

# Nuclear structure (theory) related to NUSTAR and FAIR

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**University of Barcelona  
Institute of Cosmos Sciences**

**FAIRness 2024, 8<sup>th</sup> FAIRness workshop**

**Donji Seget, 27<sup>th</sup> September 2024**

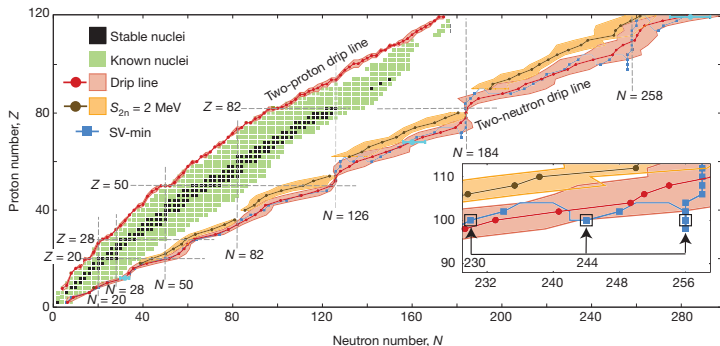


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BARCELONA



# Nuclear landscape

The goal of nuclear theory is a unified description of nuclear structure, across the nuclear chart and based on nuclear forces



~ 3000 isotopes measured

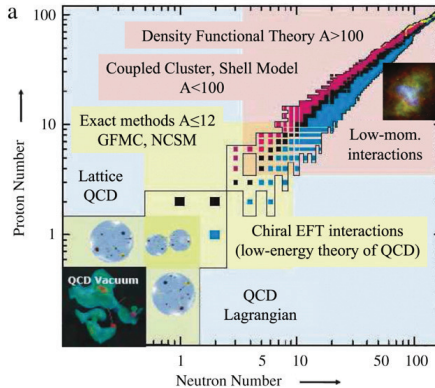
~ 7000 predicted

Erler et al.  
 Nature 486 509 (2012)

Limits of existence, ground-state properties, shell evolution, excitation spectra, spectroscopy, shape coexistence,  $\beta$  decays, fission...

# Nuclear Structure from First Principles

All nuclear structure calculations are, to some extent, phenomenological



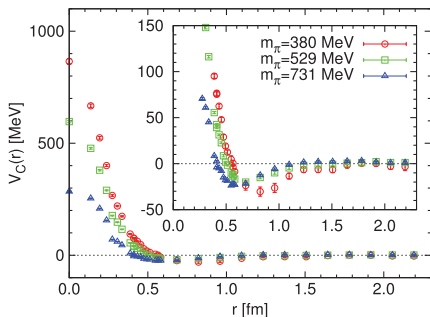
Relevant degrees of freedom:  
 protons and neutrons  
 Many-body problem  
 too hard in general,  
 approximations are needed

Nuclear force at low  
 (nuclear structure) energies:  
 adjustments to reproduce  
 finite nuclei needed

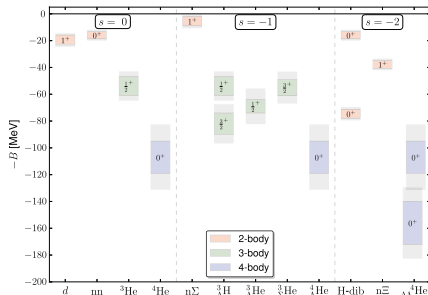
**Can we connect  
 nuclear structure  
 calculations to quantum  
 chromodynamics (QCD)?**

# Lattice QCD

QCD non-perturbative at low energies relevant for nuclear structure  
 Lattice QCD solves the QCD Lagrangian in discretized space-time lattice



HALQCD Collaboration



NPLQCD Collaboration

Nuclear potentials, and lightest nuclei and hypernuclei solved  
 at non-physical pion mass  $m_\pi \sim 400 - 800$  MeV, ongoing improvements

