Ab initio calculations around neutron-rich shell closures

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TRIUMF Advanced Rare Isotope Laboratory (ARIEL)

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LOEWE Exzellente Forschung für Hessens Zukunft

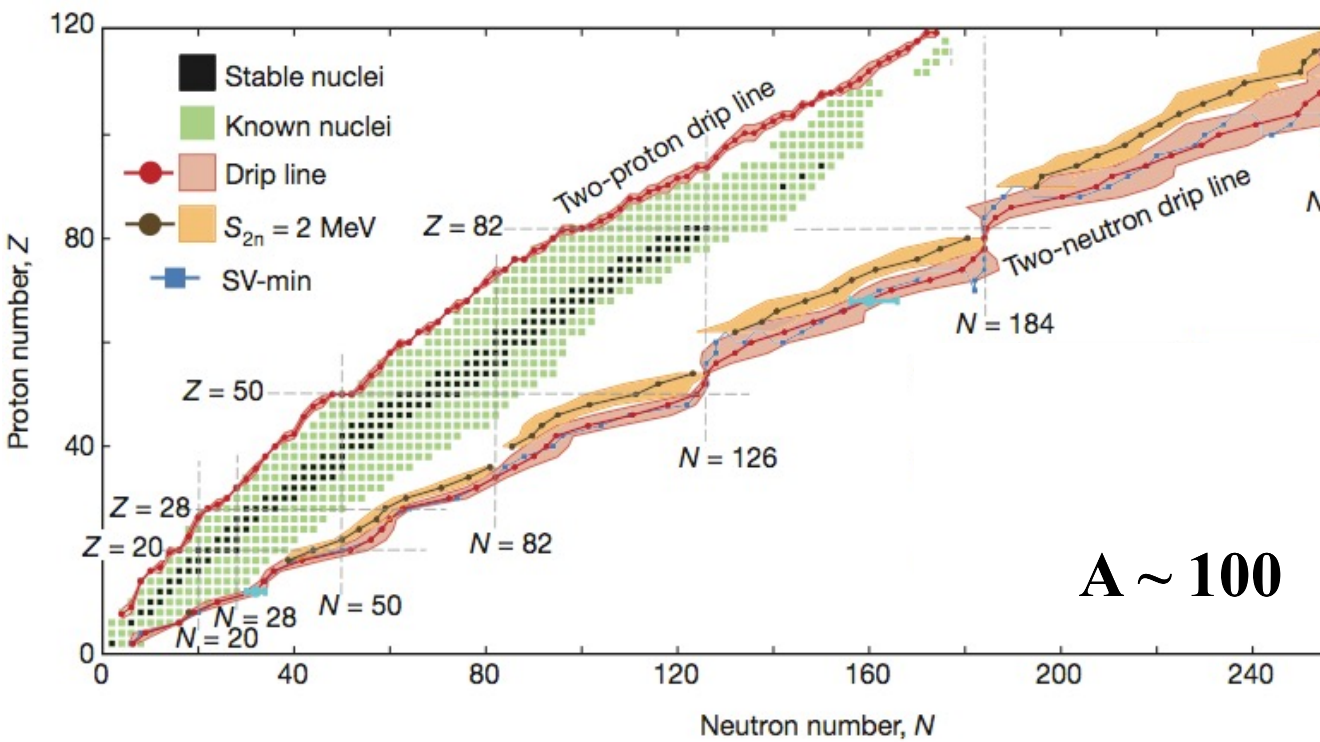
Structure of nuclei and dense matter in neutron stars

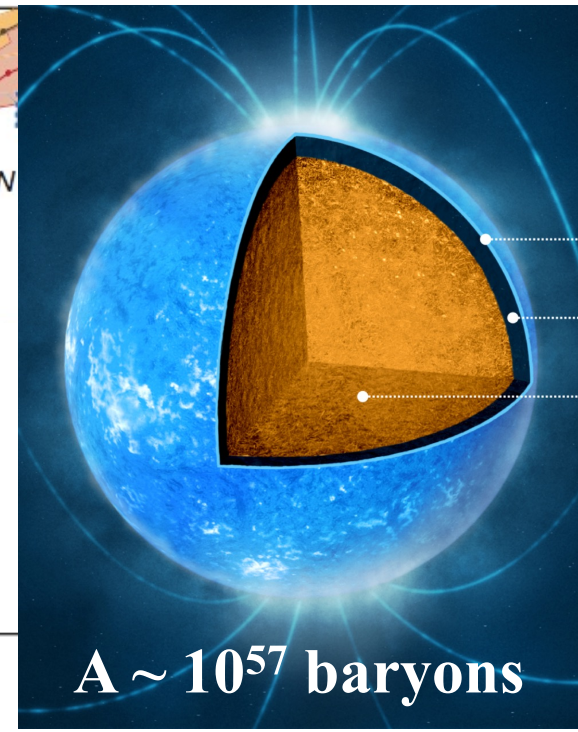
doi:10.1038/nature11188

The limits of the nuclear landscape

Jochen Erler[1,2], Noah Birge[1], Markus Kortelainen[1,2,3], Witold Nazarewicz[1,2,4], Erik Olsen[1,2], Alexander M. Perhac[1] & Mario Stoitsov[1,2]‡

~ 4000±500 nuclei unknown, extreme neutron-rich





Extreme neutron-rich matter in neutron stars

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The limits of the nuclear landscape

