# Large-scale shell-model challenges within the RIB era

Luigi Coraggio

Istituto Nazionale di Fisica Nucleare - Sezione di Napoli

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Luigi Coraggio



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#### 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

E. Caurier and A. P. Zuber Groupe de Physique Théorique, Centre de Rocherches Nucléaires, Institut National de Physique Sucléaire et de Physique des Particles, Centre National de la Rocherche Scientifique, Université Louis Pasteu Boile Pastel 29, 6-20137 Strasburg-Cedes, France

A. Poves and G. Martínez-Pinedo Departamento de Física Teórica C-XI, Universidad Autónoma de Madrid, E-28049 Madrid, Spain (Received 18 December 1993)

VOLUME 77, NUMBER 16

PHYSICAL REVIEW LETTERS

14 OCTOBER 1996

#### Nuclear Shell Model by the Quantum Monte Carlo Diagonalization Method

Michioi Honma,<sup>1</sup> Takahim Mizusaki<sup>2</sup> and Takahuru Ousuk<sup>2-3</sup>.
<sup>1</sup>Center for Mathematical Science, University of Aixa, Turruga, Ikki muchi, Aizu Wakamatu, Fakushima 965, Japan
<sup>2</sup>Department of Physics, University of Tokyo, Hongy, Tokyo 113, Japan
<sup>3</sup>RIKEN, Hirosawa, Wako-shi, Saitama 351.01, Japan
(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.



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#### Collective behavior



NATHAN shell-model code



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### 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,<sup>1</sup> Takaharu Otsuka,<sup>1,2,3</sup> Noritaka Shimizu,<sup>2</sup> Michio Honma,<sup>4</sup> and Yutaka Utsuno<sup>5</sup>

## Shape evolution in Ni isotopes



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#### Islands of inversion

PHYSICAL REVIEW C 90, 014302 (2014)

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

E. Caurier,<sup>1</sup> F. Nowacki,<sup>1</sup> and A. Poves<sup>2,3</sup> <sup>1</sup>IPHC, IN2P3-CNRS and Université Louis Posteur, F-6703 Strasbourg, France <sup>2</sup>Departamento de Física and IFT-UAM/CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain <sup>3</sup>Iolde (CERN) 1211 Genève 23, Switzerland Merging of the N = 20 and N = 28 islands of inversion in Mg isotopes



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### Shell evolution

RAPID COMMUNICATIONS

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

Quenching of the neutron N = 82 shell gap near <sup>120</sup>Sr with monopole-driving core excitations

Han-Kui Wang<sup>1,2</sup> Kazmari Kancko,<sup>2</sup> and Yang Sun<sup>2,4,4</sup>
School of Physics and Mechanical and Electrical Engineering. Zhuokaw Normal University, Henau 64000, People's Republic of China <sup>2</sup>Department of Physics and Attorneys, Shanghal 2005, University, Shanghal 200240, People's Republic of China <sup>3</sup>Department of Physics, Ryshink Sangyo University, Fakudoa 813-8303, Japan <sup>4</sup>PENS Collaborative Innovation Center, Shanghal 2005, Tong University, Shanghai 200240, People's Republic of China Study of the N = 82 shell evolution as a function of the neutron shell gap



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- 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 <sup>48</sup>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<sup>10</sup>
- In calculations [4] only one valence-neutron is allowed to occupy the  $1f_{7/2}$ ,  $2p_{3/2}$ .



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INFN Millen Macorale d'Fabre Machary

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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.





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#### 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<sub>eff</sub> theoretically





### An example: <sup>19</sup>F



- 9 protons & 10 neutrons interacting
- spherically symmetric mean field (e.g. harmonic oscillator)
- 1 valence proton & 2 valence neutrons interacting in a truncated model space



The degrees of freedom of the core nucleons and the excitations of the valence ones above the model space are not considered explicitly.

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#### Effective shell-model hamiltonian

The shell-model hamiltonian has to take into account in an effective way all the degrees of freedom not explicitly considered

#### Two alternative approaches

- phenomenological
- microscopic

$$V_{NN}$$
 (+ $V_{NNN}$ )  $\Rightarrow$  many-body theory  $\Rightarrow$   $H_{eff}$ 

#### Definition

The eigenvalues of  $\textit{H}_{\rm eff}$  belong to the set of eigenvalues of the full nuclear hamiltonian



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### Workflow for a realistic shell-model calculation

- Choose a realistic NN potential (NNN)
- Oetermine the model space better tailored to study the system under investigation
- Oerive the effective shell-model hamiltonian by way of the many-body theory
- Calculate the physical observables (energies, e.m. transition probabilities, ...)





