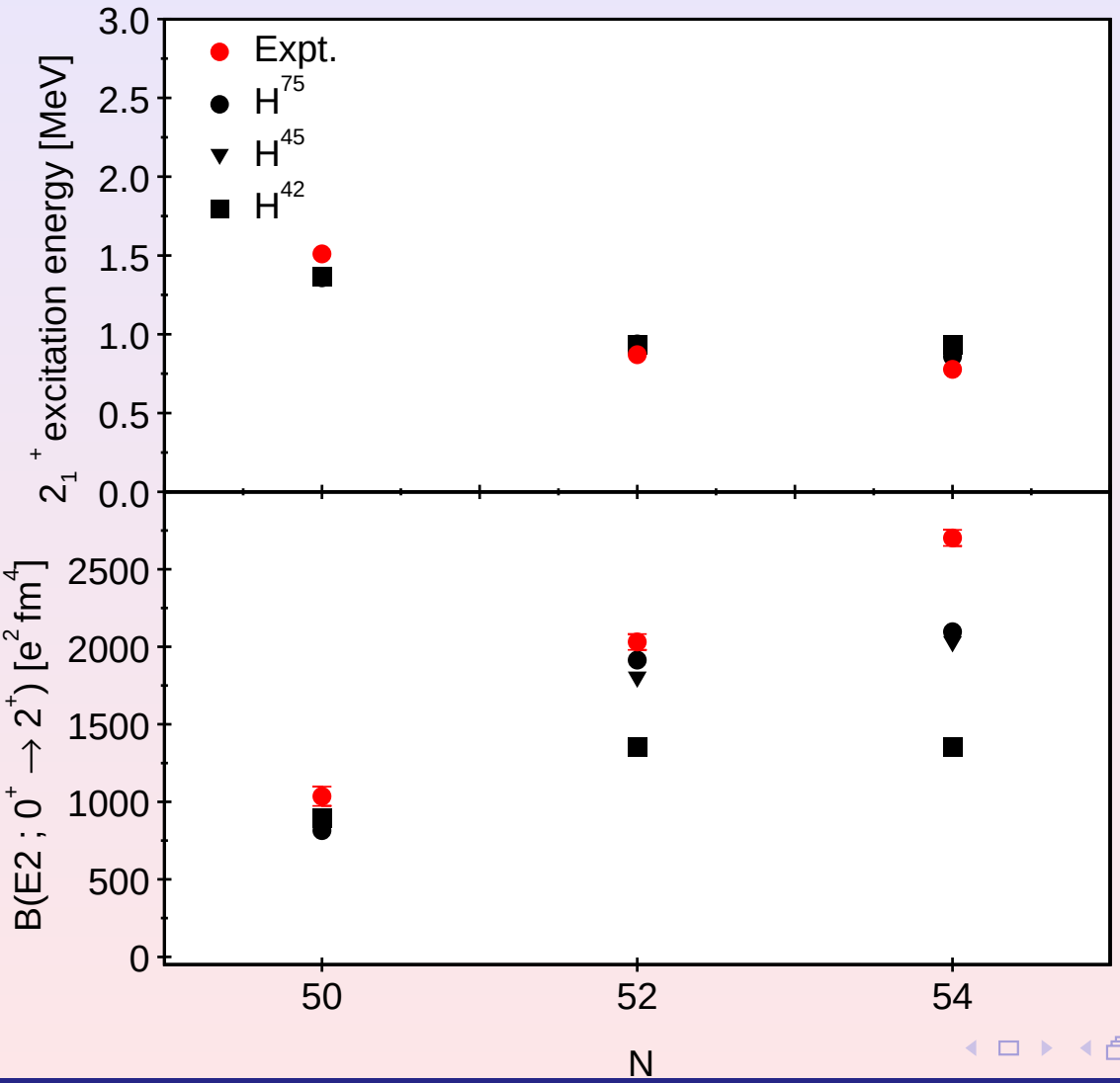
$$V^{4n} = \sum_{k=1}^{d}(E_k - E_0)|\phi_k\rangle\langle\tilde{\phi}_k| \ ,$$

where $|\tilde{\phi}_k\rangle$ are biorthogonal states defined as $|\tilde{\phi}_k\rangle\langle\phi_{k'}| = \delta_{kk'}$

