Modelli Teorici per Studi di Struttura Nucleare II

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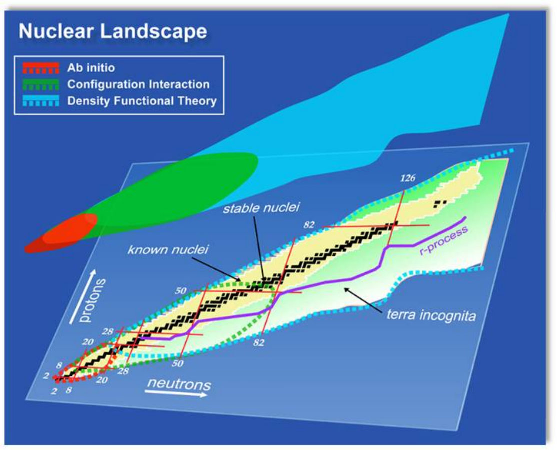
Microscopic nuclear structure calculations

- Common background: the starting point is a realistic nuclear potential.
- Main tasks:
  - take into account, as much as possible, all degrees of freedom of the interacting nucleons;
  - keep under control the needed approximations: evaluation of theoretical errors;
  - parameter-free approach to the nuclear structure;
  - enhance the predictiveness.
- Notable models: No-core shell model, coupled-cluster approach, realistic shell model.

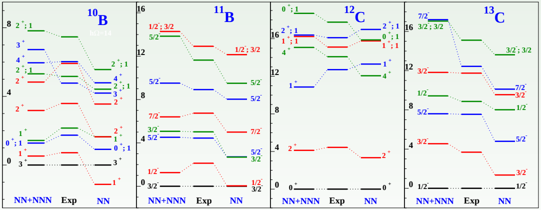

Nuclear Landscape
Ab initio
Configuration Interaction
Density Functional Theory
stable nuclei
known nuclei
r-process
terra incognita
protons
neutrons
126
82
50
28
20
8
2

No-Core Shell Model

The starting point: $A-$nucleons hamiltonian, that includes also the center-of-mass potential

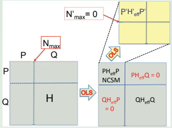
$$H_A^{\omega} = \sum_{i=1}^{A} \left[\frac{p_i^2}{2m} + \frac{1}{2}\omega^2 r_i^2 \right] + \sum_{i<j=1}^{A} \left[V(\mathbf{r}_i - \mathbf{r}_j) - \frac{m\omega^2}{2A}(\mathbf{r}_i - \mathbf{r}_j)^2 \right]$$

- Problem: too big to be diagonalized, even for light nuclei
- Solution: The Hilbert space is then truncated to those states with harmonic oscillator quanta N less or equal than a fixed $N_{\rm max}$
- $\Rightarrow$ An effective hamiltonian $H_{\rm eff}$ that acts in this truncated model space is derived by way of the Lee-Suzuki unitary transformation.

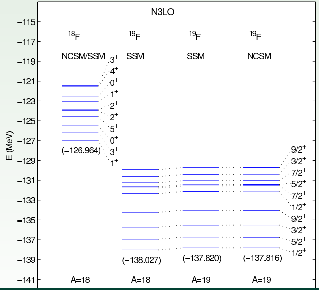


No-Core Shell Model

- Limitations: NCSM, within present computer technology, provides reliable nuclear structure only for light nuclear systems.
- Evolution: with a double-step procedure, an effective shell-model hamiltonian for a shell-model calculation (a few valence nucleons in a reduced model space) may be obtained.



- ⇒ This extension may applied to heavier nuclei.



Coupled-Cluster Approach

Within the coupled-cluster theory (F. Coester,1958) the correlated function of the many-body system is written as

$$|\Psi\rangle = \exp(-T)|\Psi_0\rangle \quad ,$$

where the correlation operator $T = T_1 + T_2 + ... + T_A$ is expressed as a sum of correlation operators

$$T_1 = \sum_{i<\epsilon_f, a>\epsilon_f} t_i^a a_a^\dagger a_i \qquad T_2 = \sum_{ij<\epsilon_f, ab>\epsilon_f} t_{ij}^{ab} a_a^\dagger a_b^\dagger a_i a_j \qquad ...$$

