Perspectives of large-scale shell model with realistic effective hamiltonians

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- A. Gargano (INFN)
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- L. C. (INFN)

Framework

- 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.
- The computational complexity of dealing with large model spaces and many interacting valence nucleons is the main problematic to be tackled.

Large-scale shell model

PHYSICAL REVIEW C VOLUME 50, NUMBER 1 JULY 1994

Full pf shell model study of A=48 nuclei

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(Received 16 December 1993)

VOLUME 77, NUMBER 16 PHYSICAL REVIEW LETTERS 14 OCTOBER 1996

Nuclear Shell Model by the Quantum Monte Carlo Diagonalization Method

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(Received 29 April 1996)

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.

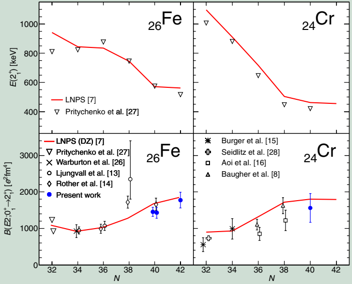
Collective behavior

PRL **110,** 242701 (2013) PHYSICAL REVIEW LETTERS week ending 14 JUNE 2013

Quadrupole Collectivity in Neutron-Rich Fe and Cr Isotopes

H. L. Crawford,[1] R. M. Clark,[1] P. Fallon,[1] A. O. Macchiavelli,[1] T. Baugher,[2,3] D. Bazin,[2] C. W. Beausang,[4] J. S. Berryman,[2] D. L. Bleuel,[5] C. M. Campbell,[1] M. Cromaz,[1] G. de Angelis,[6] A. Gade,[2,3] R. O. Hughes,[4] I. Y. Lee,[1] S. M. Lenzi,[7] F. Nowacki,[8] S. Paschalis,[1] M. Petri,[1] A. Poves,[9] A. Ratkiewicz,[2,3] T. J. Ross,[4] E. Sahin,[6] D. Weisshaar,[2] K. Wimmer,[2,10] and R. Winkler[2]

Onset of collectivity at $N = 40$



Model space

- 4 proton orbitals: $0f_{7/2}, 1p_{3/2}, 1p_{1/2}, 0f_{5/2}$
- 5 neutron orbitals: $1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$

NATHAN shell-model code

Novel collective feaures

RAPID COMMUNICATIONS

PHYSICAL REVIEW C **89**, 031301(R) (2014)

Novel shape evolution in exotic Ni isotopes and configuration-dependent shell structure

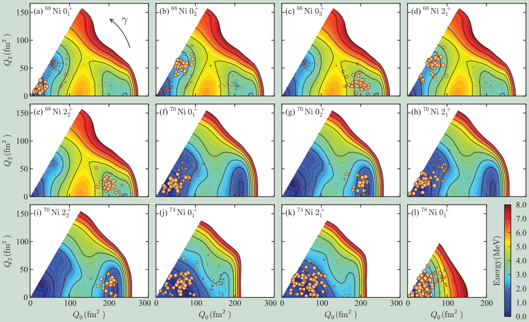
Yusuke Tsunoda,[1] Takaharu Otsuka,[1,2,3] Noritaka Shimizu,[2] Michio Honma,[4] and Yutaka Utsuno[5]

Shape evolution in Ni isotopes

Model space

- 6 proton orbitals:
  $0f_{7/2}, 1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$
- 6 neutron orbitals:
  $0f_{7/2}, 1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$

Monte Carlo shell model



Islands of inversion

PHYSICAL REVIEW C **90**, 014302 (2014)

Merging of the islands of inversion at $N = 20$ and $N = 28$

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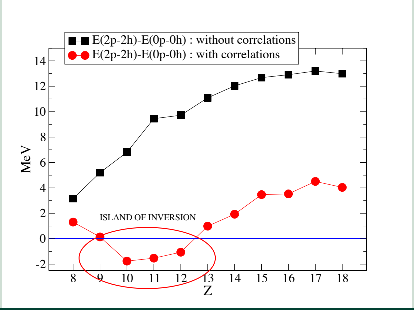
Merging of the $N = 20$ and $N = 28$ islands of inversion in Mg isotopes