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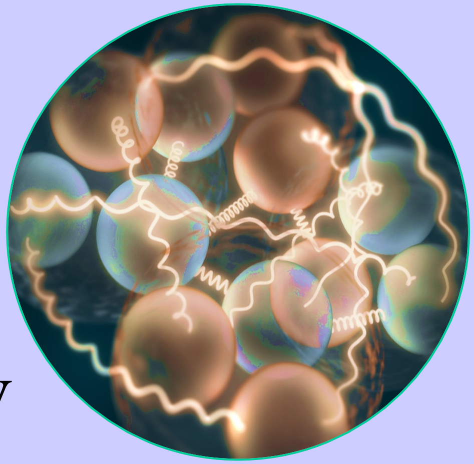
~ 4000 ± 500 nuclei unknown, extreme neutron-rich

rich physics with nucleons
as degrees of freedom

microphysics of nuclei
macrophysics of neutron stars

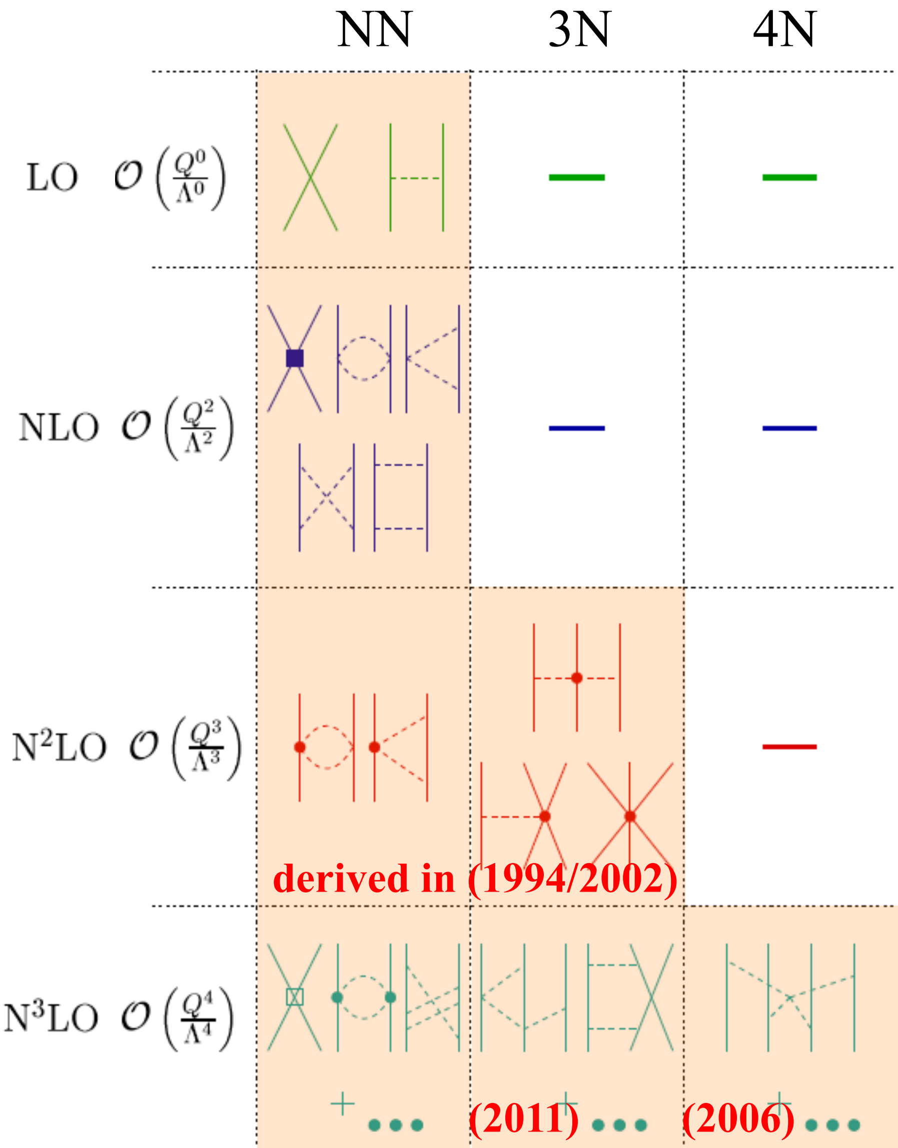
typical momenta Q ~ 200 MeV
~ **pion** mass m_π

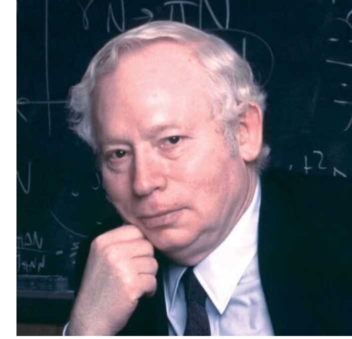


Extreme neutron-rich matter in neutron stars

Chiral effective field theory for nuclear forces

Systematic expansion in low momenta $(Q/\Lambda_b)^n$





based on symmetries of strong interaction (QCD)

long-range interactions governed by pion exchanges

powerful approach for many-body interactions

all 3- and 4-neutron forces predicted to N^3LO

Tews et al., PRL (2013)

enables uncertainty quantification from higher orders and input data

Weinberg (1990,91), van Kolck, Kaplan, Savage, Wise, Bernard, Epelbaum, Kaiser, Meißner,…