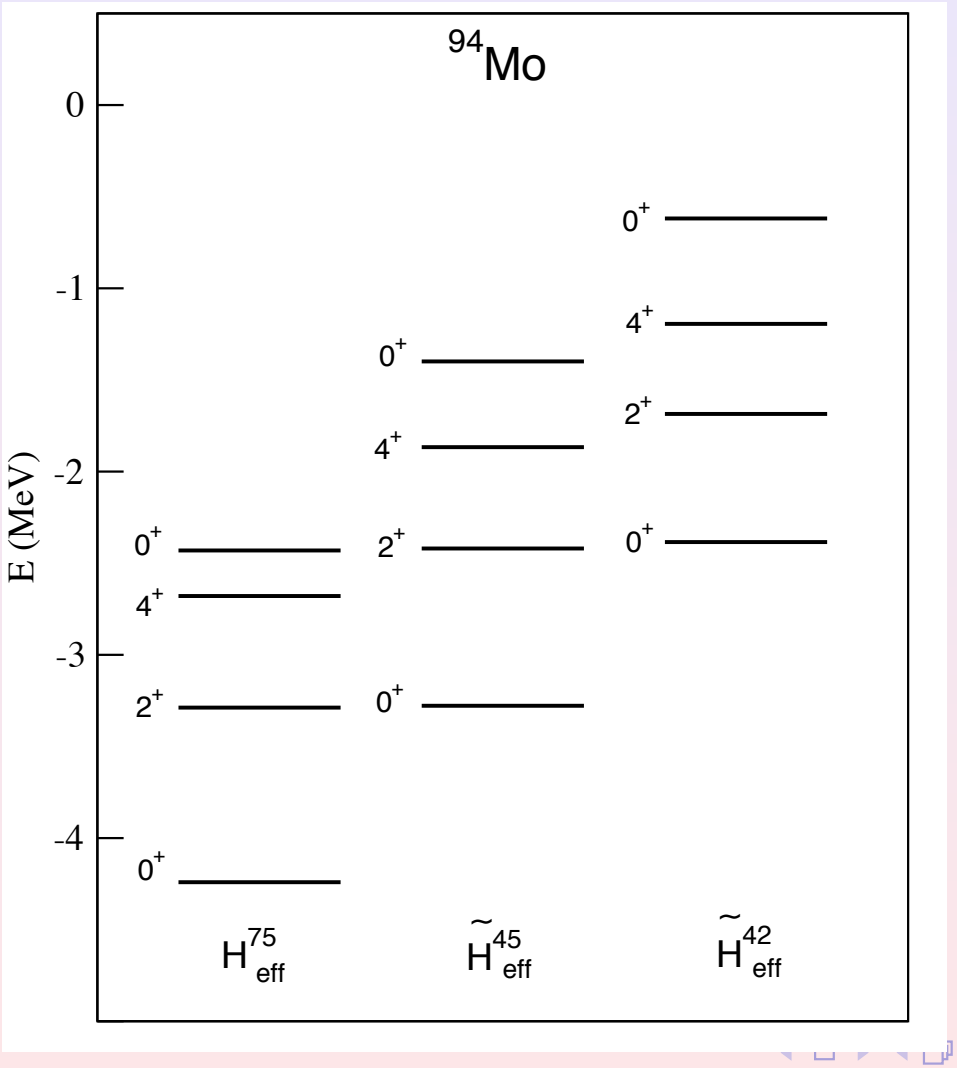
Results for Zr isotopes



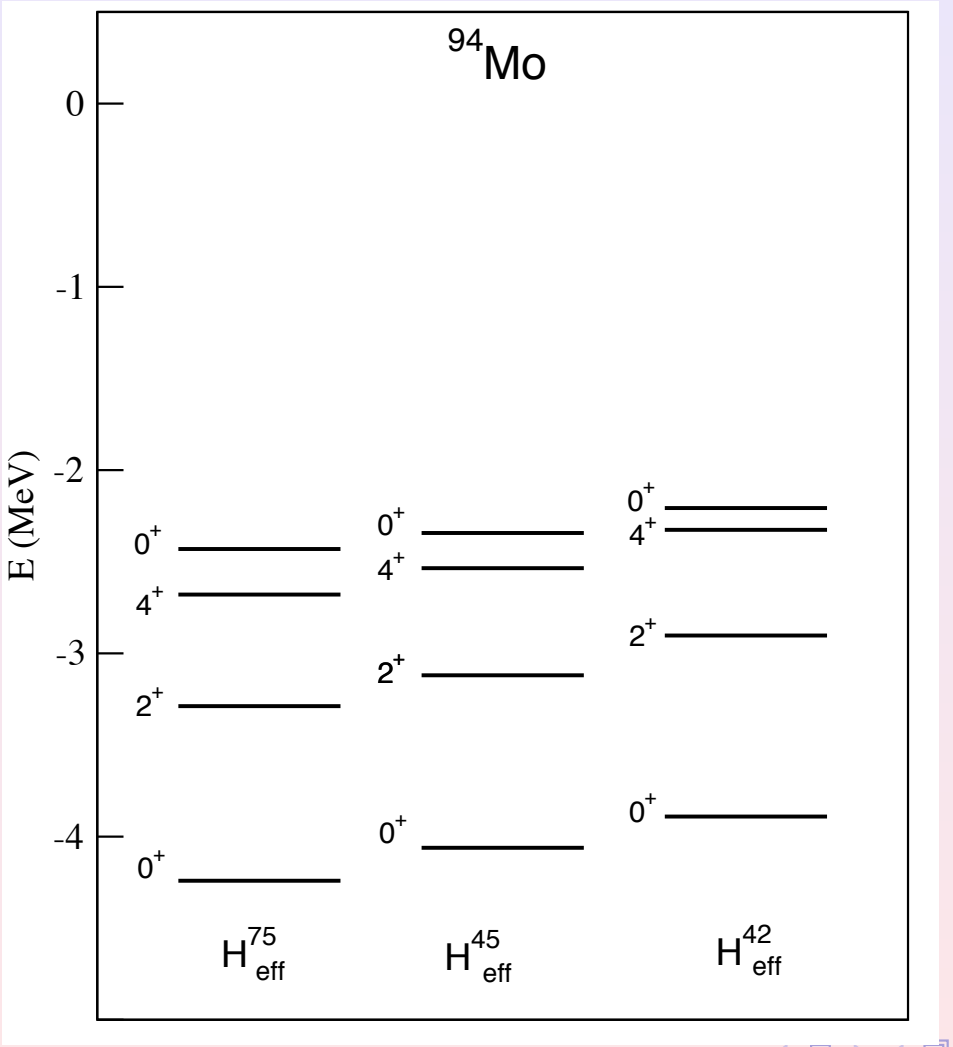
Results for Mo isotopes



A closer look to ^{94}Mo



A closer look to ^{94}Mo



Application to light tin isotopes

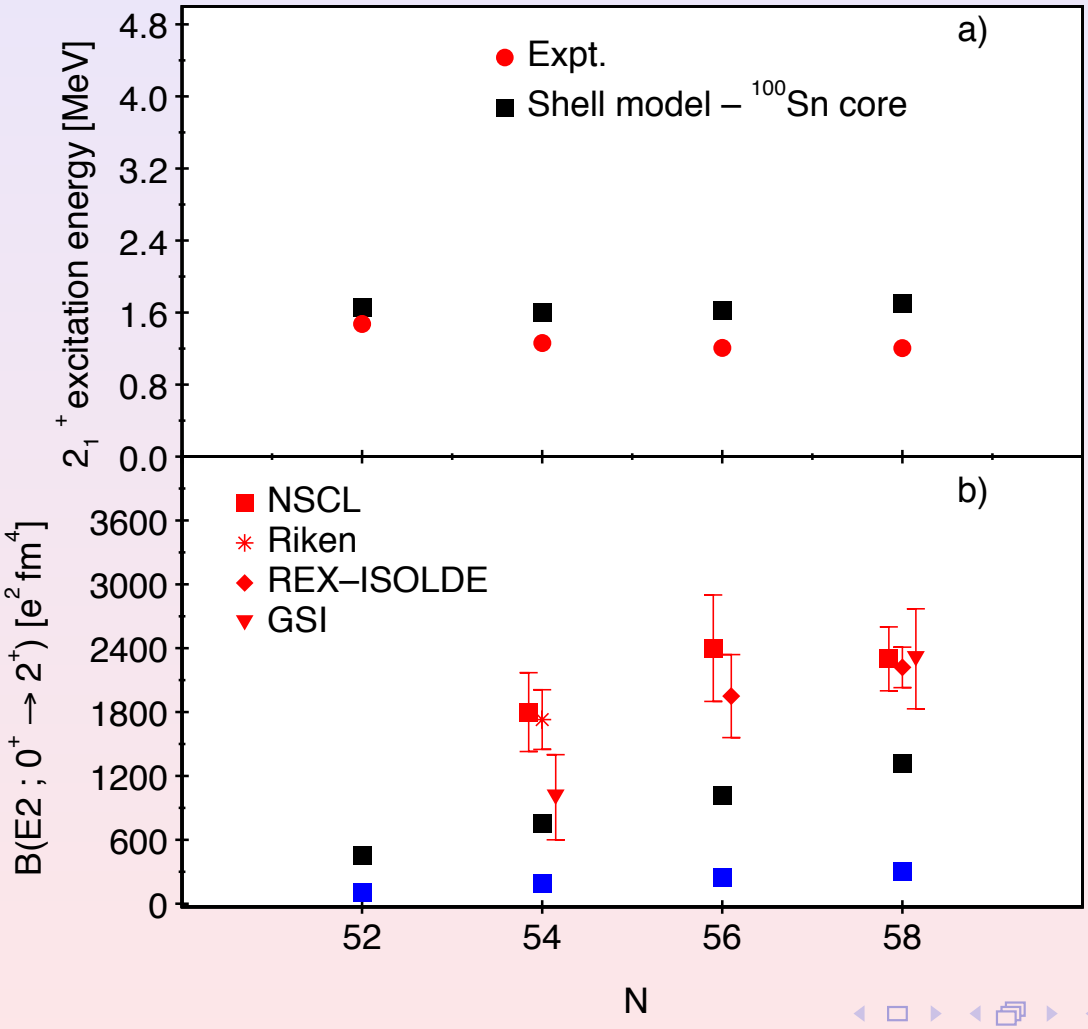
- At present there is a renewed experimental interest in the physics of light tin isotopes:
  1. A. Banu *et al.*, Phys. Rev. C **72**, 061305 (2005).
  2. G. Guastalla *et al.*, Phys. Rev. Lett. **110**, 172501 (2013).
  3. V. M. Bader *et al.*, Phys. Rev. C **88**, 051301 (2013).
  4. P. Doornenbal *et al.*, Phys. Rev. C **90**, 061302 (2014).
- Observed quadrupole collectivity: a challenge for shell-model calculations.
- To investigate the ability of realistic many-body calculations to explain the mechanism of the enhanced $B(E2)$ values

Results with neutron degrees of freedom only

orbital	single-particle energy
$0g_{7/2}$	0.0
$1d_{5/2}$	0.1
$1d_{3/2}$	1.3
$2s_{1/2}$	1.9
$0h_{11/2}$	4.1

$n_a l_a j_a$	$n_b l_b j_b$	$\langle a\|e_n\|b\rangle$
$0g_{7/2}$	$0g_{7/2}$	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