Coupled-Cluster Approach

The amplitudes *t* of the correlation operators are calculated using the variational principle. This procedure leads to the following set of equations:

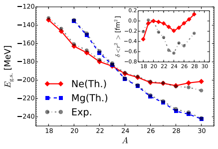
$$
\begin{aligned}
\langle \Psi_0 | \exp(T) H \exp(-T) | \Psi_i^a \rangle &= 0 \\
\langle \Psi_0 | \exp(T) H \exp(-T) | \Psi_{ij}^{ab} \rangle &= 0 \\
&\dots
\end{aligned}
$$

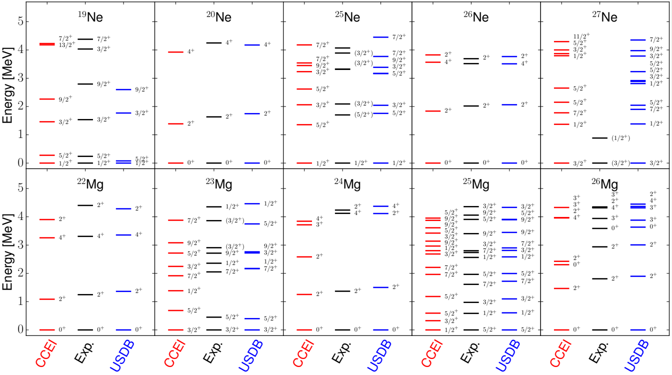
These equations may be calculated using the Baker-Hausdorf relation:

$$
\begin{aligned}
\exp(T) H \exp(-T) &= H + [H, T_1] + [H, T_2] + \frac{1}{2} [[H, T_1], T_1] + \\
&+ \frac{1}{2} [[H, T_2], T_2] + [[H, T_1], T_2]
\end{aligned}
$$

Coupled-Cluster Approach

This method may be more easily extended to heavier systems





The realistic shell model

- The derivation of the shell-model effective hamiltonian using the many-body perturbation theory may provide a useful tool to study nuclei in the full range of nuclear masses
- 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_{eff} theoretically

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

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

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

1. Choose a realistic *NN* potential (*NNN*)
2. Set up the model space which is better tailored to study the nuclear system under investigation
3. Derive the effective shell-model hamiltonian by way of the many-body theory
4. Calculate the physical observables (energies, e.m. transition probabilities, ...)

The shell-model effective hamiltonian

A-nucleon system Schrödinger equation

$$H|\Psi_\nu\rangle = E_\nu|\Psi_\nu\rangle$$

with

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

Model space

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

Model-space eigenvalue problem

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

The shell-model effective hamiltonian

$$\left(\begin{array}{c|c} PHP & PHQ \\ \hline QHP & QHQ \end{array}\right) \quad \overset{\mathcal{H}=X^{-1}HX}{\underset{Q\mathcal{H}P=0}{\Longrightarrow}} \quad \left(\begin{array}{c|c} P\mathcal{H}P & P\mathcal{H}Q \\ \hline 0 & Q\mathcal{H}Q \end{array}\right)$$

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

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

$$H_1^{\rm eff}(\omega) = PH_1P + PH_1Q\frac{1}{\epsilon - QHQ}QH_1P - $$
$$-PH_1Q\frac{1}{\epsilon - QHQ}\omega H_1^{\rm eff}(\omega)$$

The shell-model effective hamiltonian

Folded-diagram expansion

$\hat{Q}$-box vertex function

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

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

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

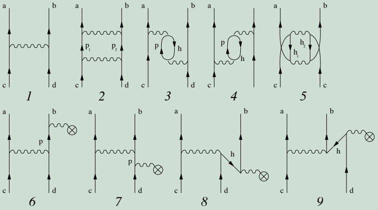
The perturbative approach to the shell-model H^{eff}

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

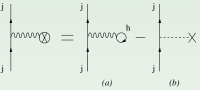
The $\hat{Q}$-box can be calculated perturbatively

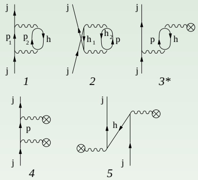
$$\frac{1}{\epsilon - QHQ} = \sum_{n=0}^{\infty} \frac{(QH_1Q)^n}{(\epsilon - QH_0Q)^{n+1}}$$