# Theory for nuclear forces

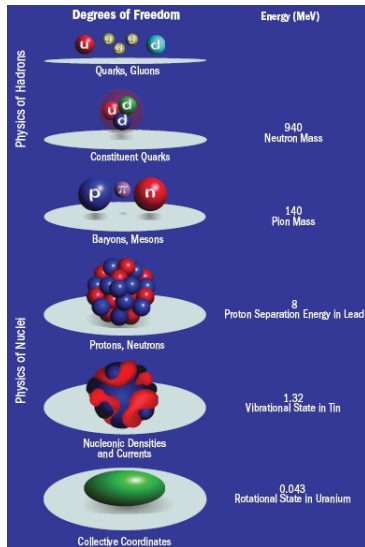
Difficult to find NN potential with consistent NNN forces and connected to QCD...

Use concept of separation of scales!

The energy scale relevant determines the degrees of freedom

For nuclear structure, typical energies of interest point to nucleons and pions (pions are particularly light mesons!)

Effective theory with nucleons and pions as degrees of freedom, with connection to QCD



# Effective theories

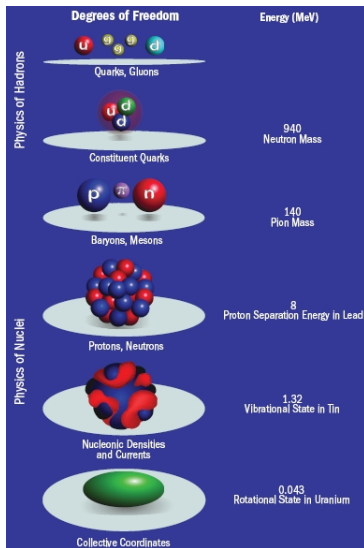
Effective theory:  
approximation of the full theory  
valid at relevant scales

Expansion in terms of small  
parameter: typical scale /  
breakdown scale

In an effective theory  
the physics resolved  
at relevant energies is explicit

Terms at different orders given by  
symmetries of the full theory

Unresolved physics  
encoded in Low Energy Couplings

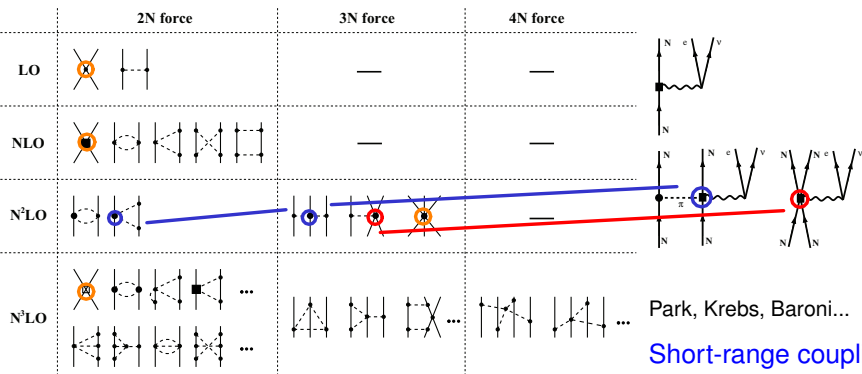


# Chiral Effective Field Theory (EFT)

Chiral EFT: low energy approach to QCD, nuclear structure energies

Approximate chiral symmetry: pion exchanges, contact interactions

Systematic expansion: nuclear forces and electroweak currents



Park, Krebs, Baroni...

Short-range couplings fitted to experiment once

Weinberg, van Kolck, Kaplan, Savage, Wise, Meißner, Epelbaum...

# Ab initio many-body methods

Oxygen dripline using chiral NN+3N forces correctly reproduced  
 ab-initio calculations treating explicitly all nucleons  
 excellent agreement between different approaches

No-core shell model  
 (Importance-truncated)

In-medium SRG

Hergert et al. PRL110 242501(2013)

Self-consistent Green's function

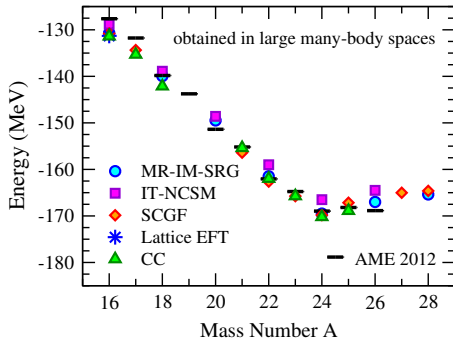
Cipollone et al. PRL111 062501(2013)

