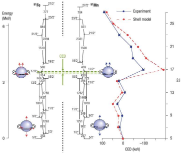
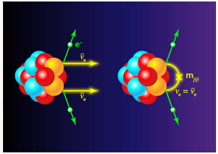
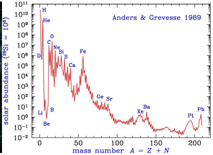
CI methods for nuclear structure and reactions

F. Nowacki, K. Sieja (IPHC), N. Smirnova (CENBG), P. Van Isacker (GANIL)

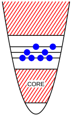






Atelier Physique Théorique des deux infinis

CI calculations: broad spectrum of applications



- define effective interaction
- $\mathscr{H}_{\text{eff}}\Psi_{\text{eff}} = E\Psi_{\text{eff}}$
- build and diagonalize energy matrix

Nuclear forces and nuclear structure

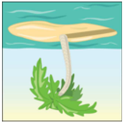
- Shell evolution: from stability to dripline
- Isospin symmetry breaking
- Emergence of quadrupole collectivity, superdeformation
- Vibrational modes
- Dipole resonances
- Symmetries

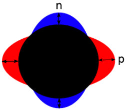
Weak processes

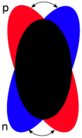
- β decay $\Longleftrightarrow$ fundamental interactions
  $\Longleftrightarrow$ nucleosynthesis
- $\beta\beta$ decay $\Longleftrightarrow$ nature of neutrino
- e capture $\Longleftrightarrow$ supernovae

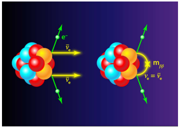
Particle capture reactions

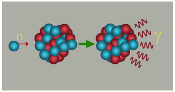
- Neutron-capture rates $\Longleftrightarrow$ r-process
- Proton-capture rates $\Longleftrightarrow$ rp-process
  $\Longleftrightarrow$ novae



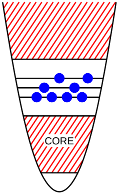








CI (LSSM) calculations: giant computations



$$H_{eff}|\Psi_{eff}\rangle = E|\Psi_{eff}\rangle$$

$$|\Psi_{eff}\rangle = \sum_{ph} C_{ph}|\Phi_{ph}\rangle$$

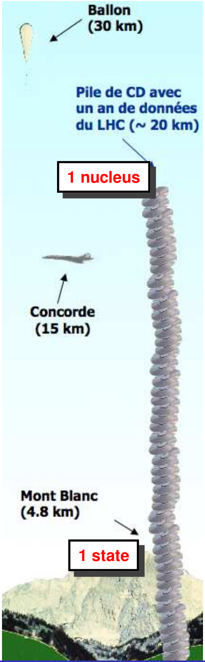
$$|\Phi_{ph}\rangle = \phi_{\alpha_1}(\vec{r}_1)\phi_{\alpha_2}(\vec{r}_2)...\phi_{\alpha_n}(\vec{r}_n)$$

$$E = \sum_{pp'hh'} C^*_{p'h'}\langle\Phi_{p'h'}|H_{eff}|\Phi_{ph}\rangle C_{ph}$$

- Exponential growth of basis dimensions: $D \sim \begin{pmatrix} d_\pi \\ p \end{pmatrix} \cdot \begin{pmatrix} d_\nu \\ n \end{pmatrix}$

  In *pf* shell :
  ^{56}Ni **1,087,455,228**
  In *pf*-*sdg* space :
  ^{78}Ni **210,046,691,518**

- Actual limits in giant diagonalizations: **0.2 10^{12}** (^{114}Sn)
- Largest matrices up to now: $\sim 10^{14}$ non-zero matrix elements
- More than 1,000,000 CD-ROM's to store a single matrix !
- Can not be stored on hard disk: computed on the fly
- Strasbourg LSSM codes: **ANTOINE** and **NATHAN**



PHYSICAL REVIEW C **100**, 054329 (2019)