Great progress in ab initio calculations of nuclei

systematic interaction expansion + systematic many-body expansion

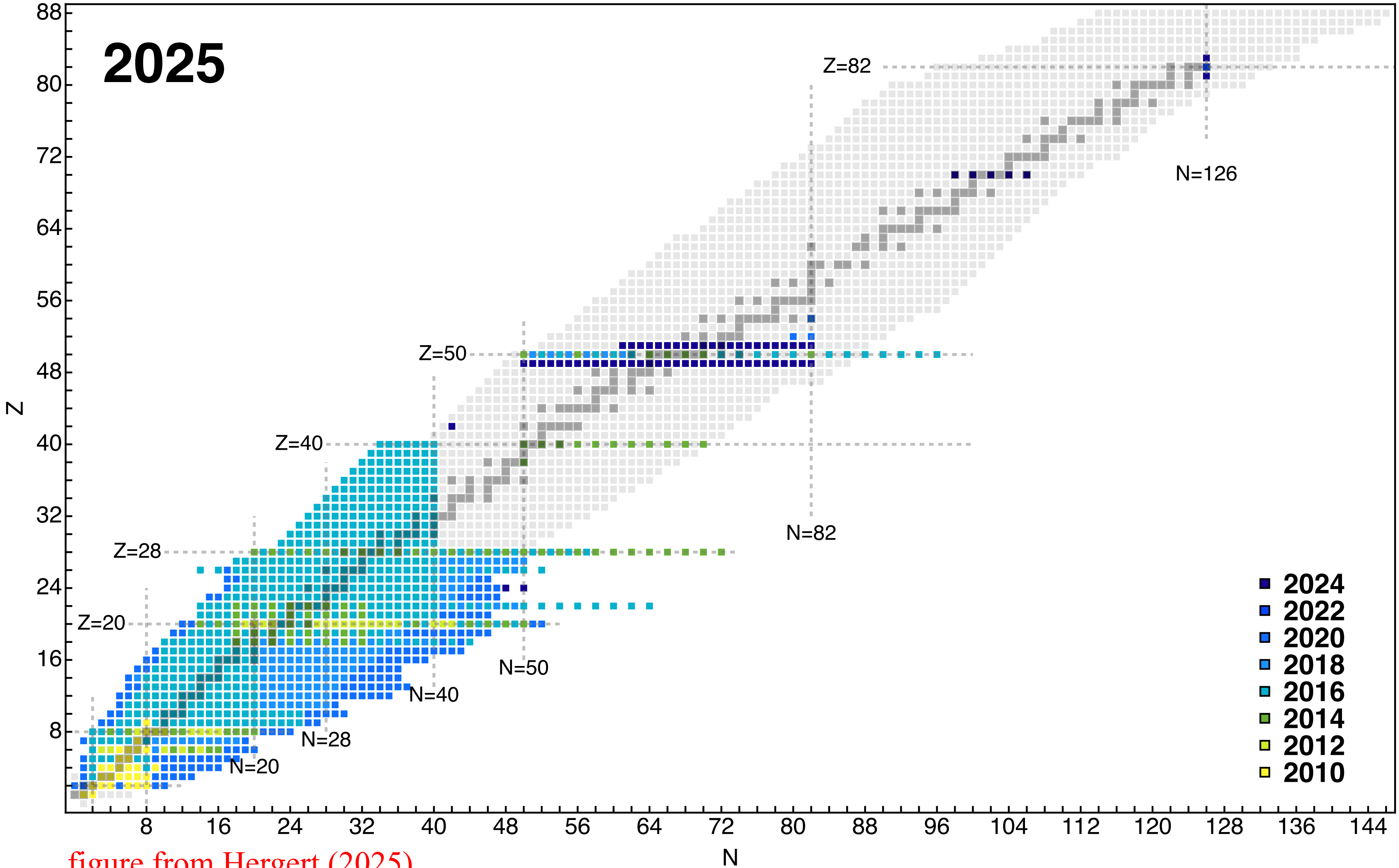
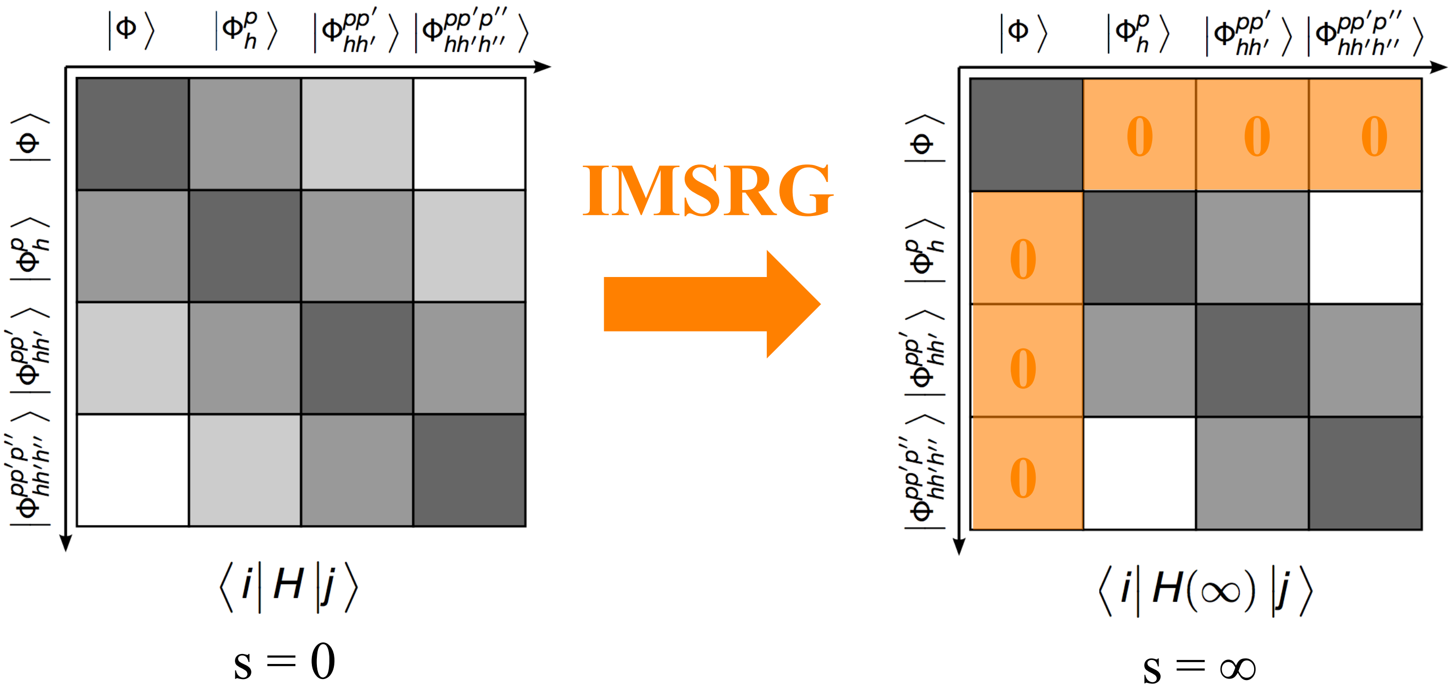


figure from Hergert (2025)