Coupled-clusters

Jansen et al. PRL113 142502(2014)

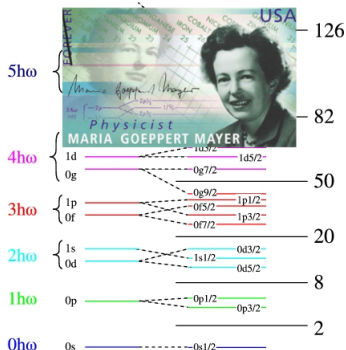
Recent application to  $^{208}\text{Pb}$

Hu, Jiang, Miyagi et al. Nature Phys. 18, 1196 (2022)





# Nuclear shell model



Nuclear shell model configuration space only keep essential degrees of freedom

- High-energy orbitals: always empty
- **Valence space:** where many-body problem is solved
- Inert core: always filled

$$H|\Psi\rangle = E|\Psi\rangle \rightarrow H_{\text{eff}}|\Psi\rangle_{\text{eff}} = E|\Psi\rangle_{\text{eff}}$$

$$|\Psi\rangle_{\text{eff}} = \sum_{\alpha} c_{\alpha} |\phi_{\alpha}\rangle, \quad |\phi_{\alpha}\rangle = a_{i_1}^{\dagger} a_{i_2}^{\dagger} \dots a_{i_A}^{\dagger} |0\rangle$$

Shell model diagonalization:

$\sim 10^{10}$  Slater det. Caurier et al. RMP77 (2005)

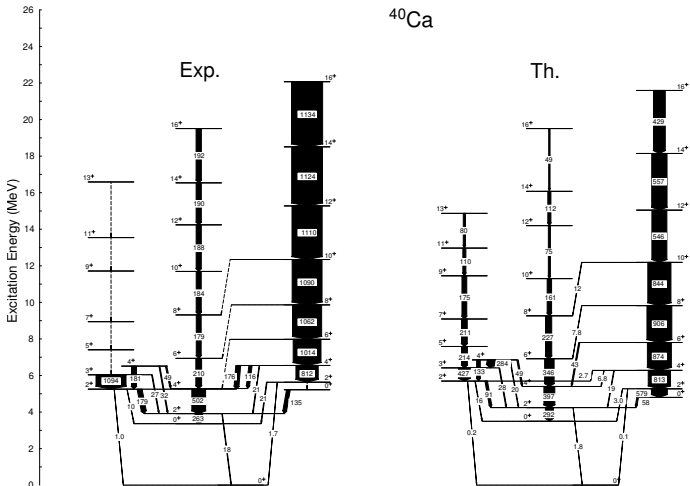
$\gtrsim 10^{24}$  Slater det. with Monte Carlo SM

Otsuka, Shimizu, Y.Tsunoda

$H_{\text{eff}}$  includes effects of

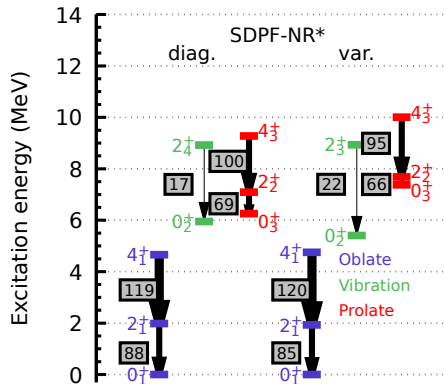
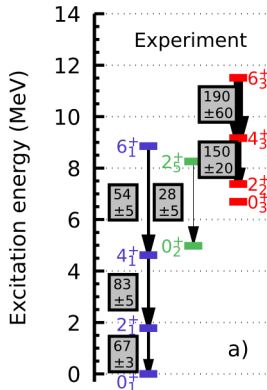
- inert core
- high-energy orbitals

