Shell model calculations for exotic nuclei with realistic potentials: reliability and predictiveness

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## Part I

### The theoretical framework



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### What is a realistic effective shell-model hamiltonian ?



### 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.



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  $H_{\rm eff}$  belong to the set of eigenvalues of the full nuclear hamiltonian



### Workflow for a realistic shell-model calculation

- Choose a realistic NN potential (NNN)
- 2 Determine 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, ...)



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

### How to handle the short-range repulsion ?

- Brueckner G matrix
- EFT inspired approaches

# Strong short-range repulsion





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

# Strong short-range repulsion



- Brueckner G matrix
- EFT inspired approaches
  - $V_{\text{low}-k}$
  - SRG
  - chiral potentials



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# Strong short-range repulsion



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  - SRG
  - chiral potentials



### 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

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

### The shell-model effective hamiltonian

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

 $H_{\rm eff} = P \mathcal{H} P$ 

Suzuki & Lee  $\Rightarrow X = e^{\omega}$  with  $\omega = \left( \begin{array}{c|c} 0 & 0 \\ \hline Q \omega P & 0 \end{array} \right)$ 

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



### 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, ...)

$${\cal H}_{
m eff} = \hat{Q} - \hat{Q}^{\prime} \int \hat{Q} + \hat{Q}^{\prime} \int \hat{Q} \int \hat{Q} - \hat{Q}^{\prime} \int \hat{Q} \int \hat{Q} \int \hat{Q} \int \hat{Q} \cdots,$$



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

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

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

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

### The diagrammatic expansion of the $\hat{Q}$ -box





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### The shell-model effective operators

Consistently, any shell-model effective operator may be calculated

It has been demonstrated that, for any bare operator  $\Theta$ , a non-Hermitian effective operator  $\Theta_{eff}$  can be written in the following form:

$$\Theta_{\rm eff} = (P + \hat{Q}_1 + \hat{Q}_1 \hat{Q}_1 + \hat{Q}_2 \hat{Q} + \hat{Q} \hat{Q}_2 + \cdots)(\chi_0 + \chi_1 + \chi_2 + \cdots) ,$$

where

$$\hat{Q}_m = rac{1}{m!} rac{d^m \hat{Q}(\epsilon)}{d\epsilon^m} \Big|_{\epsilon=\epsilon_0} \; ,$$

 $\epsilon_0$  being the model-space eigenvalue of the unperturbed hamiltonian  $H_0$ 

K. Suzuki and R. Okamoto, Prog. Theor. Phys. 93, 905 (1995)



### The shell-model effective operators

. . .

The  $\chi_n$  operators are defined as follows:

$$\begin{split} \chi_{0} &= (\hat{\Theta}_{0} + h.c.) + \Theta_{00} , \\ \chi_{1} &= (\hat{\Theta}_{1}\hat{Q} + h.c.) + (\hat{\Theta}_{01}\hat{Q} + h.c.) , \\ \chi_{2} &= (\hat{\Theta}_{1}\hat{Q}_{1}\hat{Q} + h.c.) + (\hat{\Theta}_{2}\hat{Q}\hat{Q} + h.c.) + \\ (\hat{\Theta}_{02}\hat{Q}\hat{Q} + h.c.) + \hat{Q}\hat{\Theta}_{11}\hat{Q} , \end{split}$$

and

$$\hat{\Theta}(\epsilon) = P\Theta P + P\Theta Q \frac{1}{\epsilon - QHQ} QH_1 P ,$$

$$\hat{\Theta}(\epsilon_1; \epsilon_2) = P\Theta P + PH_1 Q \frac{1}{\epsilon_1 - QHQ} \times Q\Theta Q \frac{1}{\epsilon_2 - QHQ} QH_1 P ,$$

$$\hat{\Theta}_m = \frac{1}{m!} \frac{d^m \hat{\Theta}(\epsilon)}{d\epsilon^m} \Big|_{\epsilon = \epsilon_0} , \quad \hat{\Theta}_{nm} = \frac{1}{n!m!} \frac{d^n}{d\epsilon_1^n} \frac{d^m}{d\epsilon_2^m} \hat{\Theta}(\epsilon_1; \epsilon_2) \Big|_{\epsilon_1 = \epsilon_0, \epsilon_2 = \epsilon_0} \quad \text{if is the set of a set of$$