Model space: full sdfp orbitals

NATHAN shell-model code



Shell evolution

RAPID COMMUNICATIONS

PHYSICAL REVIEW C **91**, 021303(R) (2015)

Quenching of the neutron $N = 82$ shell gap near ^{120}Sr with monopole-driving core excitations

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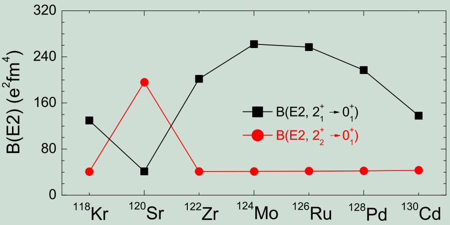
Study of the $N = 82$ shell evolution as a function of the neutron shell gap

6 proton orbitals:
$0f_{5/2}, 1p_{3/2}, 1p_{1/2}, 0g_{9/2}, 0g_{7/2}, 1d_{5/2}$

6 neutron orbitals:
$0g_{7/2}, 1d_{5/2}, 1d_{3/2}, 2s_{1/2}, 0h_{11/2}, 1f_{7/2}, 2p_{3/2}$

NuShellX code



- 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. In the *m*-scheme the dimension of the basis is $\simeq 10^{24}$, reduced to 50 by the importance sampling of the shell-model basis performed within the Monte Carlo Shell Model (MCSM) approach.
- In calculations [3] only neutron $N = 20$ cross-shell excitations are taken into account. Shell model basis has a dimension up to 10^{10}
- In calculations [4] only one valence-neutron is allowed to occupy the $1f_{7/2}, 2p_{3/2}$.

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.

The realistic shell model

- The derivation of the shell-model hamiltonian using the many-body theory may provide a reliable approach
- The model space may be “shaped” according to the computational needs of the diagonalization of the shell-model hamiltonian
- In such a case, the effects of the neglected degrees of freedom are taken into account by the effective hamiltonian $H_{\rm eff}$ theoretically

The shell-model effective hamiltonian

The effective hamiltonian $H_{\rm eff}$ is derived from a realistic *NN* potential 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 $H_{\rm eff}$ is expressed as

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

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

Our recipe for realistic shell model

- Input V_{NN}: $V_{\rm low-k}$ derived from the high-precision *NN* CD-Bonn potential with a cutoff: $\Lambda = 2.6$ fm^{-1}.
- $H_{\rm eff}$ obtained calculating the *Q*-box up to the 3rd order in $V_{\rm low-k}$.
- Effective electromagnetic operators are consistently derived by way of the the MBPT

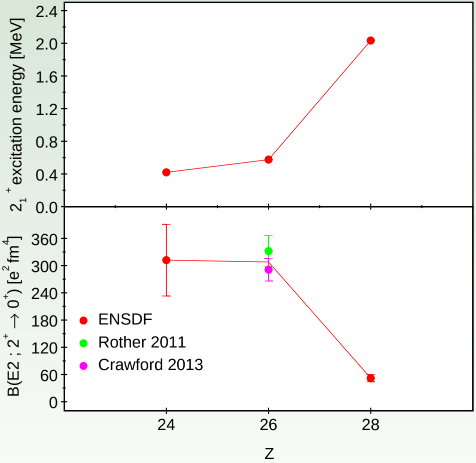
Double-step approach

However, it may occur that $H_{\rm eff}$ can be diagonalized for a certain class of nuclei, but not for other with a larger number of valence nucleons

Recently, we have started to explore the possibility to perform a double-step approach to the renormalization of the shell-model hamiltonian

More precisely, after we have derived $H_{\rm eff}$ in a certain model space P, starting from this one we generate a new $H_{\rm eff}^{\rm new}$ acting in a truncated subspace $P^{\rm new} \subset P$

First example: the collectivity at $N = 40$



The collectivity at $N = 40$: the model space

Within the shell-model framework the key role for the onset/disappearance of the $N = 40$ collectivity is played by the interaction between the quadrupole partners $\nu 0g_{9/2}, \nu 1d_{5/2}$