# Test of shell-model calculations, $^{40}\text{Ca}$



Caurier, JM, Nowacki, Poves, PRC 75, 054317 (2007)

# Test of shell-model calculations, $^{28}\text{Si}$

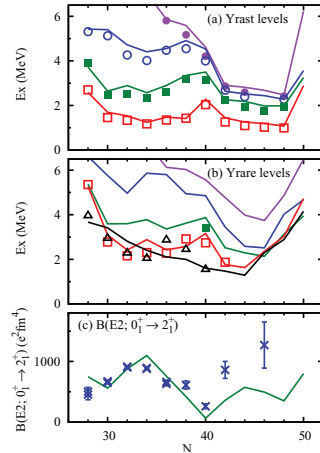
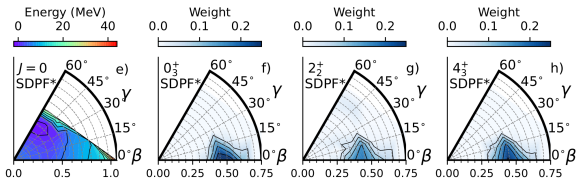
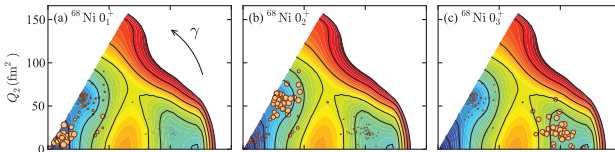


Frycz et al. arXiv:2404.14506

Good description of both oblate and prolate bands simultaneously!

# Nuclear shell model: energy surfaces

The Shell Model is the method of choice for shell model nuclei:  
energies, deformation, electromagnetic and beta transition rates...

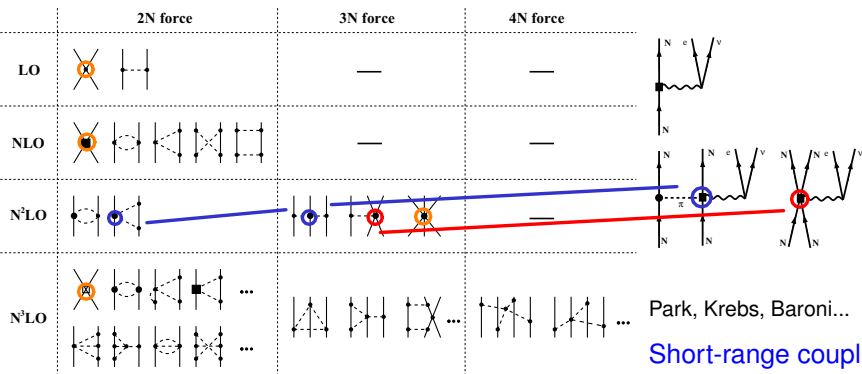


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# Effective shell-model interactions

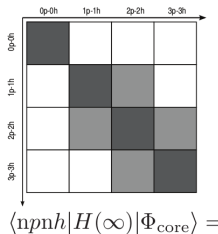
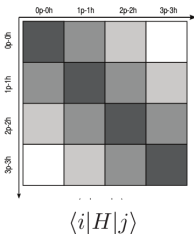
Coupled Cluster:

Solve coupled-cluster equations for core (reference state  $|\Phi\rangle$ ),  $A + 1$  and  $A + 2$  systems

Project the coupled-cluster solution into valence space (Okubo-Lee-Suzuki transformation)

Jansen et al. Phys. Rev. Lett. 113, 142502 (2014)

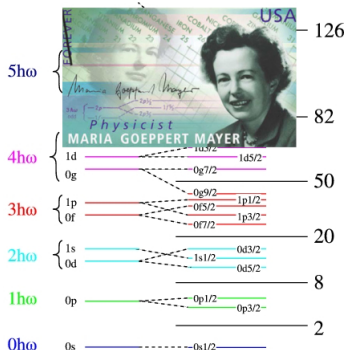
In-medium similarity  
renormalization group  
decouple  
core from excitations  
decouple  $A$  particles in  
valence space from rest



Stroberg et al.