### The shell-model effective operators

We arrest the  $\chi$  series at  $\chi_0$ , and expand it perturbatively:







### 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*<sub>eff</sub> obtained calculating the *Q*-box up to the 3rd order in perturbation theory.
- Effective operators are consistently derived by way of the the MBPT



# Part II

# Reliability



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### Large-scale realistic shell-model calculations

### Neutron-rich isotopic chains

Approaching neutron drip line:

Shell-model study of the onset of collectivity at N = 40

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

### Proton-rich isotopic chains

Approaching proton drip line:

Enhanced quadrupole collectivity of neutron-deficient tin isotopes

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



### Collectivity at N = 40



 $\Rightarrow$  shell-model study of neutron-rich isotopic chains outside <sup>48</sup>Ca  $\Rightarrow$  Collective behavior framed within the quasi-SU(3) approximate symmetry

 $\Rightarrow$  Two model spaces with <sup>48</sup>Ca inert core, including or not the neutron  $1d_{5/2}$  orbital



### The collectivity at N = 40

#### PHYSICAL REVIEW C 81, 051304(R) (2010)

#### Collectivity at N = 40 in neutron-rich <sup>64</sup>Cr

A. Gade, "R. V.F. Janssen," J. Bangher, "J. D. Bang," B. A. Brows, "J. M. Pequence," C. J. Charg, "A. N. Docons," J. S. Perrem, G. Storger, C. R. Morris, "B. P. Kay, "F. G. Konder, "L. Lamitens," B. Mohand, "J. K. Mohand, "A. N. Docons," J. P. Kay, "R. C. Konder, "L. Lamitens," B. Mohand, "D. K. Mohand, "E. K. Mohand, "D. K. Mandad, "Manghand, "D. K. K. Mohand, "D. K. Mandad, "D. K. K

"Be-indeed inclusic scattering of  $^{42.44}$ Fe and  $^{40.24}$ Cr was performed at intermediate beam energies. Excited states in  $^{46}$ Cr were measured for the first time. Energies and population patterns of excited states in these neutron-ick Fe and Cr ancle in compared and interpreted in the framework of targs-scale skell-andel calculations in different model spaces. Evidence for increased collectivity and for distinct structural changes between the neighboring Fear ACT (storage chains near  $^{-1}$  and to p strements).

#### PHYSICAL REVIEW C 81, 061301(R) (2010)

#### Onset of collectivity in neutron-rich Fe isotopes: Toward a new island of inversion?

J. J. Japael, "A. Gauga, A. Oscadi, W. Wann, P. Chann, Y. G. Marna, Y. Japael, A. Bangal, Z. Markan, Y. Lawar, K. Sangal, Y. Lawar, Y

The lifetime of the first costs 2<sup>-1</sup> stars in <sup>10</sup>Fa and <sup>10</sup>Fa have been meansule for the first interardig the nuclei drames (Dopfer drift module all resultations) means the means in the interaction is a interaction. In the interaction is a interaction of the interaction. The interaction means are used on the interaction is the interaction in the inte

#### PHYSICAL REVIEW C 88, 024326 (2013)

#### Collectivity of neutron-rich Ti isotopes

H. Sandi, "S. And, "F. Eakons, "A. F. Maraka," S. Soh, "H. Back, "K. Barky, "L. Barky

The ensure of the average of the matrixes  $^{12}$  max investigated to prove indexis average in average of the 24 MeV/related  $N_{\rm F}$  material phi denois (in  $\mu$  mays (the fractionity  $\nu$  rays, there matches with the scapped or (1004) (11 MeV (1004)) and (1002) (12 MeV are indexisted). The adjust suggests are straightforware indexisted in the adjust suggest and the scale of the straightforware indexisted in t