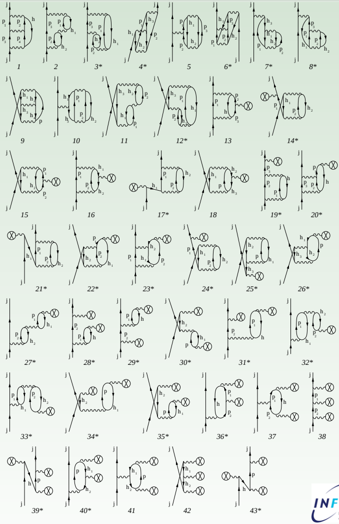
The diagrammatic expansion of the $\hat{Q}$-box



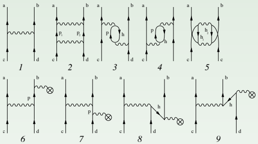
$\hat{Q}$-box perturbative expansion: 1-body diagrams

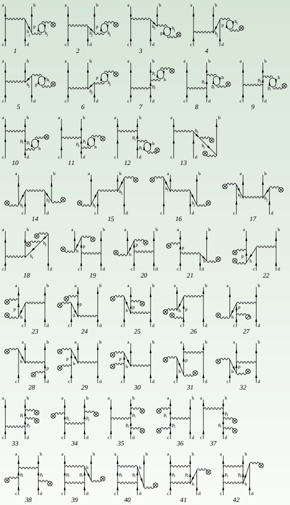




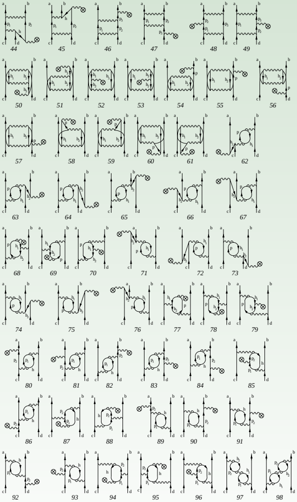


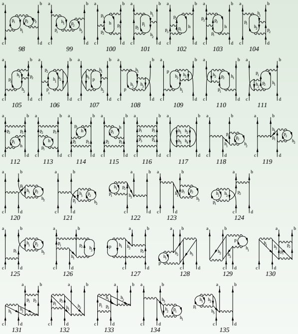
$\hat{Q}$-box perturbative expansion: 2-body diagrams





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





Our recipe for realistic shell model

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

Large-scale shell model

- 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. Zuker
Groupe de Physique Théorique, Centre de Recherches Nucléaires, Institut National de Physique Nucléaire et de Physique des Particles, Centre National de la Recherche Scientifique, Université Louis Pasteur Boîte Postale 20, F-67037 Strasbourg-Cedex, France

A. Poves and G. Martínez-Pinedo
Departamento de Física Teórica C-XI, Universidad Autónoma de Madrid, E-28049 Madrid, Spain
(Received 16 December 1993)

VOLUME 77, NUMBER 16 PHYSICAL REVIEW LETTERS 14 OCTOBER 1996

Nuclear Shell Model by the Quantum Monte Carlo Diagonalization Method

Michio Honma,[1] Takahiro Mizusaki,[2] and Takaharu Otsuka[2,3]
[1]*Center for Mathematical Sciences, University of Aizu, Tsuruga, Ikki-machi, Aizu-Wakamatsu, Fukushima 965, Japan*
[2]*Department of Physics, University of Tokyo, Hongo, Tokyo 113, Japan*
[3]*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.

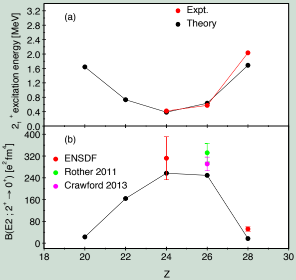
Collective behavior

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

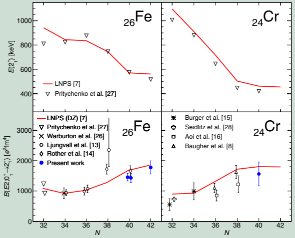
Quadrupole Collectivity in Neutron-Rich Fe and Cr Isotopes