Annu. Rev. Nucl. Part. Sci. 69, 307 (2019)

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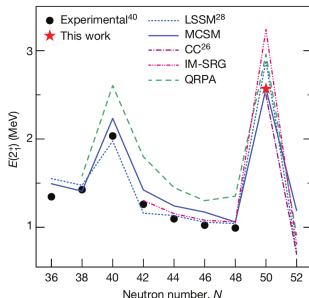
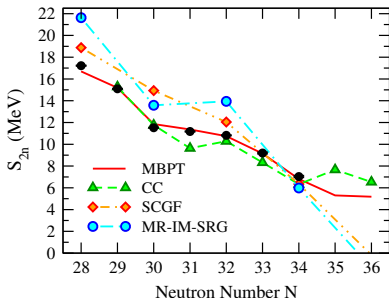
Otsuka, Shimizu, Y.Tsunoda

$H_{\text{eff}}$  includes effects of

- inert core
- high-energy orbitals

# Shell evolution in medium-mass nuclei

Calculations with NN+3N forces predict doubly-magic  $^{52}\text{Ca}$ ,  $^{54}\text{Ca}$ ,  $^{78}\text{Ni}$  groundbreaking mass /  $2^+$  measurements at ISOLDE / RIBF



## 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>1</sup>, Ch. Borgmann<sup>1</sup>, M. Brettenfeldt<sup>1</sup>, R. B. Cakirli<sup>1,3</sup>, S. George<sup>2</sup>, F. Herfurth<sup>1</sup>, J. D. Holt<sup>4,5</sup>, M. Kowalka<sup>1</sup>, S. Kreisel<sup>6</sup>, D. Lunney<sup>7</sup>, V. Mann<sup>2</sup>, J. Meininger<sup>8,9</sup>, D. Noidner<sup>1</sup>, M. Rosenbusch<sup>1</sup>, L. Schwickard<sup>1</sup>, A. Schwent<sup>1</sup>, J. Simons<sup>10</sup>, J. Stanje<sup>11</sup>, M. N. Wolf<sup>1</sup> & K. Zuber<sup>1</sup>