#### PHYSICAL REVIEW C 82, 054301 (2010)

#### Island of inversion around 64Cr

S. M. Leasti, F. Nowacki, <sup>2</sup> A. Poves,<sup>3</sup> and K. Sieja<sup>5,4</sup> <sup>1</sup>Dipariments di Fuis and Thimerinia and MFW, Segime di Panhora, 1-53131 Padowa, Indy <sup>1</sup>PIPC, ICMF-KMSE to Lineraria di Samburge, F-5703 Samburg, France <sup>2</sup>Diparimento de Fritera Toriera et FF-UMICSE, Universidad Automas de Madrid, E-2009 Madrid, Spain (Receival O Sementre 2000; mblinded 2 November 2010)

We say the development of calculation prior the startme each make in some M = 40, where the experiment of the brochest calculates are prior plot plot appearing prior the plot calculates of the startment of the startment of the startment of the startment of the plot calculates of the startment startment of the startment of th



### Collectivity at N = 40





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### Enhanced quadrupole collectivity in light tin isotopes



 $\Rightarrow$  shell-model study of neutron-deficient tin isotopes using  $^{88}\mathrm{Sr}$  as a core

 $\Rightarrow$  Quadrupole collectivity enhanced by the Z = 50 cross-shell excitations

 $\Rightarrow$  Model space spanned by proton  $1p_{1/2}, 0g_{9/2}, 0g_{7/2}, 1d_{5/2}$  and  $0g_{7/2}, 1d_{5/2}$  orbitals

 $\Rightarrow$  <u>Theoretical</u> single-particle energies, two-body matrix elements and effective charges have been employed

### Calculation of the effective charges

### Proton effective charges

n <sub>a</sub> l <sub>a</sub> j <sub>a</sub> n <sub>b</sub> l <sub>b</sub> j <sub>b</sub>	$\langle a e_{ ho} b angle$
0 <i>g</i> <sub>9/2</sub> 0 <i>g</i> <sub>9/2</sub>	1.62
$0g_{9/2} 0g_{7/2}$	1.67
0g <sub>9/2</sub> 1d <sub>5/2</sub>	1.60
$0g_{7/2} 0g_{7/2}$	1.73
0g <sub>7/2</sub> 1d <sub>5/2</sub>	1.74
0g <sub>7/2</sub> 1d <sub>3/2</sub>	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

Neutron effective charge	s	
n <sub>a</sub> laja n <sub>b</sub> l <sub>bjb</sub>	$\langle a e_n b\rangle$	
$0g_{7/2} 0g_{7/2}$	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	



### Enhanced quadrupole collectivity in light tin isotopes





# Part III

## Predictiveness



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### Nuclear models and predictive power



RIBs & advances in detection techniques  $\Rightarrow$  unknown structure of nuclei towards the drip lines





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# realistic shell-model calculations in different mass regions $$\Downarrow$$ results in good agreement with experimental data

### Can realistic shell-model calculations be predictive ? few selected examples



### Few selected physics cases

- Sn isotopes beyond N = 82
- heavy calcium isotopes
- neutron-rich titanium and nickel isotopes

Single-particle energies from the experiment  $\Rightarrow$  reduced role of 3N force





 10th International Spring Seminar on Nuclear Physics: New Quests in Nuclear Structure
 IOP Publishing

 Journal of Physics: Conference Series 267 (2011) 012019
 doi:10.1088/1742-6596/267/1/012019

# Shell-model study of exotic Sn isotopes with a realistic effective interaction

A Covello<sup>1,2</sup>, L Coraggio<sup>2</sup>, A Gargano<sup>2</sup> and N Itaco<sup>1,2</sup> <sup>1</sup>Dipartimento di Scienze Fisiche, Università di Napoli Federico II, Complesso Universitario di Monte S. Angelo, I-80126 Napoli, Italy <sup>2</sup>Istituto Nazionale di Fisica Nucleare, Complesso Universitario di Monte S. Angelo, I-80126 Napoli, Italy

- $\Rightarrow$  shell-model study of Sn isotopes beyond N = 82
- $\Rightarrow$  V<sub>low-k</sub> from CD-Bonn *NN* potential
- $\Rightarrow h_{9/2} fpi_{13/2}$  model space with <sup>132</sup>Sn inert core
- $\Rightarrow$  SP energies from <sup>133</sup>Sn



 10th International Spring Seminar on Nuclear Physics: New Quests in Nuclear Structure
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### $\Rightarrow$ shell-model study of Sn isotopes beyond N = 82

... It is the aim of our study to compare the results of our calculations with the available experimental data and to make predictions for the neighboring heavier isotopes ...