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 $N = 40$



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



Collective behavior

PRL **110**, 172501 (2013) PHYSICAL REVIEW LETTERS week ending 26 APRIL 2013

Coulomb Excitation of ^{104}Sn and the Strength of the ^{100}Sn Shell Closure

G. Guastalla,[1] D. D. DiJulio,[2] M. Górska,[3] J. Cederkäll,[2] P. Boutachkov,[1,3] P. Golubev,[2] S. Pietri,[3] H. Grawe,[3] F. Nowacki,[4] K. Sieja,[4] A. Algora,[5,6] F. Ameil,[3] T. Arici,[7,3] A. Atac,[8] M. A. Bentley,[9] A. Blazhev,[10] D. Bloor,[9] S. Brambilla,[11] N. Braun,[10] F. Camera,[11] Zs. Dombrádi,[6] C. Domingo Pardo,[5] A. Estrade,[3] F. Farinon,[3] J. Gerl,[3] N. Goel,[3,1] J. Grębosz,[12] T. Habermann,[3,13] R. Hoischen,[2] K. Jansson,[2] J. Jolie,[10] A. Jungclaus,[14] I. Kojouharov,[3] R. Knoebel,[3] R. Kumar,[15] J. Kurcewicz,[16] N. Kurz,[3] N. Lalović,[3] E. Merchan,[1,3] K. Moschner,[10] F. Naqvi,[3,10] B. S. Nara Singh,[9] J. Nyberg,[17] C. Nociforo,[3] A. Obertelli,[18] M. Pfützner,[3,16] N. Pietralla,[1] Z. Podolyák,[19] A. Prochazka,[3] D. Ralet,[1,3] P. Reiter,[10] D. Rudolph,[2] H. Schaffner,[3] F. Schirru,[19] L. Scruton,[9] D. Sohler,[6] T. Swaleh,[2] J. Taprogge,[10,20] Zs. Vajta,[6] R. Wadsworth,[9] N. Warr,[10] H. Weick,[3] A. Wendt,[10] O. Wieland,[11] J. S. Winfield,[3] and H. J. Wollersheim[3]

PHYSICAL REVIEW C **88**, 051301(R) (2013)

Quadrupole collectivity in neutron-deficient Sn nuclei: ^{104}Sn and the role of proton excitations

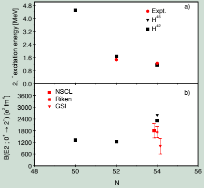
V. M. Bader,[1,2] A. Gade,[1,2] D. Weisshaar,[1,2] B. A. Brown,[1,2] T. Baugher,[1,2] D. Bazin,[1] J. S. Berryman,[1] A. Ekström,[1,3] M. Hjorth-Jensen,[1,2,3] S. R. Stroberg,[1,2] W. B. Walters,[4] K. Wimmer,[1,5] and R. Winkler[1,*]

PHYSICAL REVIEW C **90**, 061302(R) (2014)

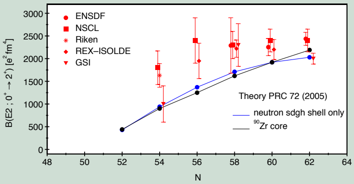
Intermediate-energy Coulomb excitation of ^{104}Sn: Moderate $E2$ strength decrease approaching ^{100}Sn

P. Doornenbal,[1,*] S. Takeuchi,[1] N. Aoi,[2] M. Matsushita,[3,4] A. Obertelli,[5] D. Steppenbeck,[3] H. Wang,[1,6] L. Audirac,[5] H. Baba,[1] P. Bednarczyk,[7] S. Boissinot,[5] M. Ciemala,[7,†] A. Corsi,[5] T. Furumoto,[8] T. Isobe,[1] A. Jungclaus,[9] V. Lapoux,[5] J. Lee,[1] K. Matsui,[10] T. Motobayashi,[1] D. Nishimura,[11] S. Ota,[3] E. C. Pollacco,[5] H. Sakurai,[1,10] C. Santamaria,[5] Y. Shiga,[4] D. Sohler,[12] and R. Taniuchi[10]