In-medium similarity renormalization group (IMSRG)

Tsukiyama, Bogner, AS, PRL (2011), Hergert et al., Phys. Rep. (2016), Stroberg et al., PRL (2017)

flow equations to decouple higher-lying particle-hole states ($s = 0 \rightarrow \infty$)



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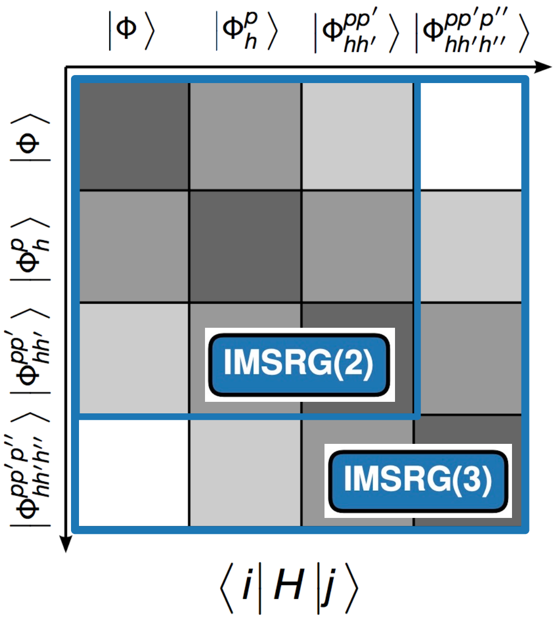
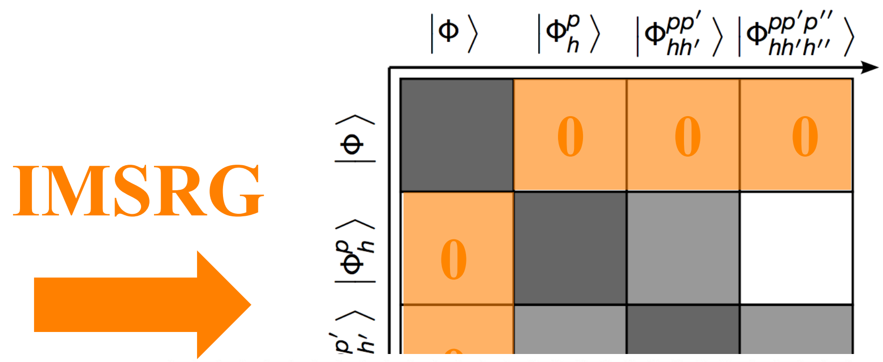
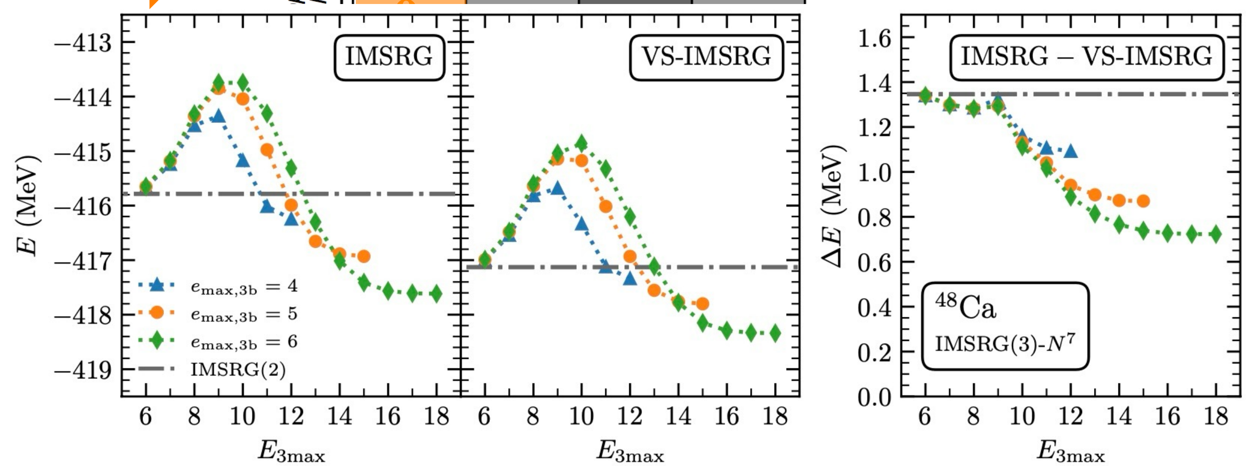