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#### Several realistic potentials $\chi^2/datum \simeq 1$ : CD-Bonn, Argonne V18, Nijmegen, ...

## Strong short-range repulsion



How to handle the short-range repulsion ?

- Brueckner G matrix
- EFT inspired approaches



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*V*<sub>low-k</sub>, SRG
chiral potentials

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- Brueckner G matrix
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  - $V_{low-k}$ , SRG
  - chiral potentials

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## Strong short-range repulsion





#### The shell-model effective hamiltonian

A-nucleon system Schrödinger equation

 $|H|\Psi_{
u}
angle=E_{
u}|\Psi_{
u}
angle$ 

with

$$H = H_0 + H_1 = \sum_{i=1}^{A} (T_i + U_i) + \sum_{i < j} (V_{ij}^{NN} - U_i)$$

Model space

$$|\Phi_i\rangle = [a_1^{\dagger}a_2^{\dagger} \dots a_n^{\dagger}]_i |c\rangle \Rightarrow P = \sum_{i=1}^d |\Phi_i\rangle\langle\Phi_i|$$

#### Model-space eigenvalue problem

$$H_{\rm eff} P |\Psi_{\alpha}\rangle = E_{\alpha} P |\Psi_{\alpha}\rangle$$



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#### The shell-model effective hamiltonian

$$\begin{pmatrix} PHP & PHQ \\ \hline QHP & QHQ \end{pmatrix} \begin{array}{c} \mathcal{H} = X^{-1}HX \\ \Longrightarrow \\ Q\mathcal{H}P = 0 \end{array} \begin{pmatrix} P\mathcal{H}P & P\mathcal{H}Q \\ \hline 0 & Q\mathcal{H}Q \end{pmatrix}$$

$$H_{
m eff} = P\mathcal{H}P$$
  
Suzuki & Lee  $\Rightarrow X = e^{\omega}$  with  $\omega = \left( egin{array}{c|c} 0 & 0 \ \hline Q\omega P & 0 \end{array} 
ight)$ 

$$H_{1}^{\text{eff}}(\omega) = PH_{1}P + PH_{1}Q \frac{1}{\epsilon - QHQ}QH_{1}P - PH_{1}Q \frac{1}{\epsilon - QHQ}\omega H_{1}^{\text{eff}}(\omega)$$



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### The shell-model effective hamiltonian

#### Folded-diagram expansion

 $\hat{Q}$ -box vertex function

$$\hat{Q}(\epsilon) = PH_1P + PH_1Qrac{1}{\epsilon-QHQ}QH_1P$$

 $\Rightarrow$  Recursive equation for  $H_{\rm eff} \Rightarrow$  iterative techniques (Krenciglowa-Kuo, Lee-Suzuki, ...)

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



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#### The perturbative approach to the shell-model $H^{\text{eff}}$

$$\hat{Q}(\epsilon) = PH_1P + PH_1Q rac{1}{\epsilon - QHQ}QH_1P$$

The  $\hat{Q}$ -box can be calculated perturbatively

$$\frac{1}{\epsilon - QHQ} = \sum_{n=0}^{\infty} \frac{(QH_1Q)^n}{(\epsilon - QH_0Q)^{n+1}}$$



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### $\hat{Q}$ -box perturbative expansion: 1-body diagrams









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### $\hat{Q}$ -box perturbative expansion: 2-body diagrams







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### $\hat{Q}$ -box perturbative expansion: 2-body diagrams

H H H H888679 -BBBB j.O O. No • <u>0</u> • <u>0</u> 0 0 0 0 0 a a propriate 



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#### **Benchmark calculation**

A benchmark calculation has been performed for light *p*-shell nuclei, comparing realistic shell-model calculations with those of NCSM, starting from chiral two-body potential  $N^{3}LO$ .