Quadrupole collectivity in light tin isotopes



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



Novel collective feaures

RAPID COMMUNICATIONS

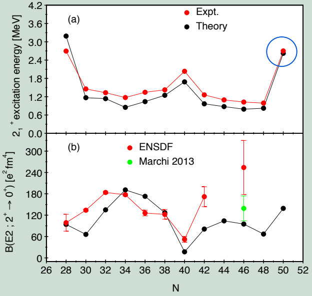
PHYSICAL REVIEW C **89**, 031301(R) (2014)

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

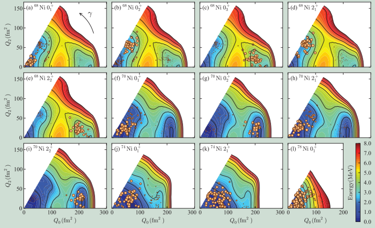
Yusuke Tsunoda,[1] Takaharu Otsuka,[1,2,3] Noritaka Shimizu,[2] Michio Honma,[4] and Yutaka Utsuno[5]

Shape evolution in Ni isotopes

Realistic shell-model



Monte Carlo shell model



Islands of inversion

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

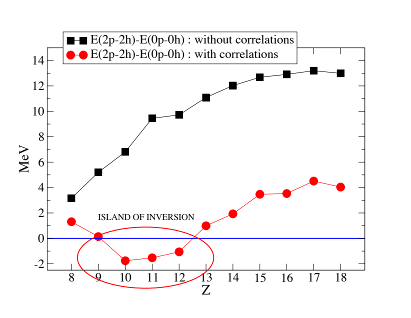
Merging of the islands of inversion at $N = 20$ and $N = 28$

E. Caurier,[1] F. Nowacki,[1] and A. Poves[2,3]
[1] *IPHC, IN2P3-CNRS and Université Louis Pasteur, F-67037 Strasbourg, France*
[2] *Departamento de Física Teórica and IFT-UAM/CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain*
[3] *Isolde (CERN) 1211 Genève 23, Switzerland*

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

Model space: full sdfp shell

Shell model basis has a dimension up to 10^{10}



Shell evolution

PHYSICAL REVIEW C **87**, 034309 (2013)

Evolution of single-particle states beyond ^{132}Sn

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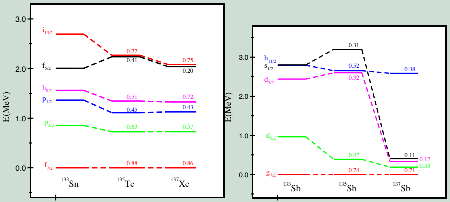
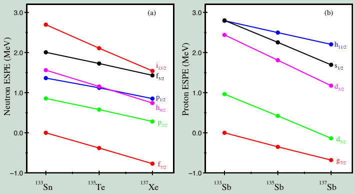
[2]*Dipartimento di Fisica, Università di Napoli Federico II, Complesso Universitario di Monte S. Angelo, I-80126 Napoli, Italy*

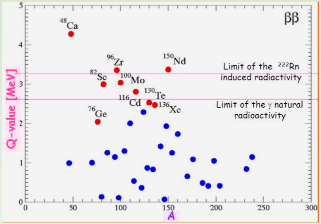
(Received 15 January 2013; published 7 March 2013)

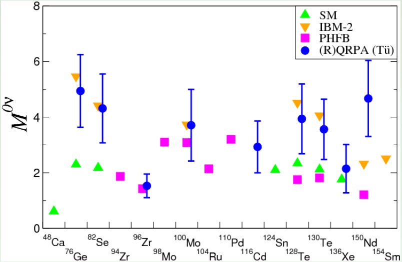
Evolution of single-particle structure beyond doubly-closed ^{132}Sn