## ARTICLE

https://doi.org/10.1038/nature13354

### $^{78}\text{Ni}$ revealed as a doubly magic stronghold against nuclear deformation

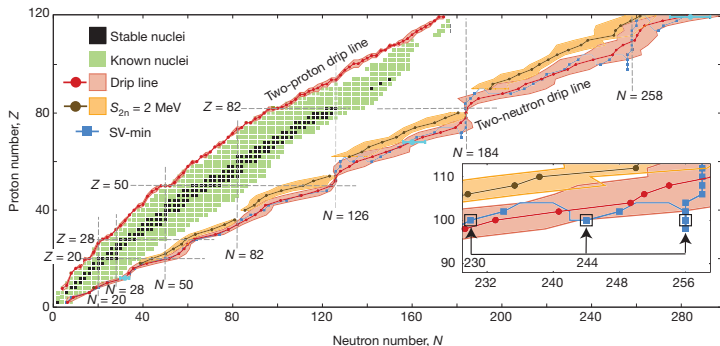
R. Tanaka<sup>1,2</sup>, C. Santamaria<sup>1,2</sup>, P. Dierckx<sup>1,2,3</sup>, A. Oberst<sup>1,2,4</sup>, K. Yoneda<sup>5</sup>, G. Juthwa<sup>6</sup>, H. Baba<sup>7</sup>, D. Cabot<sup>8</sup>, F. Chéreau<sup>9</sup>, A. Corradi<sup>10</sup>, G. Dubau<sup>11</sup>, T. M. Eicher<sup>12</sup>, A. Gilibert<sup>13</sup>, J. D. Holt<sup>14</sup>, Z. Inak<sup>15</sup>, Y. Igarashi<sup>16</sup>, M. Itatani<sup>17</sup>, T. Motobara<sup>18</sup>, S. Moriyama<sup>19</sup>, T. Motokawa<sup>20</sup>, M. Nakazawa<sup>21</sup>, Y. Niwa<sup>22</sup>, K. Ogata<sup>23</sup>, H. Otsu<sup>24</sup>, T. Ozuwa<sup>25</sup>, C. Perone<sup>26</sup>, S. Pirro<sup>27</sup>, A. Poves<sup>28</sup>, E. C. Rafferty<sup>29</sup>, A. Poves<sup>30</sup>, L. V. Sarantsev<sup>31</sup>, H. Sakurai<sup>32</sup>, J. Schweig<sup>33,34</sup>, Y. Shiga<sup>35</sup>, J. Simons<sup>36,37</sup>, S. K. Sonzogni<sup>38</sup>, S. Takahashi<sup>39</sup>, Y. Taniuchi<sup>40</sup>, T. Taniuchi<sup>41</sup>, F. Tassler<sup>42</sup>, R. Teruya<sup>43</sup>, L. X. Chen<sup>44</sup>, Z. Dong<sup>45</sup>, S. Franchose<sup>46</sup>, F. Gillibert<sup>47</sup>, A. Gottardo<sup>48</sup>, K. Hagino<sup>49</sup>, K. Katakura<sup>50</sup>, Z. Sertkan<sup>51</sup>, S. Soma<sup>52</sup>, Y. Takemasa<sup>53</sup>, M. Leitzner<sup>54</sup>, C. Linares<sup>55</sup>, R. Long<sup>56</sup>, M. Matsuoka<sup>57</sup>, T. Motokawa<sup>58</sup>, S. Nishizawa<sup>59</sup>, J. Okura<sup>60</sup>, S. Ono<sup>61</sup>, E. Paul<sup>62</sup>, E. Saba<sup>63</sup>, C. Sherrill<sup>64</sup>, A. Söderström<sup>65</sup>, I. Stefan<sup>66</sup>, D. Steppenbeck<sup>67</sup>, T. Suzuki<sup>68</sup>, Z. Vajta<sup>69</sup>, V. Werner<sup>70</sup>, J. Wu<sup>71</sup> & Z. Y. Xu<sup>72</sup>





# Nuclear landscape

The goal of nuclear theory is a unified description of nuclear structure, across the nuclear chart and based on nuclear forces



~ 3000 isotopes measured

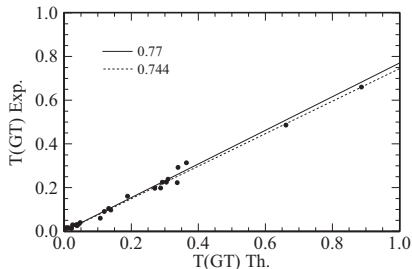
~ 7000 predicted

Erler et al.  
 Nature 486 509 (2012)

Limits of existence, ground-state properties, shell evolution, excitation spectra, spectroscopy, shape coexistence,  $\beta$  decays, fission...

# $\beta$ -decay Gamow-Teller transitions: “quenching”

$\beta$  decays ( $e^-$  capture): nuclear shell model vs ab initio

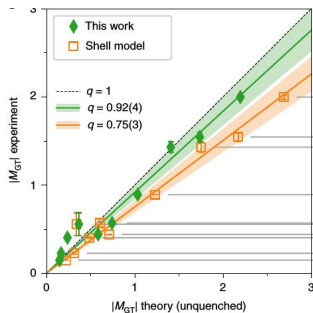


Martinez-Pinedo et al. PRC53 2602(1996)

$$\langle F | \sum_i [g_A \sigma_{iT}^-]^{\text{eff}} | I \rangle, \quad [\sigma_{iT}]^{\text{eff}} \approx 0.7 \sigma_{iT}$$

Shell model:  $\sigma_{iT}$  “quenching”

quenching: effects not in model



Gysbers et al. Nature Phys. 15 428 (2019)