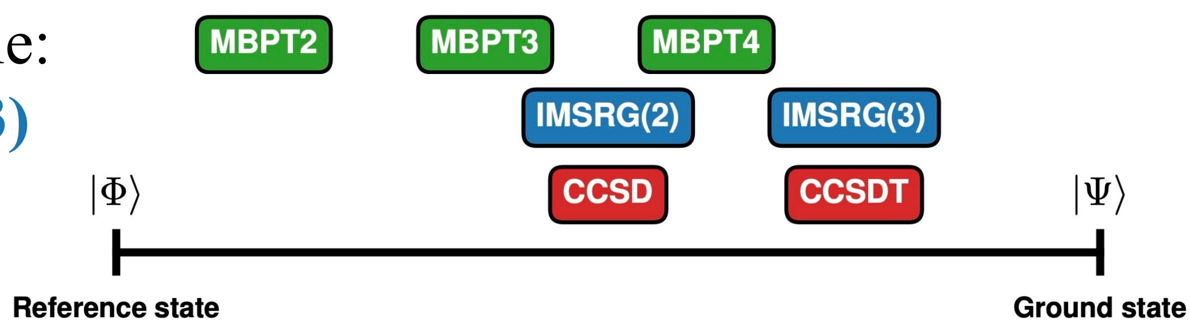


Systematically improvable:

IMSRG(2) → IMSRG(3)

Heinz et al., PRC (2021), (2025)

He, Stroberg, PRC (2024)



Great progress in ab initio calculations of nuclei

ARTICLES
https://doi.org/10.1038/s41567-022-01715-8
nature physics
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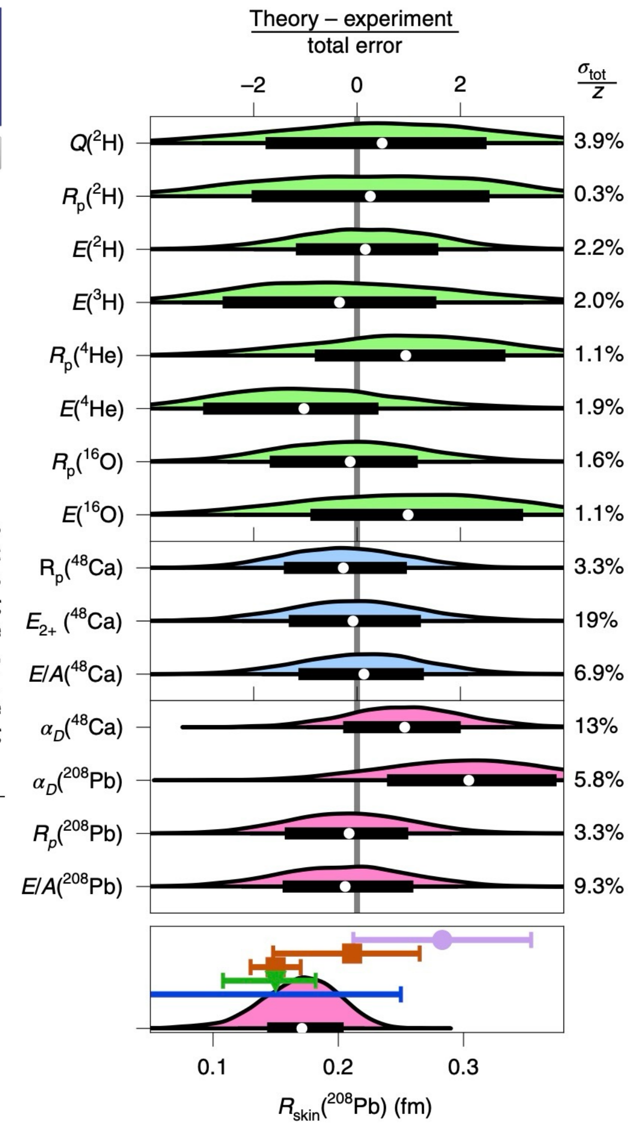
OPEN

Ab initio predictions link the neutron skin of ^{208}Pb to nuclear forces

Baishan Hu[1,11], Weiguang Jiang[2,11], Takayuki Miyagi[1,3,4,11], Zhonghao Sun[5,6,11], Andreas Ekström[2], Christian Forssén[2] ✉, Gaute Hagen[1,5,6], Jason D. Holt[1,7], Thomas Papenbrock[5,6], S. Ragnar Stroberg[8,9] and Ian Vernon[10]

Heavy atomic nuclei have an excess of neutrons over protons, which leads to the formation of a neutron skin whose thickness is sensitive to details of the nuclear force. This links atomic nuclei to properties of neutron stars, thereby relating objects that differ in size by orders of magnitude. The nucleus ^{208}Pb is of particular interest because it exhibits a simple structure and is experimentally accessible. However, computing such a heavy nucleus has been out of reach for ab initio theory. By combining advances in quantum many-body methods, statistical tools and emulator technology, we make quantitative predictions for the properties of ^{208}Pb starting from nuclear forces that are consistent with symmetries of low-energy quantum chromodynamics. We explore 10^9 different nuclear force parameterizations via history matching, confront them with data in select light nuclei and arrive at an importance-weighted ensemble of interactions. We accurately reproduce bulk properties of ^{208}Pb and determine the neutron skin thickness, which is smaller and more precise than a recent extraction from parity-violating electron scattering