In order to study this phenomenon we have chosen to perform a sort of "differential diagnosis", employing as the proton model space the $\pi 0f_{7/2}, \pi 1p_{3/2}$ orbitals, and two different neutron model spaces:

- Model space I: $1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}$
- Model space II: $1p_{3/2}, 1p_{1/2}, 0f_{5/2}, 0g_{9/2}, 1d_{5/2}$

The double-step procedure

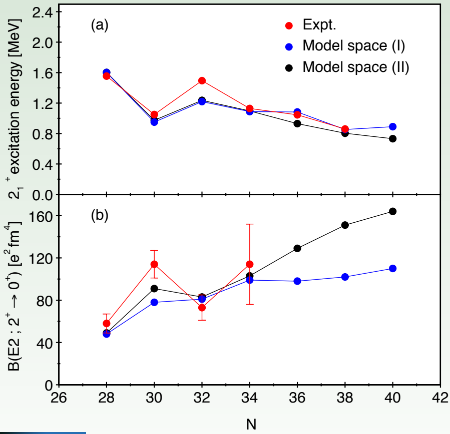
In order to make this comparison as much consistent as possible, we have followed this procedure

1. We have derived first H_{eff} - within the MBPT - in a very large model space outside the ^{40}Ca closed core, and spanned by six proton and neutron *pfgd* orbitals.
2. Then, we derive from this "mother hamiltonian" two new effective hamiltonians - again using MBPT - defined in the smaller model spaces (I) and (II).
3. Single-particle energies are taken for experimental data.

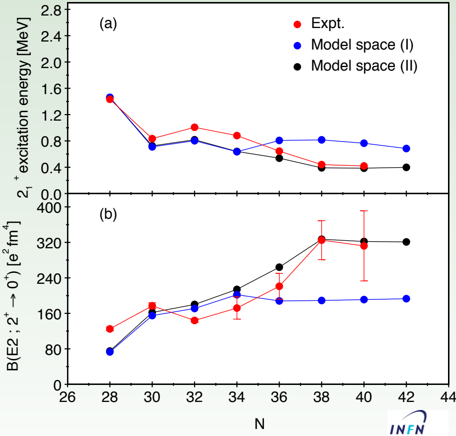
L. C., A. Covello, A. Gargano, and N. Itaco, Phys. Rev. C **89**, *024319 (2014)*