Structure and decay of exotic nuclei

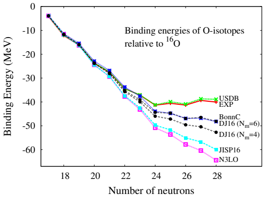
Nowadays, LSSM calculations in extended model spaces comprising a few oscillator shells
☞shell structure evolution and sudden onset of deformation in very neutron-rich nuclei

Accurate description and deep insight into nuclear structure
☞pavement for ab-initio methods

- Construction of fully microscopic interactions for valence-space calculations (Okubo-Lee-Suzuki transformation) as a path towards regions where no experimental data available
- Development of numerical techniques and state-of-the-art computations
- Search for additionnal guidelines and shortcuts using symmetry based approaches

Effective interactions in the *sd* shell

N. A. Smirnova*
CENBG (CNRS/IN2P3 - Université de Bordeaux), 33175 Gradignan cedex, France

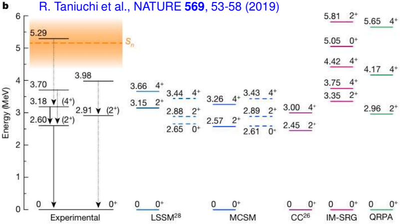


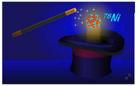
ARTICLE

https://doi.org/10.1038/s41586-019-1155-x

^{78}Ni revealed as a doubly magic stronghold against nuclear deformation

R. Taniuchi et al., NATURE **569**, 53-58 (2019)





PRL

Shape Coexistence in ^{78}Ni as the Portal to the Fifth Island of Inversion

F. Nowacki, A. Poves, E. Caurier, and B. Bounthong

Phys. Rev. Lett. **117**, 272501 (2016) - Published 27 December 2016

PRL Featured in Physics Editors' Suggestion

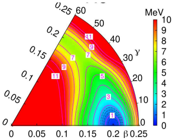
Binding Energy of ^{79}Cu: Probing the Structure of the Doubly Magic ^{78}Ni from Only One Proton Away

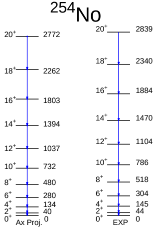
A. Welker, N. A. S. Althubiti, D. Atanasov, K. Blaum, T. E. Cocolios, F. Herfurth, S. Kreim, D. Lunney, V. Manea, M. Mougeot, D. Neidherr, F. Nowacki, A. Poves, M. Rosenbusch, L.

BSM: New opportunities for nuclear structure studies

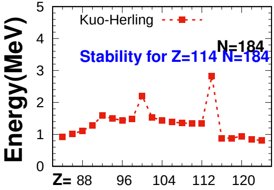
Synergies between Large Scale Shell Model & Projected Generator Coordinate Method

Application to studies of:
-Octupole shapes
-N=Z nuclei
-Heavy and superheavy nuclei
-$\beta\beta$ decay
-r-process nucleosynthesis





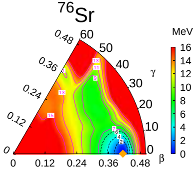
- Technical aspects with Taurus/DFSM codes
- Optimal selection of GCM states
- Center of mass decoupling
- Ab-initio interactions



Collaboration with Universidad Autonoma Madrid
& IRN ASTRANUCAP

B. Bounthong, IPHC, PhD Thesis (2016)
D. Dao, IPHC, Post-Doc (2021)

BSM: New opportunities for nuclear structure studies



Synergies between Large Scale Shell Model & Projected Generator Coordinate Method

Application to studies of:
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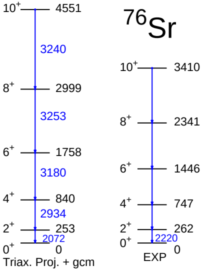
Triax. proj. + GCM:

Strongly deformed 8p8h structure



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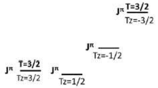
Collaboration with Universidad Autonoma Madrid & IRN ASTRANUCAP

D. Dao, IPHC, Post-Doc (2021)

Isospin symmetry breaking

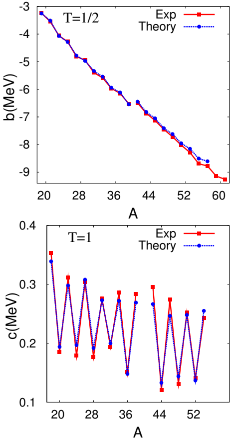
$$M(\alpha,T) = a(\alpha,T) + b(\alpha,T)T_Z + c(\alpha,T)T_Z^2$$