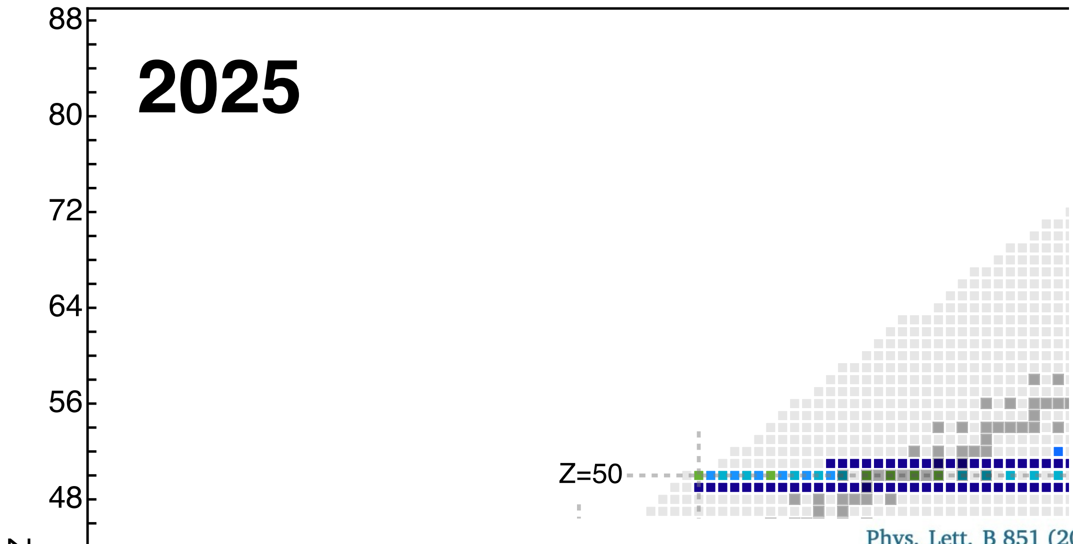


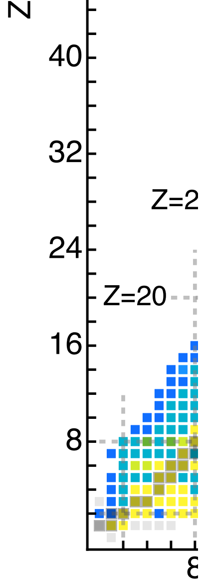
PHYSICAL REVIEW C **105**, 014302 (2022)

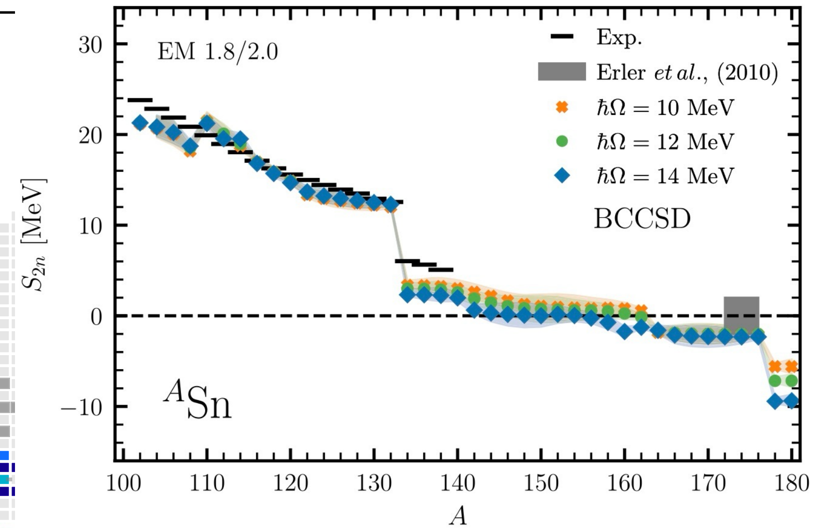
Converged *ab initio* calculations of heavy nuclei

T. Miyagi[1,*] S. R. Stroberg[2,†] P. Navrátil[1,‡] K. Hebeler[3,4,5,§] and J. D. Holt[1,6,‖]
[1]*TRIUMF, 4004 Wesbrook Mall, Vancouver, BC V6T 2A3, Canada*
[2]*Department of Physics, University of Washington, Seattle, Washington 98195, USA*
[3]*Technische Universität Darmstadt, 64289 Darmstadt, Germany*
[4]*ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*
[5]*Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*
[6]*Department of Physics, McGill University, 3600 Rue University, Montréal, QC H3A 2T8, Canada*

Great progress in ab initio calculations of nuclei







Phys. Lett. B 851 (2024) 138571

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Letter

Towards heavy-mass *ab initio* nuclear structure: Open-shell Ca, Ni and Sn isotopes from Bogoliubov coupled-cluster theory

Check for updates

A. Tichai [a,b,c,*], P. Demol [d], T. Duguet [e,d]

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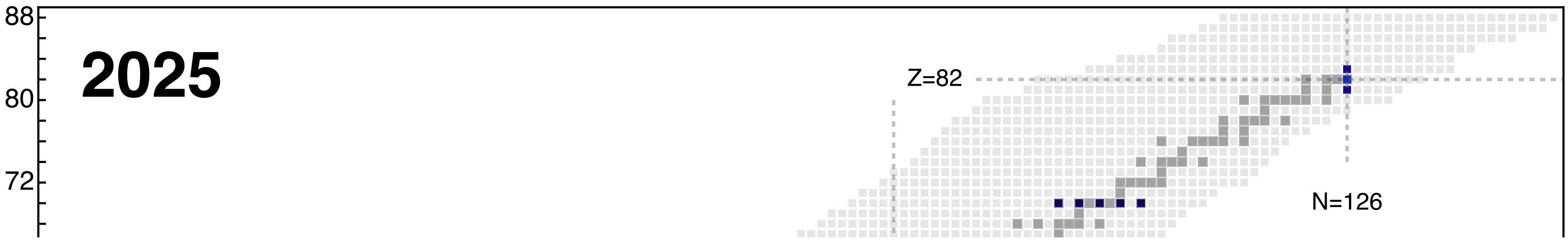
[b] ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany
[c] Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany
[d] KU Leuven, Instituut voor Kern- en Stralingsfysica, 3001 Leuven, Belgium
[e] IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France

figures

Great progress in ab initio calculations of nuclei



PHYSICAL REVIEW LETTERS **134,** 063002 (2025)