$B(E2)$s in ligth tin isotopes

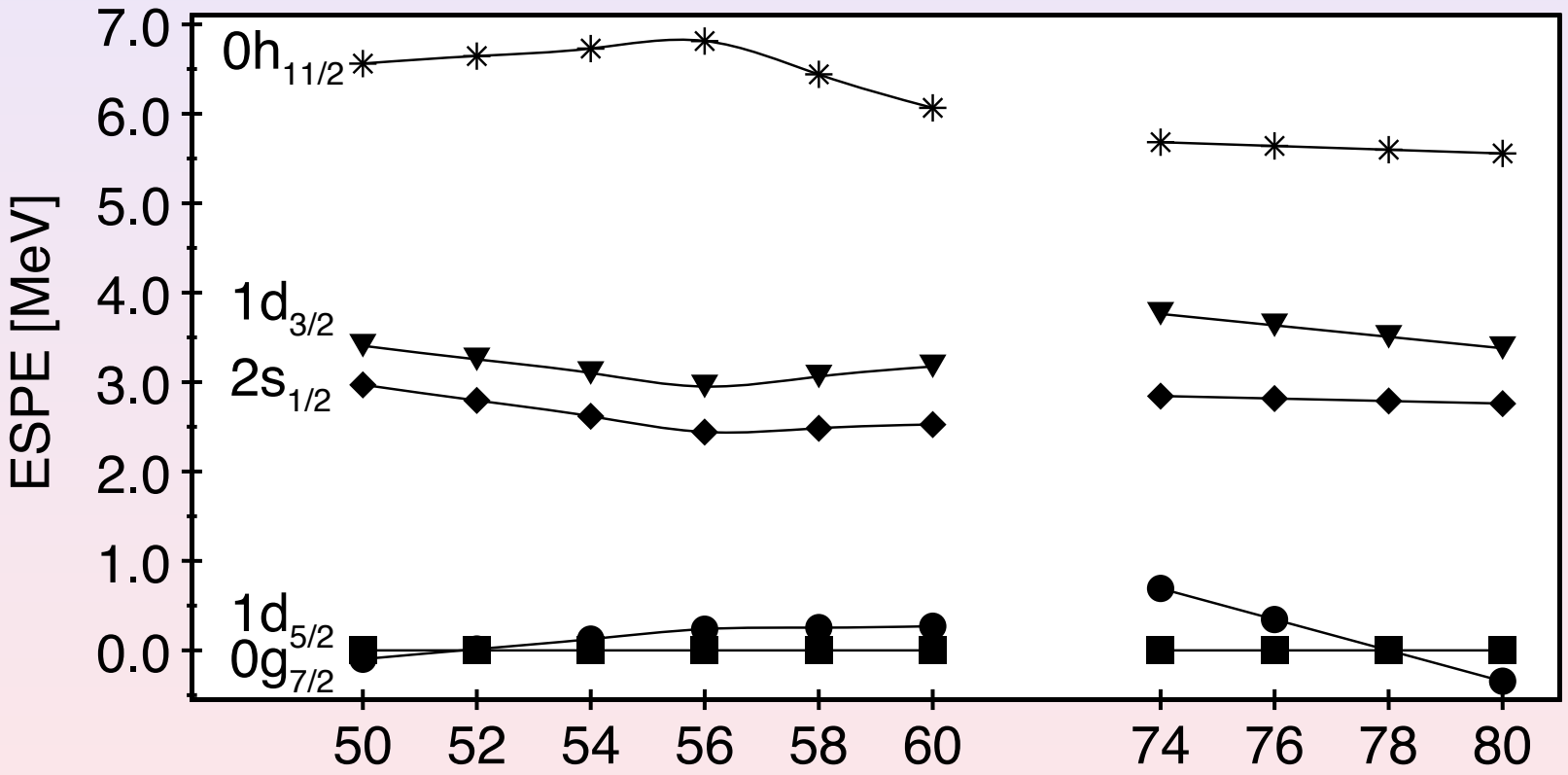


Evidence: even if the theoretical neutron effective charges are larger than empirical ones, the calculated $B(E2)$s are deficient with respect the experimental ones.