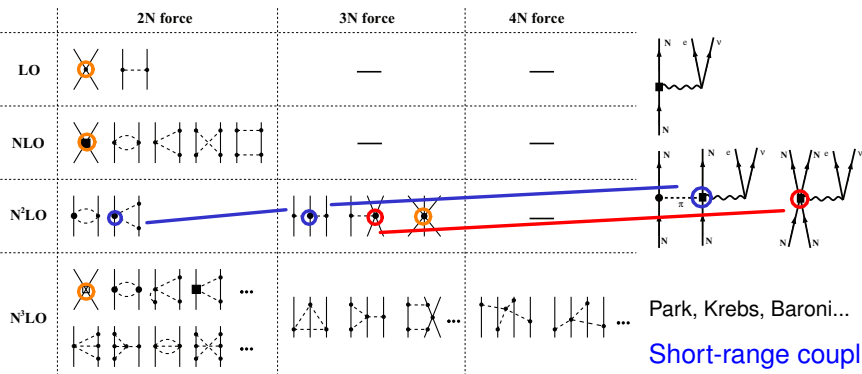
Ab initio calculations including meson-exchange currents and additional nuclear correlations do not need “quenching”

# Chiral effective field theory

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Approximate chiral symmetry: pion exchanges, contact interactions

Systematic expansion: nuclear forces and electroweak currents



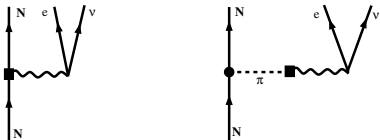
Park, Krebs, Baroni...

Short-range couplings  
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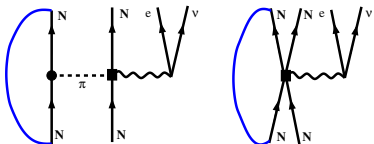
# Axial 1b and 2b currents

One-body currents receive contribution from two-body currents



$$\mathbf{J}_{i,1b}^3 = \frac{1}{2} \tau_i^3 \left( G_A^3(\mathbf{q}^2) \boldsymbol{\sigma}_i - \frac{G_P^3(\mathbf{q}^2)}{4m_N^2} (\mathbf{q} \cdot \boldsymbol{\sigma}_i) \mathbf{q} \right)$$

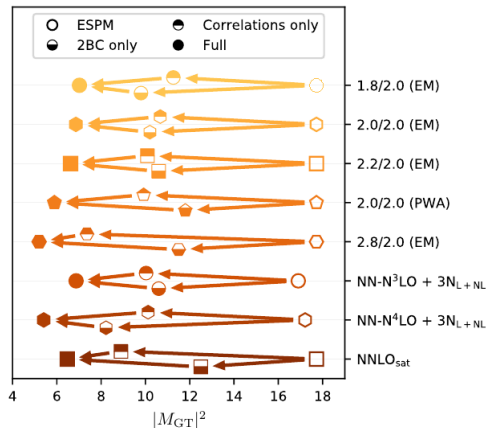
Approximate in medium-mass nuclei:  
 normal-ordered 1b part with respect to spin/isospin symmetric Fermi gas



$$\mathbf{J}_{i,2b}^{\text{eff}}(\rho, \mathbf{q}) = g_A \frac{\tau_i^3}{2} \left[ \delta a(\mathbf{q}^2) \boldsymbol{\sigma}_i + \frac{\delta a^P(\mathbf{q}^2)}{\mathbf{q}^2} (\mathbf{q} \cdot \boldsymbol{\sigma}_i) \mathbf{q} \right]$$

# Origin of $\beta$ decay “quenching”

Which are main effects missing in conventional  $\beta$ -decay calculations?  
 Test case: GT decay of  $^{100}\text{Sn}$

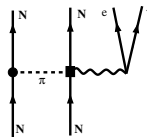


Relatively similar  
 and complementary  
 impact of

- nuclear correlations
- meson-exchange currents

Gysbers et al.