(a) not translationally invariantHamiltonian(b) purely intrinsic hamiltonian



L.C., A. Covello, A. Gargano, N. Itaco, and T. T. S. Kuo, Ann. Phys. **327**, 2125-2151 (2012)



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#### Our recipe for realistic shell model

- Input  $V_{NN}$ :  $V_{low-k}$  derived from the high-precision NN CD-Bonn potential with a cutoff:  $\Lambda = 2.6 \text{ fm}^{-1}$ .
- $H_{\rm eff}$  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





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





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#### First example: the collectivity at N = 40





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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<sub>3/2</sub>, 1p<sub>1/2</sub>, 0f<sub>5/2</sub>, 0g<sub>9/2</sub>
- Model space II: 1p<sub>3/2</sub>, 1p<sub>1/2</sub>, 0f<sub>5/2</sub>, 0g<sub>9/2</sub>, 1d<sub>5/2</sub>





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

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



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



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#### Collectivity at N = 40



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#### Collectivity at N = 40



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#### Collectivity at N = 40





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# 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 <sup>88</sup>Sr.

Model space of the "mother hamiltonian":

Proton orbitals	Neutron orbitals
1 <i>p</i> <sub>1/2</sub>	
0 <i>g</i> <sub>9/2</sub>	
$1d_{5/2}$	1 <i>d</i> <sub>5/2</sub>
0 <i>g</i> <sub>7/2</sub>	0 <i>g</i> <sub>7/2</sub>
$1d_{3/2}$	$1d_{3/2}$
$2s_{1/2}$	$2s_{1/2}$
$0h_{11/2}$	$0h_{11/2}$



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## 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", and locate the relevant degrees of freedom (single-particle orbitals).
- Second step: perform a unitary transformation of the "mother hamiltonian" into a reduced model space, so to obtain an effective hamiltonian that is computationally.

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



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

L. C., A. Gargano, and N. Itaco, Phys. Rev. C 93, 064328 (2016)



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# Single-particle properties with H<sup>75</sup>

orbital	proton s.p.e.
1 <i>p</i> <sub>1/2</sub>	0.0
0 <i>g</i> <sub>9/2</sub>	1.5
0 <i>g</i> <sub>7/2</sub>	5.7
1 <i>d</i> <sub>5/2</sub>	6.4
1 <i>d</i> <sub>3/2</sub>	8.8
$2s_{1/2}$	8.7
0 <i>h</i> <sub>11/2</sub>	10.2
orbital	neutron s.p.e.
1 <i>d</i> <sub>5/2</sub>	0.0
0 <i>g</i> <sub>7/2</sub>	1.5
$2s_{1/2}$	2.2
1 <i>d</i> <sub>3/2</sub>	3.4
$0h_{11/2}$	5.1

n <sub>a</sub> l <sub>a</sub> j <sub>a</sub> n <sub>b</sub> l <sub>b</sub> j <sub>b</sub>	$\langle a e_p b\rangle$	
0g <sub>9/2</sub> 0g <sub>9/2</sub>	1.62	
$0g_{9/2} 0g_{7/2}$	1.67	n <sub>a</sub> l <sub>a</sub> j <sub>a</sub> n <sub>b</sub> l <sub>b</sub> j <sub>b</sub>
$0g_{9/2} \ 1d_{5/2}$	1.60	$0g_{7/2} 0g_{7/2}$
/ -/	1.73	0 <i>g</i> <sub>7/2</sub> 1 <i>d</i> <sub>5/2</sub>
$0g_{7/2} 0g_{7/2}$		$0g_{7/2} 1d_{3/2}$
0g <sub>7/2</sub> 1d <sub>5/2</sub>	1.74	$1d_{5/2} 1d_{5/2}$
0 <i>g</i> <sub>7/2</sub> 1 <i>d</i> <sub>3/2</sub>	1.76	$1d_{5/2} 1d_{3/2}$
1 <i>d</i> <sub>5/2</sub> 1 <i>d</i> <sub>5/2</sub>	1.73	
$1d_{5/2} \ 1d_{3/2}$	1.72	$1d_{5/2} 2s_{1/2}$
$1d_{5/2} 2s_{1/2}$	1.76	$1d_{3/2} 1d_{3/2}$
	1.74	$1d_{3/2} 2s_{1/2}$
$1d_{3/2} 1d_{3/2}$		$0h_{11/2} 0h_{11/2}$
$1d_{3/2} 2s_{1/2}$	1.76	
$0h_{11/2} 0h_{11/2}$	1.72	



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#### Proton ESPE





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### Neutron ESPE





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## 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  $H_{\text{eff}}^{4n}$  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.