Collectivity at $N = 40$

Titanium isotopes

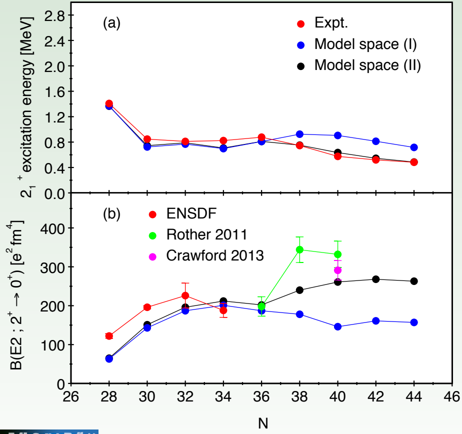


Chromium isotopes

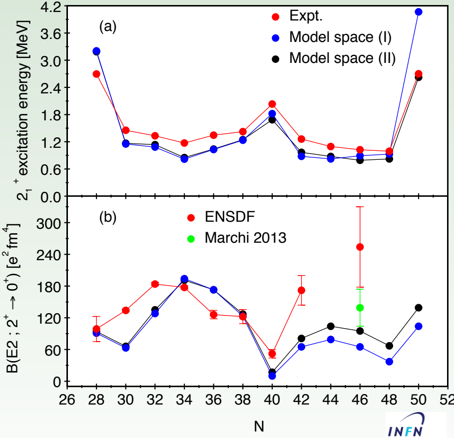


Collectivity at $N = 40$

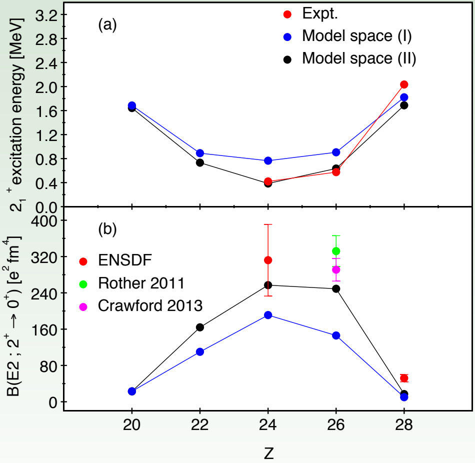
Iron isotopes



Nickel isotopes



Collectivity at $N = 40$



A second example: quadrupole collectivity around $Z = 50$

Our interest: to study the quadrupole collectivity due to $Z = 50$ cross-shell excitations in even-mass isotopic chains above ^{88}Sr.

Model space of the "mother hamiltonian":

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

A modest proposal

A "Poor Man's Approach" to lighten the computational complexity of diagonalizing the "mother hamiltonian" H^{75} 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.

Single-particle energies, effective two-body matrix elements, and effective electromagnetic operators are all derived from theory

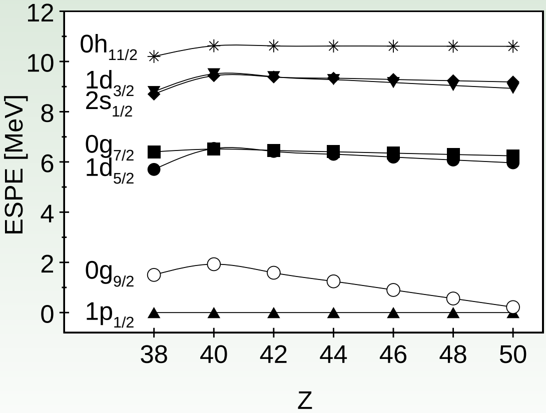
Single-particle properties with H^{75}

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

$n_a l_a j_a \;\; n_b l_b j_b$	$\langle a \vert e_p \vert b \rangle$
$0g_{9/2}\ 0g_{9/2}$	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

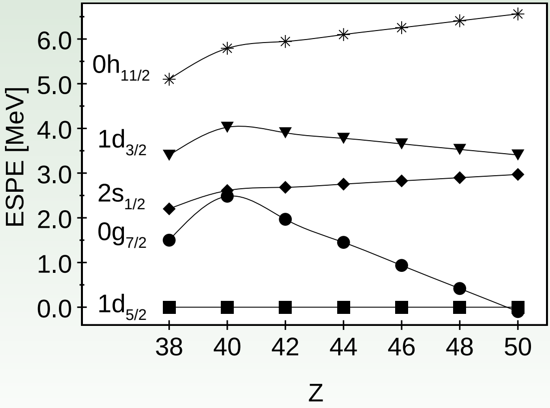
$n_a l_a j_a \;\; n_b l_b j_b$	$\langle a \vert e_n \vert b \rangle$
$0g_{7/2}\ 0g_{7/2}$	0.94
$0g_{7/2}\ 1d_{5/2}$	0.96
$0g_{7/2}\ 1d_{3/2}$	0.95
$1d_{5/2}\ 1d_{5/2}$	0.94
$1d_{5/2}\ 1d_{3/2}$	0.97
$1d_{5/2}\ 2s_{1/2}$	0.79
$1d_{3/2}\ 1d_{3/2}$	0.96
$1d_{3/2}\ 2s_{1/2}$	0.79
$0h_{11/2}\ 0h_{11/2}$	0.87

Proton ESPE



ESPE [MeV]
12
10
8
6
4
2
0
0h11/2
1d3/2
2s1/2
0g7/2
1d5/2
0g9/2
1p1/2
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 second step

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

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

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

$$H_0 = PH_0P + QH_0Q \quad .$$

The second step

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 $|\phi_k\rangle = P|\psi_k\rangle$.