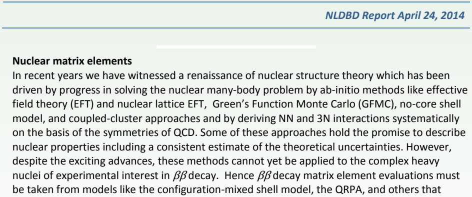




The detection of the $0\nu\beta\beta$-decay







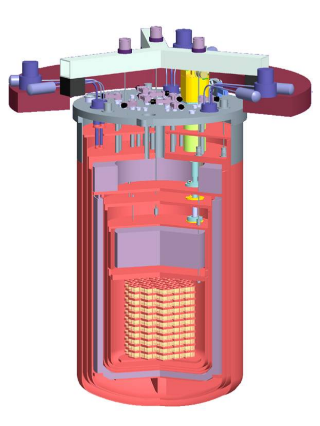
NLDBD Report April 24, 2014

Nuclear matrix elements

In recent years we have witnessed a renaissance of nuclear structure theory which has been driven by progress in solving the nuclear many-body problem by ab-initio methods like effective field theory (EFT) and nuclear lattice EFT, Green's Function Monte Carlo (GFMC), no-core shell model, and coupled-cluster approaches and by deriving NN and 3N interactions systematically on the basis of the symmetries of QCD. Some of these approaches hold the promise to describe nuclear properties including a consistent estimate of the theoretical uncertainties. However, despite the exciting advances, these methods cannot yet be applied to the complex heavy nuclei of experimental interest in $\beta\beta$ decay. Hence $\beta\beta$ decay matrix element evaluations must be taken from models like the configuration-mixed shell model, the QRPA, and others that

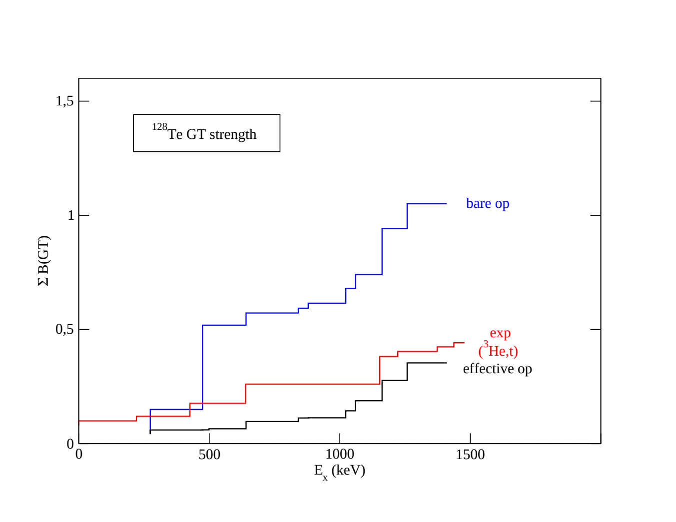
The spread of nuclear structure calculations evidences inconsistencies among results obtained with different models

CUORE@LNGS

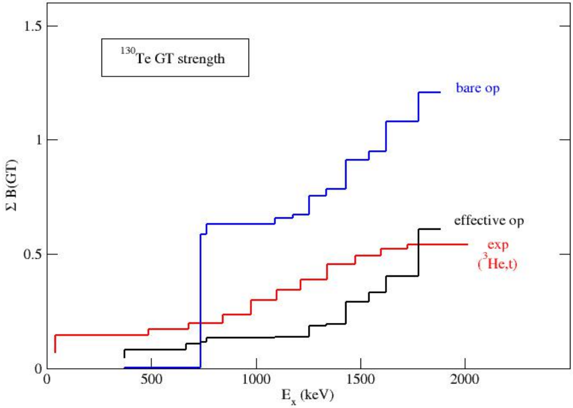


- TeO_2 crystals used as low heat capacity bolometers, arranged into towers and cooled in a large cryostat to approximately 10 m°K with a dilution refrigerator.
- The detectors are isolated from backgrounds by ultrapure low-radioactivity shielding.
- Temperature spikes from electrons emitted in Te $0\beta\beta$ are collected for spectrum analysis.

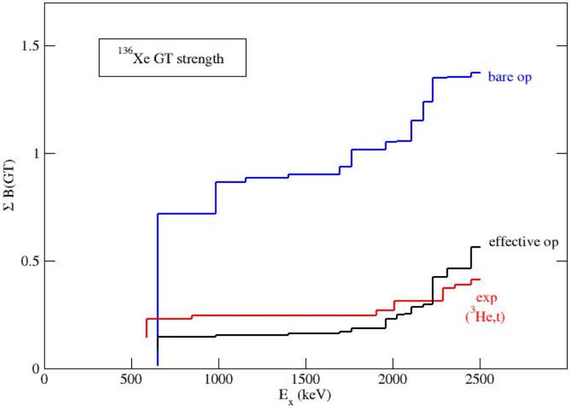
Realistic shell model: ^{128}Te Gamow-Teller strengths