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#### The second step

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

The eigenvalue problem for  $H^{75}$  is:

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

 $H^{75}$  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:

 $H_0 = PH_0P + QH_0Q \ .$ 





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#### 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  $|\phi_k\rangle = \boldsymbol{P}|\psi_k\rangle$ .

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  $E_k$ ,  $\psi_k$ .

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

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

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



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#### Results for Zr isotopes



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#### **Results for Mo isotopes**



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## A closer look to <sup>96</sup>Mo



a)  $H_{\rm eff}^{45}$  and  $H_{\rm eff}^{42}$  with double-step procedure;



- $\tilde{H}^{45}, \tilde{H}^{42}_{eff}$  derived by way of the many-body perturbation theory;
- c) the hamiltonian  $H^{75}$ , but constraining the calculations to model spaces [45], [42].

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b)

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### Results for Ru isotopes



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#### Results for Pd isotopes



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#### Results for Cd isotopes



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#### Results for Sn isotopes



## Last example: open-shell nuclei around <sup>132</sup>Sn

Our goal: to study the structure of nuclei that are currently of exeperimental interest to detect the neutrinoless double-beta decay.

Model space of the "mother hamiltonian":

Proton orbitals	Neutron orbitals	
1 <i>d</i> <sub>5/2</sub>	1 <i>d</i> <sub>5/2</sub>	
$0g_{7/2}$	0 <i>g</i> <sub>7/2</sub>	
$1d_{3/2}$	$1d_{3/2}$	
$2s_{1/2}$	$2s_{1/2}$	
$0h_{11/2}$	$0h_{11/2}$	





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# Single-particle properties with H55

orbital	proton s.p.e.
0 <i>g</i> <sub>7/2</sub>	0.0
$1d_{5/2}$	0.3
1 <i>d</i> <sub>3/2</sub>	1.5
$2s_{1/2}$	1.5
$0h_{11/2}$	1.8
orbital	neutron s.p.e.
0 <i>g</i> <sub>7/2</sub>	0.0
1 <i>d</i> <sub>5/2</sub>	0.6
1 <i>d</i> <sub>5/2</sub>	0.6 1.5
1 <i>d</i> <sub>5/2</sub> 1 <i>d</i> <sub>3/2</sub> 2 <i>s</i> <sub>1/2</sub>	
1 <i>d</i> <sub>5/2</sub>	1.5

n <sub>a</sub> l <sub>a</sub> j <sub>a</sub> n <sub>b</sub> l <sub>b</sub> j <sub>b</sub>	$\langle a e_{ ho} b angle$	n <sub>a</sub> l <sub>a</sub> j <sub>a</sub> n <sub>b</sub> l <sub>b</sub> j <sub>b</sub>	$\langle a e_n b\rangle$
0g <sub>7/2</sub> 0g <sub>7/2</sub>	1.42	0g <sub>7/2</sub> 0g <sub>7/2</sub>	1.00
0g <sub>7/2</sub> 1d <sub>5/2</sub>	1.40	0g <sub>7/2</sub> 1d <sub>5/2</sub>	1.03
0g <sub>7/2</sub> 1d <sub>3/2</sub>	1.40	0g <sub>7/2</sub> 1d <sub>3/2</sub>	0.98
$1d_{5/2} \ 1d_{5/2}$	1.21	$1d_{5/2} 1d_{5/2}$	0.63
1d <sub>5/2</sub> 1d <sub>3/2</sub>	1.28	$1d_{5/2} 1d_{3/2}$	0.65
1 <i>d</i> <sub>5/2</sub> 2 <i>s</i> <sub>1/2</sub>	1.23	$1d_{5/2} 2s_{1/2}$	0.62
1d <sub>3/2</sub> 1d <sub>3/2</sub>	1.26	$1d_{3/2} \ 1d_{3/2}$	0.69
$1d_{3/2} 2s_{1/2}$	1.29	$1d_{3/2} 2s_{1/2}$	0.68
0h <sub>11/2</sub> 0h <sub>11/2</sub>	1.31	$0h_{11/2} 0h_{11/2}$	0.68



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### Proton ESPE





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### Results for heavy Te isotopes



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#### Results for heavy Xe isotopes



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#### The detection of the $0\nu\beta\beta$ -decay





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## CUORE@LNGS



- TeO<sub>2</sub> crystals used as low heat capacity bolometers, arranged into towers and cooled in a large cryostat to approximately 10 m°K with a dilution refrigerator.
- The detectors are isolated from backgrounds by ultrapure low-radioactivity shielding.
- Temperature spikes from electrons emitted in Te 0ββ are collected for spectrum analysis.