### Excitation energies of the $2_1^+$ , $4_1^+$ , and $6_1^+$ states in Sn isotopes





### Excitation energies of the $2_1^+$ , $4_1^+$ , and $6_1^+$ states in Sn isotopes



#### Yrast 6<sup>+</sup> Seniority Isomers of <sup>136,138</sup>Sn

G, S. Simpson,<sup>1,2,3</sup> G. Gey,<sup>3,4,5</sup> A. Jungclaus,<sup>6</sup> J. Taprogge,<sup>6,7,5</sup> S. Nishimura,<sup>5</sup> K. Sieja,<sup>8</sup> P. Doornenbal,<sup>5</sup> G. Lorusso,<sup>5</sup> P.-A. Söderström,<sup>5</sup> T. Sumikama,<sup>9</sup> Z. Y. Xu,<sup>10</sup> H. Baba,<sup>5</sup> F. Browne,<sup>11,5</sup> N. Fukuda,<sup>5</sup> N. Inabe,<sup>5</sup> T. Isobe,<sup>5</sup> H. S. Jung,<sup>12,\*</sup> D. Kameda,<sup>5</sup> G. D. Kim,<sup>13</sup> Y.-K. Kim,<sup>13,14</sup> I. Kojouharov,<sup>15</sup> T. Kubo,<sup>5</sup> N. Kurz,<sup>15</sup> Y. K. Kwon,<sup>13</sup> Z. Li,<sup>16</sup> H. Sakurai,<sup>510</sup>



### Heavy calcium isotopes

### LETTER

doi:10.1038/nature12226

# Masses of exotic calcium isotopes pin down nuclear forces

F. Wienholtz<sup>1</sup>, D. Beck<sup>2</sup>, K. Blaum<sup>3</sup>, Ch. Borgmann<sup>3</sup>, M. Breitenfeldt<sup>4</sup>, R. B. Cakirli<sup>3,5</sup>, S. George<sup>1</sup>, F. Herfurth<sup>2</sup>, J. D. Holt<sup>6,7</sup>, M. Kowalka<sup>8</sup>, S. Kreim<sup>3,8</sup>, D. Lunney<sup>9</sup>, V. Manea<sup>3</sup>, J. Menéndez<sup>6,2</sup>, D. Neidherr<sup>2</sup>, M. Rosenbusch<sup>1</sup>, L. Schweikhard<sup>1</sup>, A. Schwenk<sup>5,4</sup>, J. Simonli<sup>5,7</sup>, J. Stanja<sup>50</sup>, R. N. Wolf<sup>8</sup> K. Zuber<sup>10</sup>

⇒ first mass measurements of  ${}^{53}$ Ca and  ${}^{54}$ Ca ⇒ new method of precision mass spectroscopy with ISOLTRAP



### Heavy calcium isotopes



### Heavy calcium isotopes

# LETTER

doi:10.1038/nature12522

# Evidence for a new nuclear 'magic number' from the level structure of $^{54}$ Ca

D. Steppenbeck<sup>1</sup>, S. Takeuchi<sup>2</sup>, N. Aoi<sup>3</sup>, P. Doornenbal<sup>2</sup>, M. Matsushita<sup>1</sup>, H. Wang<sup>2</sup>, H. Baba<sup>2</sup>, N. Fukuda<sup>2</sup>, S. Go<sup>1</sup>, M. Honma<sup>4</sup>, J. Lee<sup>4</sup>, K. Matsu<sup>2</sup>, S. Michimara<sup>5</sup>, T. Ohtobayash<sup>2</sup>, D. Nishimura<sup>6</sup>, T. Ohtsuka<sup>3,3</sup>, H. Sakura<sup>6,3</sup>, Y. Shiga<sup>1</sup>, P. -A. Söderström<sup>2</sup>, T. Sumikam<sup>3,4</sup>, H. Suzuki<sup>2</sup>, R. Tainchi<sup>4</sup>, Y. Usuro, J. J. Valience Dobon<sup>5</sup> & K. Yoneda<sup>2</sup>