Realistic shell model: ^{130}Te Gamow-Teller strengths



Realistic shell model: ^{136}Xe Gamow-Teller strengths

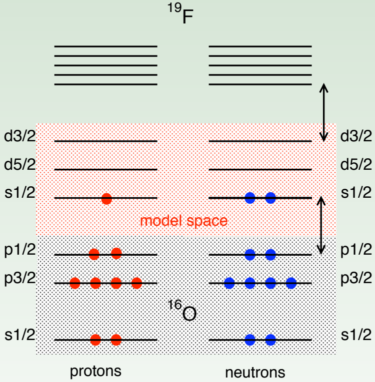


Conclusions and outlook

- The flow of experimental data coming from RIB facilities is stimulating advances in nuclear structure theory.
- Nuclear structure calculations starting from realistic nuclear potentials are now successful instruments to understand a large variety of nuclear phenomena.
- The parameter-free nature of realistic nuclear-structure calculations should provide a more reliable predictive power.
- Realistic shell model at present is the approach that provides microscopic calculations over a wider mass range, and may describe a large set of different observables.
- Application to problems in fundamental physics:, $0\nu\beta\beta$-decay, WIMP-nucleus interaction, electric-dipole moments and T-violation, etc.

Backup slides

An example: ^{19}F



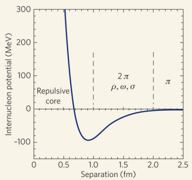
- 9 protons & 10 neutrons interacting
- spherically symmetric mean field (e.g. harmonic oscillator)
- 1 valence proton & 2 valence neutrons interacting in a truncated model space

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

Realistic nucleon-nucleon potential: V_{NN}

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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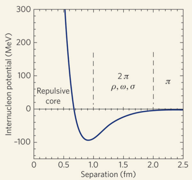

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  - V_{low-k}, SRG
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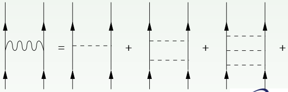

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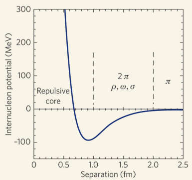

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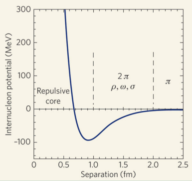

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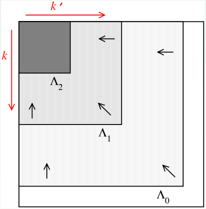

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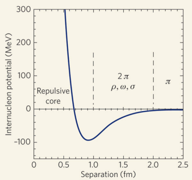

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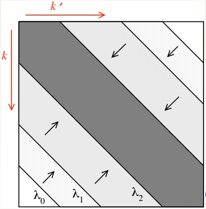

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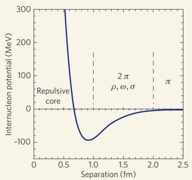

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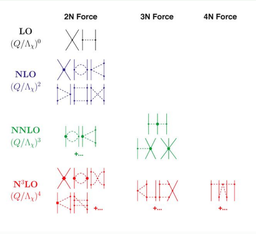

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Test case: *p*-shell nuclei

- $V_{NN} \Rightarrow$ chiral N^{3}LO potential by Entem & Machleidt (smooth cutoff $\simeq 2.5$ fm^{-1})
- $H_{\rm eff}$ for two valence nucleons outside ^{4}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)*