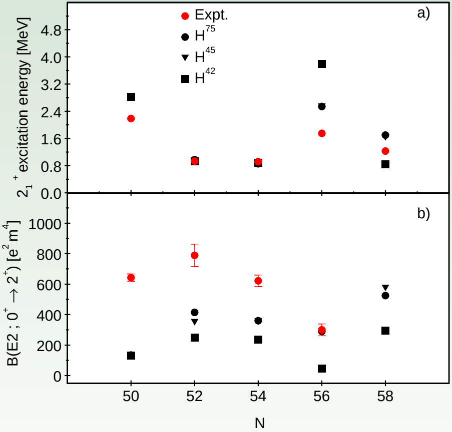
The eigenvalue problem for H^{75} can be easily solved for the two valence-nucleon systems (^{90}Zr,^{90}Sr,^{90}Y), and consequently providing the E_k, ψ_k.

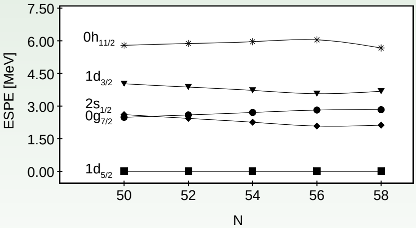
The solutions of the equation for the effective residual interaction $V^{4,n}$ are given by:

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

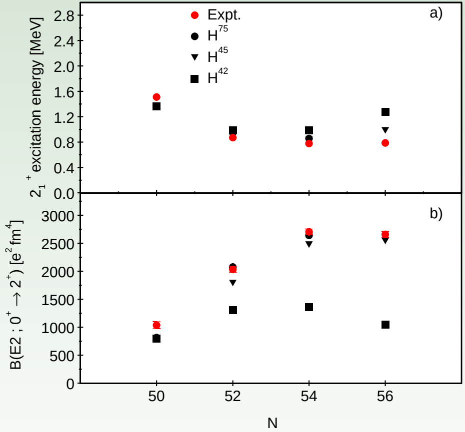
where $|\tilde{\phi}_k\rangle$ are biorthogonal states defined as $|\tilde{\phi}_k\rangle\langle\phi_{k'}| = \delta_{kk'}$