### $\Rightarrow$ spectroscopic study of <sup>54</sup>Ca

⇒ proton knockout reactions involving <sup>55</sup>Sc and <sup>56</sup>Ti projectiles





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PHYSICAL REVIEW C 80, 044311 (2009)

#### Spectroscopic study of neutron-rich calcium isotopes with a realistic shell-model interaction

L. Coraggio,<sup>1</sup> A. Covello,<sup>1,2</sup> A. Gargano,<sup>1</sup> and N. Itaco<sup>1,2</sup>

<sup>1</sup>Istituto Nazionale di Fisica Nucleare, Complesso Universitario di Monte S. Angelo, Via Cintia, I-80126 Napoli, Italy <sup>2</sup>Dipartimento di Scienze Fisiche, Università di Napoli Federico II, Complesso Universitario di Monte S. Angelo, Via Cintia, I-80126 Napoli, Italy (Received 30 July 2009; published 12 October 2009)

⇒ shell-model study of neutron-rich calcium isotopes

- $\Rightarrow$  *fp* model space with <sup>40</sup>Ca inert core
- $\Rightarrow$  predictions for the (at that time) unknown spectra of  $^{53-56}$ Ca



### Heavy calcium isotopes: shell-model results





### Heavy calcium isotopes: shell-model results



different monopole properties



### Isotopic chains "north-east" of <sup>48</sup>Ca

PHYSICAL REVIEW C 89, 024319 (2014)

#### Realistic shell-model calculations for isotopic chains "north-east" of <sup>48</sup>Ca in the (N,Z) plane

L. Coraggio,<sup>1</sup> A. Covello,<sup>2</sup> A. Gargano,<sup>1</sup> and N. Itaco<sup>1,2</sup>

<sup>1</sup> Jistinto Nazionale di Fisica Nucleare, Complesso Universitario di Monte S. Angelo, Va Cintia - I-80126 Napoli, Italy <sup>2</sup>Dipartimento di Fisica, Università di Napoli Federico II, Complesso Universitario di Monte S. Angelo, Via Cintia - I-80126 Napoli, Italy (Received 16 October 2013; revised manuscript received 9 December 2013; published 26 February 2014)

We perform realistic shell-model calculations for nuclei with valence nucleons outside <sup>44</sup>Ca, employing two different model spaces. The matrix elements of the effective two-body interaction and electromagnetic multipole operators have been calculated within the framework of many-body perturbation theory, starting from a low-momentum potential derived from the high-precision CD-Bonn free nucleon-nucleon starting. In provide the provide the test of the starting the starting of the starting test of the starting test of the starting of the starting test of test of the starting test of test of

DOI: 10.1103/PhysRevC.89.024319

PACS number(s): 21.60.Cs, 23.20.Lv, 27.40.+z, 27.50.+e

 $\Rightarrow$  shell-model study of neutron-rich isotopic chains outside <sup>48</sup>Ca

 $\Rightarrow$  fpgd model space with <sup>48</sup>Ca inert core

 $\Rightarrow$  predictions for the (at that time) unknown spectra exotic Ti isotopes and of <sup>78</sup>Ni shell closure



# Isotopic chains "north-east" of <sup>48</sup>Ca: shell-model results



### **Titanium isotopes**

Nickel isotopes



# Isotopic chains "north-east" of <sup>48</sup>Ca: shell-model results



### **Titanium isotopes**

Nickel isotopes



### Conclusions and outlook

- The agreement of our results with the experimental data testifies the reliability of a microscopic shell-model calculation with realistic potentials.
- We have now evidence of the predictive power of realistic shell model
- Role of real three-body forces and three-body correlations should be investigated.
- Perspectives: benchmark calculations with other many-body approaches.





These terms introduce density dependence into the effective shell-model hamiltonian



### Conclusions and outlook

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