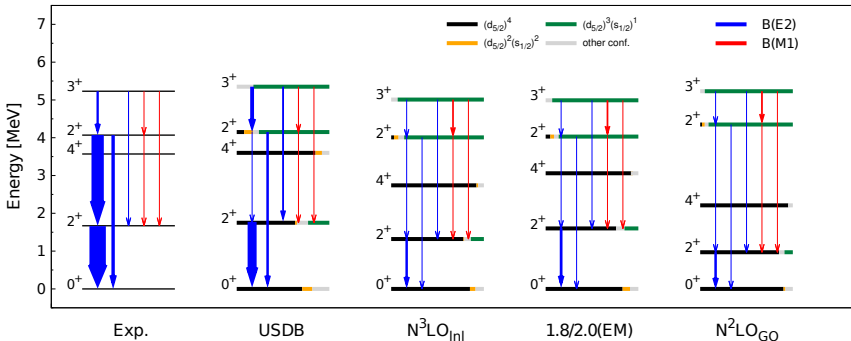
Nature Phys. 15 428 (2019)



# Electromagnetic transitions in neutron-rich nuclei

Study of B(E2) and B(M1) transitions in  $^{20}\text{O}$   
with nuclear shell model and ab initio VS-IMSRG

Zanon, Clément, Goasduff, JM, Miyagi et al. PRL 131 262501 (2023)



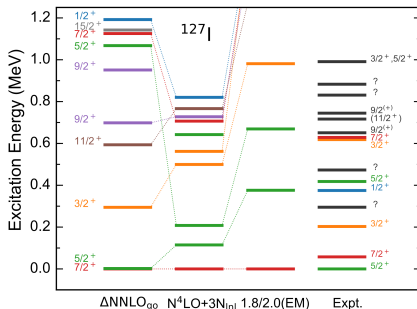
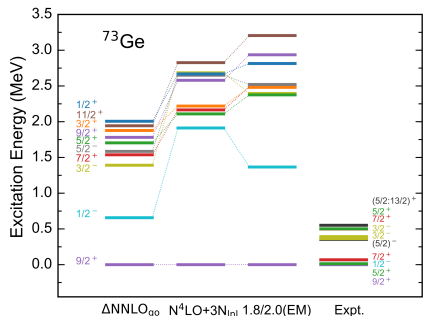
Systematic deficiency: B(E2)'s do not capture collectivity

Nuclear structure details missing:  $s - d$  mixing of  $2^+$  state

# Ab initio spectra for heavy nuclei

While VS-IMSRG calculations high quality in light nuclei (eg Na) challenges remain in heavier systems, such as  $^{73}\text{Ge}$

Interesting sensitivity to the chiral nuclear Hamiltonian used for  $^{127}\text{I}$



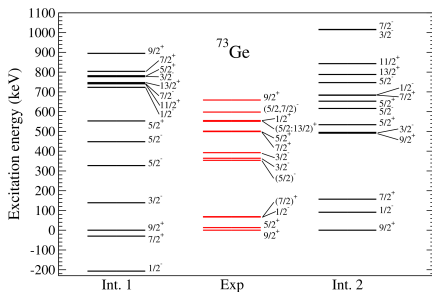
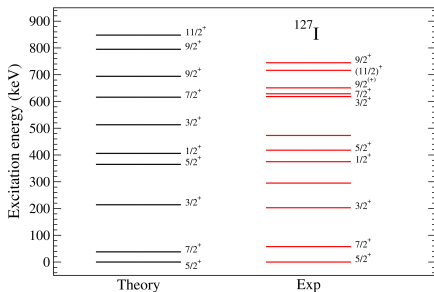
Hu et al. PRL 128, 072502 (2022)



# Shell-model spectra for heavy nuclei

Very good general agreement  
 between the properties of low-energy nuclear states  
 and nuclear shell-model calculations

However, some nuclei present challenging features  
 such as  $^{73}\text{Ge}$  ground and first-excited state, likely related to deformation



# Summary

Ab initio methods using chiral EFT forces such as the valence-space IMSRG access nuclei like nuclear shell model

Nuclear shell evolution, spectroscopy,  $\beta$  and  $\gamma$  decays with consistent operators

- Doubly-magic character of  $^{78}\text{Ni}$ ,  $^{132}\text{Sn}$ ...
- Quantified theoretical uncertainties (dominated by Hamiltonian)
- Reproduce  $\beta$  decay half-lives without adjustments (“quenching”)
- Challenge: electromagnetic decays even in light  $^{20,21}\text{O}$  nuclei
- Challenge: complex heavy nuclei