Probing New Bosons and Nuclear Structure with Ytterbium Isotope Shifts

Menno Door,[1,2,*,†] Chih-Han Yeh,[3,*,‡] Matthias Heinz,[4,5,1,§] Fiona Kirk,[3,6] Chunhai Lyu,[1] Takayuki Miyagi,[4,5,1] Julian C. Berengut,[7] Jacek Bieroń,[8] Klaus Blaum,[1] Laura S. Dreissen,[3,9] Sergey Eliseev,[1] Pavel Filianin,[1] Melina Filzinger,[3] Elina Fuchs,[3,6] Henning A. Fürst,[3,10] Gediminas Gaigalas,[11] Zoltán Harman,[1] Jost Herkenhoff,[1] Nils Huntemann,[3] Christoph H. Keitel,[1] Kathrin Kromer,[1] Daniel Lange,[1,2] Alexander Rischka,[1] Christoph Schweiger,[1] Achim Schwenk,[4,5,1] Noritaka Shimizu,[12] and Tanja E. Mehlstäubler[3,10,13]

[1]*Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*
[2]*Heidelberg University, Grabengasse 1, 69117 Heidelberg, Germany*
[3]*Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany*
[4]*Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany*
[5]*ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, Darmstadt, 64291, Germany*
[6]*Institut für Theoretische Physik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover, Germany*
[7]*School of Physics, University of New South Wales, Sydney, New South Wales 2052, Australia*
[8]*Institute of Theoretical Physics, Jagiellonian University, Kraków, 30-348, Poland*
[9]*Department of Physics and Astronomy, LaserLab, Vrije Universiteit Amsterdam, De Boelelaan 1081, Amsterdam, 1081 HV, The Netherlands*
[10]*Institut für Quantenoptik, Leibniz Universität Hannover, Welfengarten 1, 30167 Hannover, Germany*
[11]*Institute of Theoretical Physics and Astronomy, Vilnius University, Vilnius, 10222, Lithuania*
[12]*Center for Computational Sciences, University of Tsukuba, Ibaraki, 305-8577, Japan*
[13]*Laboratorium für Nano- und Quantenengineering, Leibniz Universität Hannover, Schneiderberg 39, 30167 Hannover, Germany*

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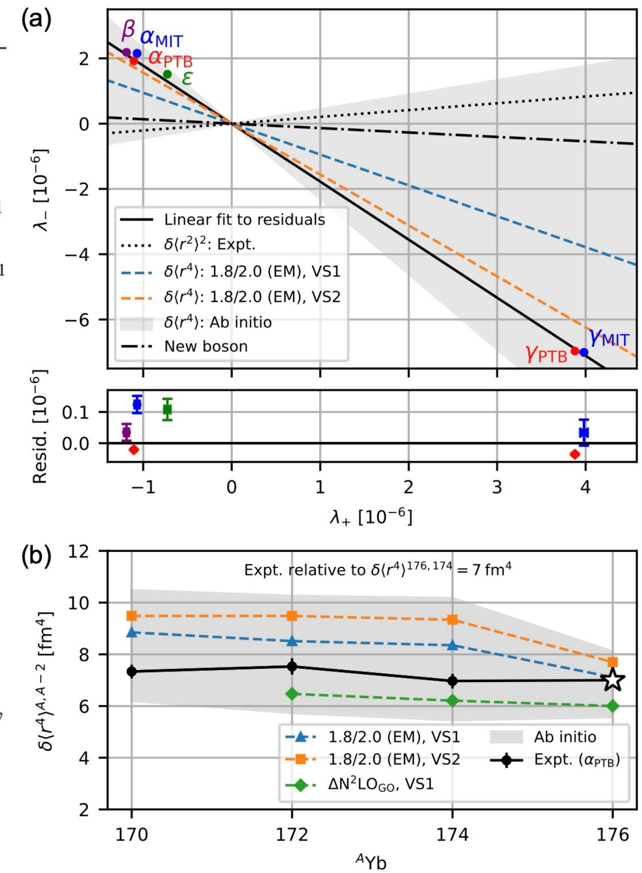
In this Letter, we present mass-ratio measurements on highly charged Yb^{42+} ions with a precision of 4×10^{-12} and isotope-shift measurements on Yb^{+} on the $^2S_{1/2} \to {}^2D_{5/2}$ and $^2S_{1/2} \to {}^2F_{7/2}$ transitions with a precision of 4×10^{-9} for the isotopes ^{168,170,172,174,176}Yb. We present a new method that allows us to extract higher-order changes in the nuclear charge distribution along the Yb isotope chain, benchmarking *ab initio* nuclear structure calculations. Additionally, we perform a King plot analysis to set bounds on a fifth force in the keV/c^2 to MeV/c^2 range coupling to electrons and neutrons.



Recent developments

Correlated mass model for calcium isotopes

Cincar, Li, Plies, Vernik, Heinz, Miyagi, AS, in prep.

Ab initio nuclear masses for r-process nucleosynthesis

across N=82: Kuske, Miyagi, Arcones, AS, arXiv:2509.19131

work on N=126: Lariviere, Vassh, Holt, et al.