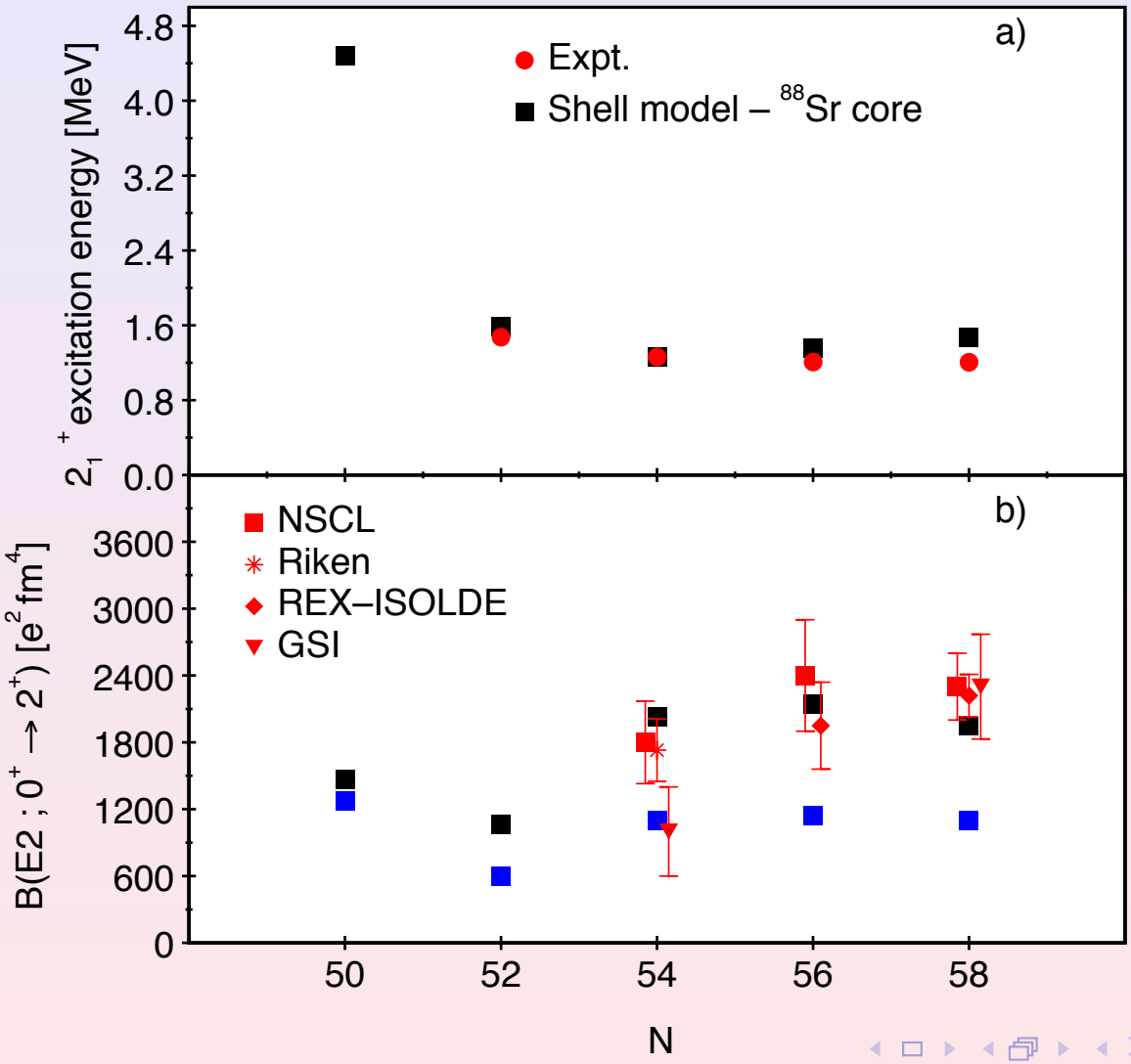
Countermeasure: to tackle this problem including explicitly the proton $Z = 50$ cross-shell excitations. We consider the model space above ^{88}Sr core.

Drawback: the H^{75} hamiltonian acts in a model space too large to diagonalize any tin isotopes.
When employing H^{45} we can diagonalize only the wavefunctions of $^{100-102}$Sn.
We need to employ the smaller model space with 4 proton and 2 neutron orbitals and diagonalize H^{42}.

ESPE of tin isotopes



Results with H^{42}



Calculated neutron effective charges

^{100}Sn core

$n_a l_a j_a$	$n_b l_b j_b$	$\langle a\|e_n\|b\rangle$
$0g_{7/2}$	$0g_{7/2}$	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

^{88}Sr core

$n_a l_a j_a$	$n_b l_b j_b$	$\langle a\|e_n\|b\rangle$
$0g_{7/2}$	$0g_{7/2}$	0.94
$0g_{7/2}$	$1d_{5/2}$	0.96
$0g_{7/2}$	$1d_{3/2}$	0.95
$1d_{5/2}$	$1d_{5/2}$	0.94
$1d_{5/2}$	$1d_{3/2}$	0.97
$1d_{5/2}$	$2s_{1/2}$	0.79
$1d_{3/2}$	$1d_{3/2}$	0.96
$1d_{3/2}$	$2s_{1/2}$	0.79
$0h_{11/2}$	$0h_{11/2}$	0.87

Conclusions

- A satisfactory description of light tin isotopes can be achieved, with shell model calculations, only taking into account $Z = 50$ cross-shell excitations explicitly.
- The introduction of a double-step procedure has allowed to reduce the complexity of the computational problem by deriving a new effective hamiltonian $H^{42}_{\rm eff}$. This may be useful for other large scale shell-model calculations.
- We have found that a crucial role is played by the calculation of both proton and neutron effective charges, in order to reproduce the experimental $B(E2)$s.