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#### Nuclear structure calculations



 The spread of nuclear structure calculations evidences inconsistencies among results obtained with different models



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INFN, Napoli

# Gamow-Teller strengths for <sup>128</sup>Te





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# Gamow-Teller strengths for <sup>130</sup>Te





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# Gamow-Teller strengths for <sup>136</sup>Xe





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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 <sup>48</sup>Ca and <sup>88</sup>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.



A parameter-free calculation of the NME for the neutrinoless double  $\beta$ -decay is in progress.



#### Present Prospects in Nuclear Structure

12th International Spring Seminar in Nuclear Physics, May 15-19 2017, Sant'Angelo d'Ischia





https://agenda.infn.it/event/spring2017



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#### Test case: *p*-shell nuclei

- V<sub>NN</sub> ⇒ chiral N<sup>3</sup>LO potential by Entem & Machleidt (smooth cutoff ≃ 2.5 fm<sup>-1</sup>)
- $H_{\rm eff}$  for two valence nucleons outside <sup>4</sup>He
- Single-particle energies and residual two-body interaction are derived from the theory. No empirical input

First, some convergence checks !

L.C., A. Covello, A. Gargano, N. Itaco, and T. T. S. Kuo, Ann. Phys. **327**, 2125-2151 (2012)





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#### Convergence checks

#### The intermediate-state space Q

Q-space is truncated: intermediate states whose unperturbed excitation energy is greater than a fixed value  $E_{max}$  are disregarded

$$|\epsilon_0 - \mathcal{QH}_0\mathcal{Q}| \leq \mathcal{E}_{ ext{max}} = \mathcal{N}_{ ext{max}} \hbar \omega$$



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#### Convergence checks

#### Order-by-order convergence



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#### Convergence checks

#### Dependence on $\hbar\omega$

Auxiliary potential  $U \Rightarrow$  harmonic oscillator potential



#### **HF-insertions**



- zero in a self-consistent basis
- neglected in most applications
- disregard of HF-insertions introduces relevant dependence on ħω

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Approximations are under control ... and what about the accuracy of the results ?

Compare the results with the "exact" ones

*ab initio* no-core shell model (NCSM) P. Navrátil, E. Caurier, Phys. Rev. C **69**, 014311 (2004)

P. Navrátil et al., Phys. Rev. Lett. 99, 042501 (2007)



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#### **Benchmark calculation**

To compare our results with NCSM we need to start from a translationally invariant Hamiltonian

$$H_{int} = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i < j=1}^{A} \left(V_{ij}^{NN} - \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{mA}\right) = \\ = \left[\sum_{i=1}^{A} \left(\frac{p_i^2}{2m} + U_i\right)\right] + \left[\sum_{i < j=1}^{A} \left(V_{ij}^{NN} - U_i - \frac{p_i^2}{2mA} - \frac{\mathbf{p}_i \cdot \mathbf{p}_j}{mA}\right)\right] \\ \xrightarrow{\substack{\text{add} \\ \text{blue} \\ \text{blue} \\ \text{blue} \\ \text{blue} \\ \text{constrained} \\ \xrightarrow{\substack{\text{constrained} \\ \text{constrained} \\ \text{constrained} \\ \text{constrained} \\ \xrightarrow{\substack{\text{constrained} \\ \text{constrained} \\ \text{constrained} \\ \xrightarrow{\substack{\text{constrained} \\ \text{constrained} \\ \text{constrained} \\ \xrightarrow{\text{constrained} \\ \text{constrained} \\ \xrightarrow{\text{constrained} \\ \text{constrained} \\ \xrightarrow{\text{constrained} \\ \xrightarrow{\text{constrained$$

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Hamiltonian

### **Benchmark calculation**

#### Remark

 ${\it H}^{\rm eff}$  derived for 2 valence nucleon systems  $\Rightarrow$  3-, 4-, ..  $\it n\text{-body}$  components are neglected



#### Benchmark calculation

#### <sup>10</sup>B relative spectrum



discrepancy ≤ 1 MeV
minor role of many-body correlations



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