Accurate description of isospin violation and associated phenomena through development of Isospin Non Conserving hamiltonians in extended valence spaces:
$((sd), (pf), (s_{1/2}d_{3/2}f_{7/2}p_{3/2})$ and beyond

$\beta - p$ and $\beta - p\gamma$ decay studies and extraction of isospin mixing in the IAS

- Development of Isospin Non Conserving hamiltonians in the $(sd - pf)$ valence space and numerous applications
- Improvement of MED and TED description within a band
- Interpretation for b and c coefficients staggering
- Support to forthcoming experimental studies



Isospin symmetry breaking

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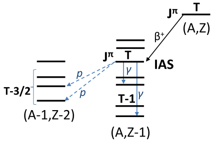

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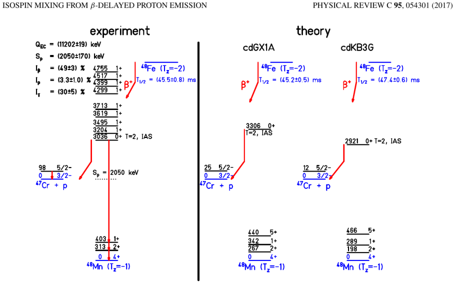


^{48}**Mn: S_{exp} = 2.7(9).10^{-3} , α_{exp} = 1.4(5)%**

Nadezda Smirnova

Isospin-symmetry breaking: exotic nuclei, fundamental interactions and astrophysics

(2017-2022) IN2P3/CENBG/IPHC/GANIL

$0^+ \to 0^+$ β-decay: a test of fundamental interactions

Large scale calculations for all emitters below A $\leq$ 40 including nuclei in the vicinity of ^{40}Ca

Use of Isospin Non Conserving hamiltonians and Woods-Saxon wave functions for untruncated *sd* and *pf* calculations

New approach of radii determination without closure approximation

Use of new effective interactions developped in Strasbourg

- Lanczos Structure Function Method for δ_C
- New $(sd - pf)$ interaction
- Effective Fermi Operator
- HF wave functions
- New emitters such as ^{58}Zn

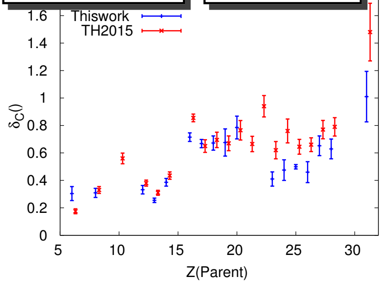
Nadezda Smirnova

-Isospin-symmetry breaking: exotic nuclei, fundamental interactions and astrophysics

(2017-2022) IN2P3/CENBG/IPHC/GANIL

$$\mathscr{F}t = (1+\delta_R)(1+\delta_{NS}-\delta_C)ft = \frac{K}{M_{F0}^2 G_F^2 |V_{ud}|^2 (1+\Delta_R)}$$

CVC hypothesis **CKM unitarity**



L. Xayavong, CENBG, PhD Thesis (2016)

L. Xayavong and N. Smirnova, PRC97 (2018) 024324; PROC. NTSE2018.

$\beta\beta$-decay and nature of neutrino

Reliable nuclear matrix elements needed to plan and fully exploit impressive experiments looking for neutrinoless double-beta decay

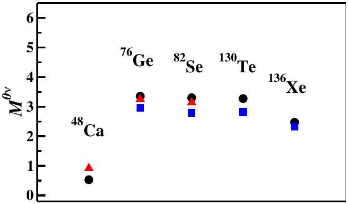
PRL Editors' Suggestion

Search for Neutrinoless Quadruple-β Decay of ^{150}Nd with the NEMO-3 Detector

R. Arnold *et al.* (NEMO-3 Collaboration)

Phys. Rev. Lett. **119**, 041801 (2017) - Published 24 July 2017

$$[T^{0\nu}_{1/2}(0^+ \rightarrow 0^+)]^{-1} = G_{0\nu}|M^{0\nu}|^2\langle m_\nu^{\beta\beta}\rangle^2$$