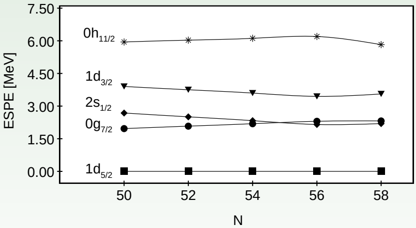
Results for Zr isotopes



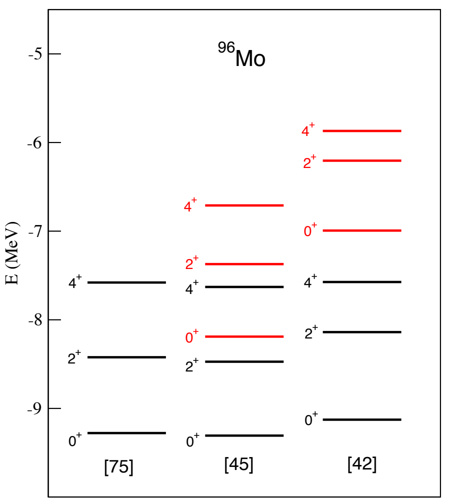


Results for Mo isotopes

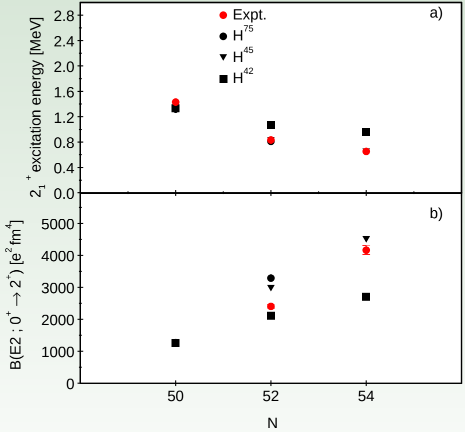


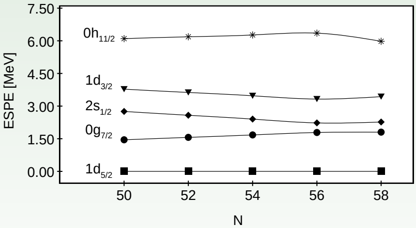


A closer look to ^{96}Mo

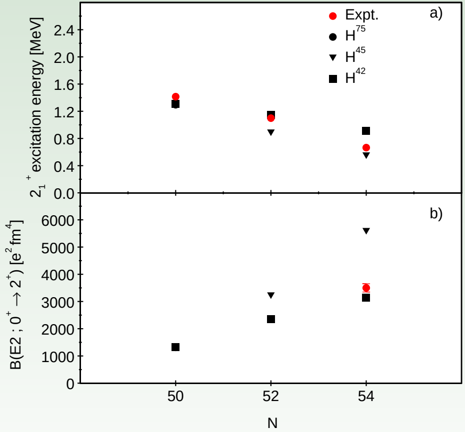


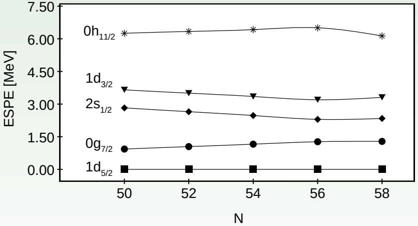
Results for Ru isotopes



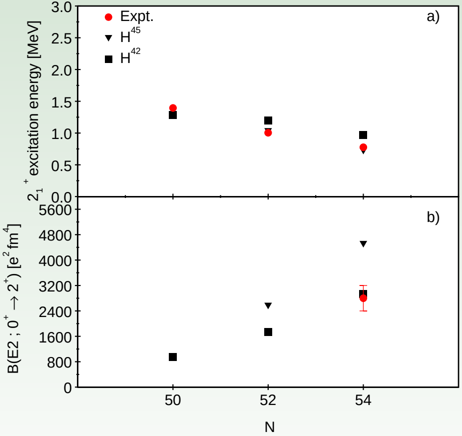


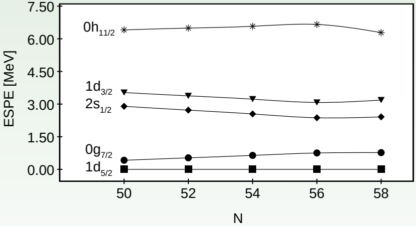
Results for Pd isotopes



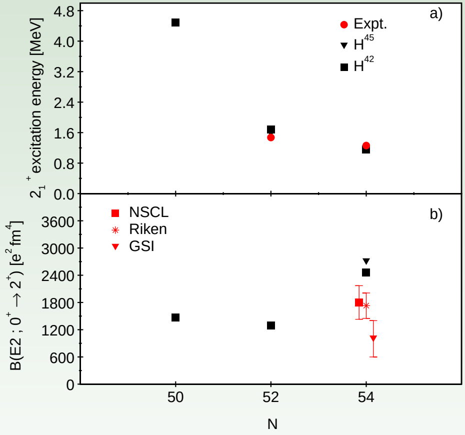


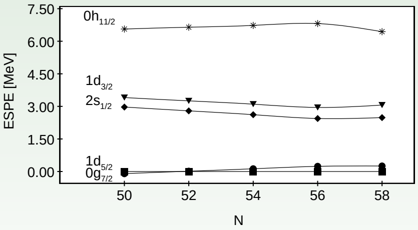
Results for Cd isotopes





Results for Sn isotopes





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Conclusions and outlook

- The introduction of a double-step procedure allows a reduction the complexity of the computational problem, and may be useful for other large scale shell-model calculations.
- Quadrupole collectivities in isotopic chains outside ^{48}Ca and ^{88}Sr cores are well reproduced.
- We are working to extend the procedure to consider also the truncation of the degrees of freedom of filled shell-model orbitals.
- The calculation of effective two-body operators are in order to improve the calculation of the electromagnetic-multipole transition rates.