INFN Istituto Nazionale di Fisica Nucleare

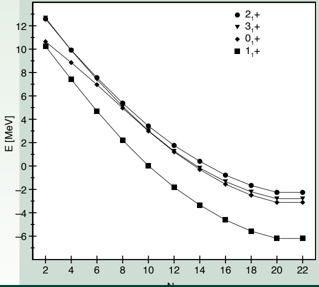
Convergence checks

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

$$|\epsilon_0 - QH_0Q| \leq E_{\max} = N_{\max}\hbar\omega$$

^{6}Li yrast states

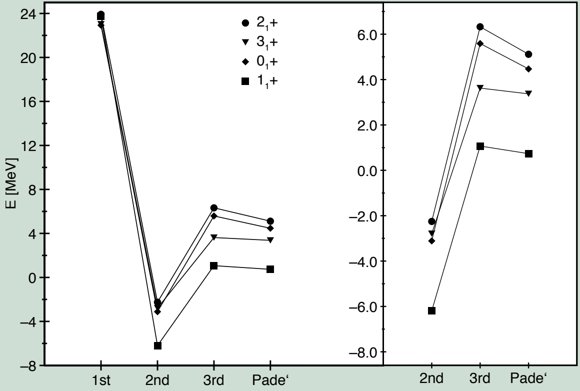


results stable for $N_{\max} \geq 20$

Convergence checks

Order-by-order convergence

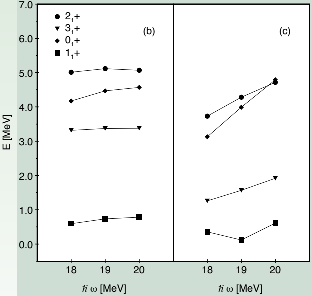
Compare results from $H^{\mathrm{eff}}_{\mathrm{1st}}$, $H^{\mathrm{eff}}_{\mathrm{2nd}}$, $H^{\mathrm{eff}}_{\mathrm{3rd}}$ and $H^{\mathrm{eff}}_{\mathrm{Padè}}$



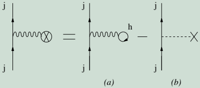
Convergence checks

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 $\hbar\omega$

Benchmark calculation

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)

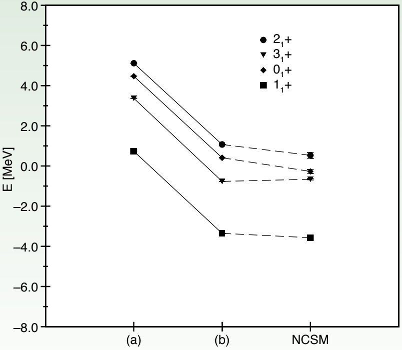
P. Navrátil *et al.*, Phys. Rev. Lett. **99**, 042501 (2007)

Benchmark calculation

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

$$H_{int} = \left(1 - \frac{1}{A}\right) \sum_{i=1}^{A} \frac{p_i^2}{2m} + \sum_{i<j=1}^{A} \left(V_{ij}^{NN} - \frac{\mathbf{p_i} \cdot \mathbf{p_j}}{mA} \right) =$$

$$= \left[\sum_{i=1}^{A} \left(\frac{p_i^2}{2m} + U_i \right) \right] + \left[\sum_{i<j=1}^{A} \left(V_{ij}^{NN} - U_i - \frac{p_i^2}{2mA} - \frac{\mathbf{p_i} \cdot \mathbf{p_j}}{mA} \right) \right]$$

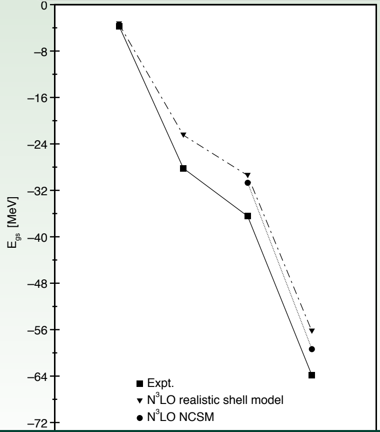


(a) not translationally invariant Hamiltonian
(b) purely intrinsic hamiltonian

Benchmark calculation

Remark

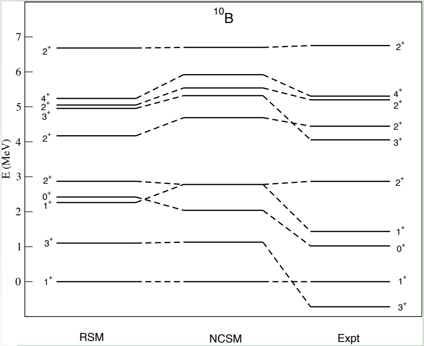
$H^{\rm eff}$ derived for 2 valence nucleon systems $\Rightarrow$ 3-, 4-, .. n-body components are neglected



- ground-state energies for $N = Z$ nuclei
- discrepancy grows with the number of valence nucleons

Benchmark calculation

^{10}B relative spectrum



- discrepancy $\leq$ 1 MeV
- minor role of many-body correlations