The calculation of the neutrinoless double-β decay matrix element within the realistic shell model

L. Coraggio,[1] A. Gargano,[1] N. Itaco,[2,1] R. Mancino,[2,1] and F. Nowacki[3,4,2]

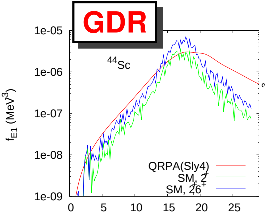
☞Talk of F. Nowacki later in this session

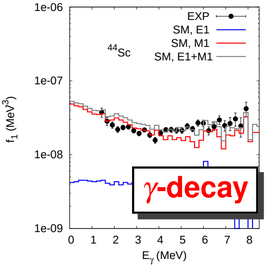
Input for reaction codes and benchmark of many-body methods

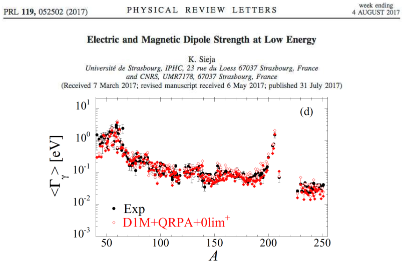
Statistical treatment of the γ de-excitation strength function
☞computations of thousands states and transitions needed

M1 and E1 treated on the same footing (application possible to any multipolarity)

Improved description of the radiative widths and CI-guided developments of fully-microscopic QRPA models






PRL 119, 052502 (2017) PHYSICAL REVIEW LETTERS week ending 4 AUGUST 2017

Electric and Magnetic Dipole Strength at Low Energy

K. Sieja
Université de Strasbourg, IPHC, 23 rue du Loess 67037 Strasbourg, France and CNRS, UMR7178, 67037 Strasbourg, France

(Received 7 March 2017; revised manuscript received 6 May 2017; published 31 July 2017)

- Microscopic nuclear structure input for reaction codes (TALYS)
- Reliable predictions of reactions rates for nucleosynthesis

Kamila Sieja
Gamma Strength
(2017-2019) IN2P3/IPHC
collaboration CEA-DAM and University of Brussels

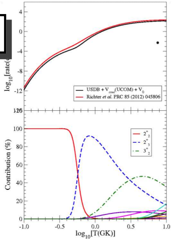
S. Goriely, S. Hilaire, S. Péru, KS, Phys.Rev.C98(2018)014327

Reaction rates and nucleosynthesis

Proton capture reaction rates for rp process (X-ray bursts) or novae

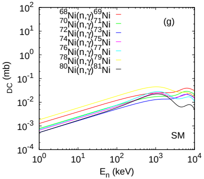
-Resonance energies (with Isospin breaking)
-Widths with respect to proton and γ emission
-Several reactions in the *sd* shell
-*pf* shell nuclei around ^{40}Ca
-Thomas-Ehrman shift in *sd* shell
-$(\alpha,\gamma),(\alpha,p),(p,\alpha)$ capture/emission modeling
-$^{22}Mg(\alpha,p)^{25}Al$ and other reactions

$^{35}Ar(p,\gamma)^{36}K$



Neutron capture reaction rates for r-process

-CI calculations as benchmark for other methods
-Input for reaction studies: spectra, spectroscopic factors, decay widths
-Systematic evaluation of direct capture rates
-Tests of Hauser-Feshbach model in neutron-rich nuclei
-Resonant capture much more difficult to treat on the neutron-rich side



☞Talk of M. Oertel in the afternoon session

Summary

- High predictive power, accurate and detailed information (structure near and far from stability, nuclear and electroweak processes)
- Success and robustness of the approach encourage further developments and applications
- Simultaneous description of multiple low-energy phenonema but need of dedicated local studies
- Intense support for future experimental programs and developments (but manpower insufficient ...)
- Existing cross fertilizing collaborations in several domains: ab-initio studies, isospin symmetry breaking, astrophysics, $\beta\beta$ decay ... and others to develop !