Beta decays and electromagnetic moments

Li, Miyagi, AS, arXiv:2509.19131, PRL in press

Miyagi, Cao, Seutin, Bacca, Garcia Ruiz, Hebeler, Holt, AS, PRL (2024)

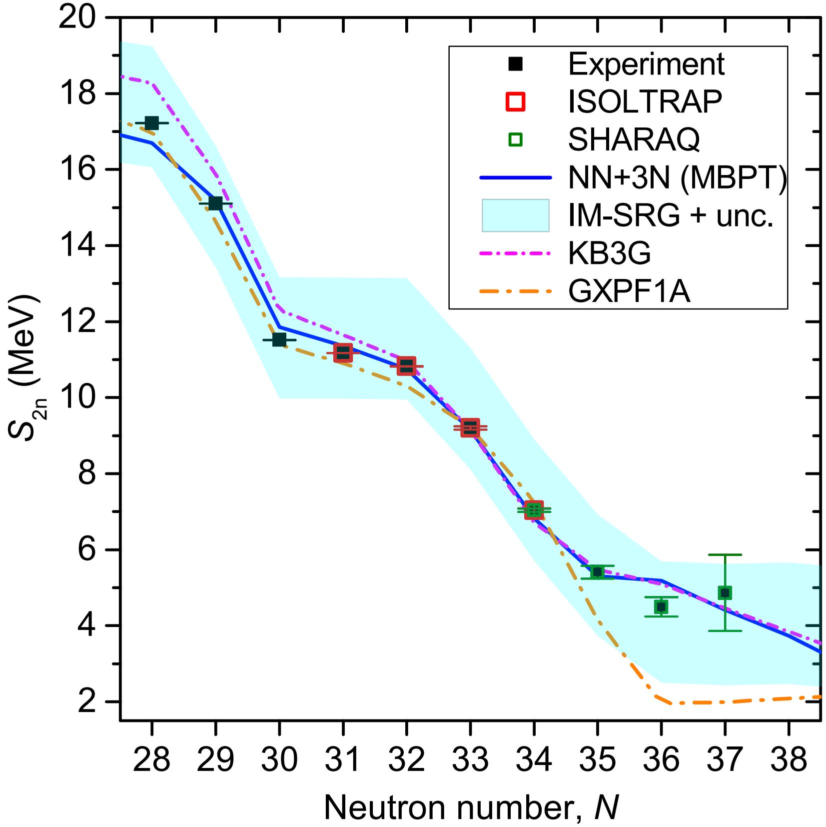
Lellinger, Vazquez Rodríguez et al.

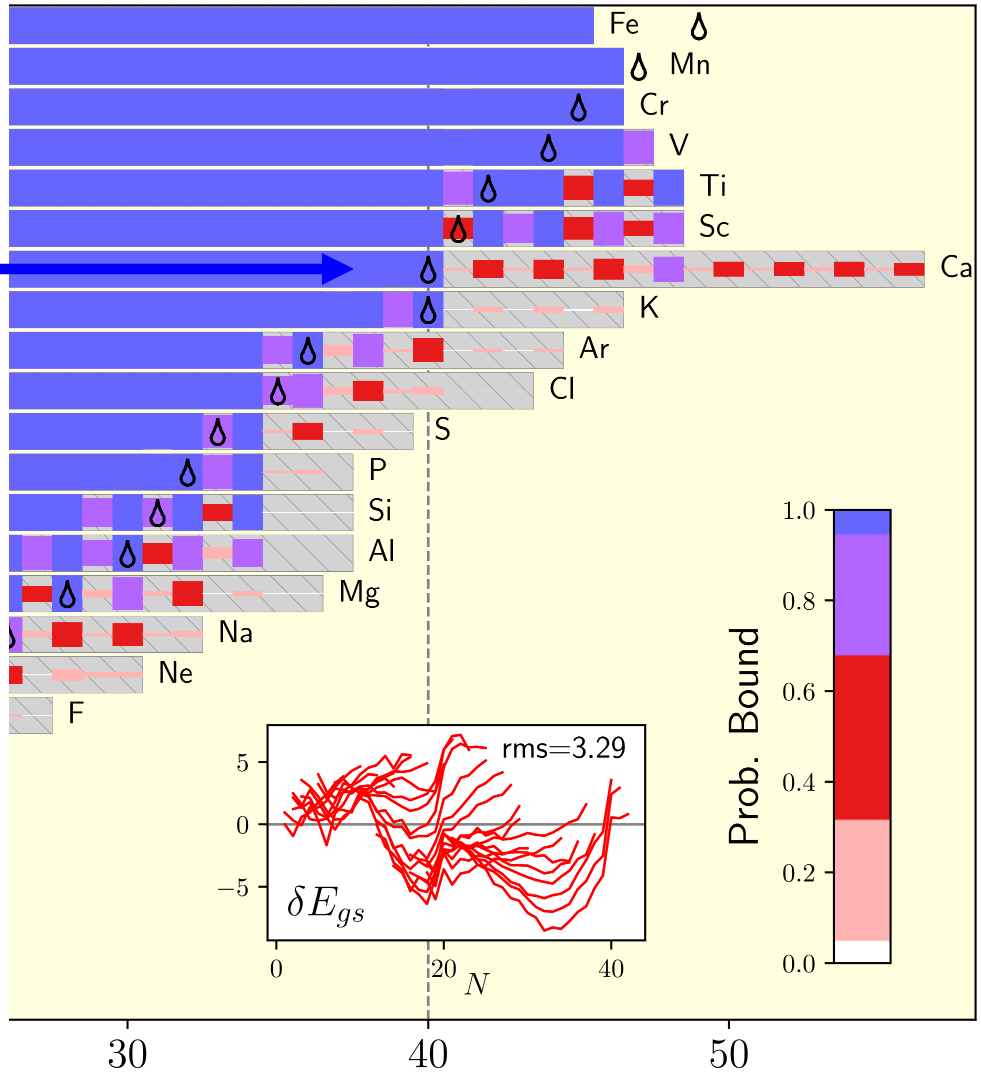
Neutron-rich calcium masses

very active exp-theory collaborations

pioneering $^{51\text{-}57}$Ca masses

Gallant et al., PRL (2012), Wienholtz et al., Nature (2013), Michimasa et al., PRL (2019)





Stroberg, Holt, AS, Simonis, PRL (2021)

Correlated mass model for calcium isotopes

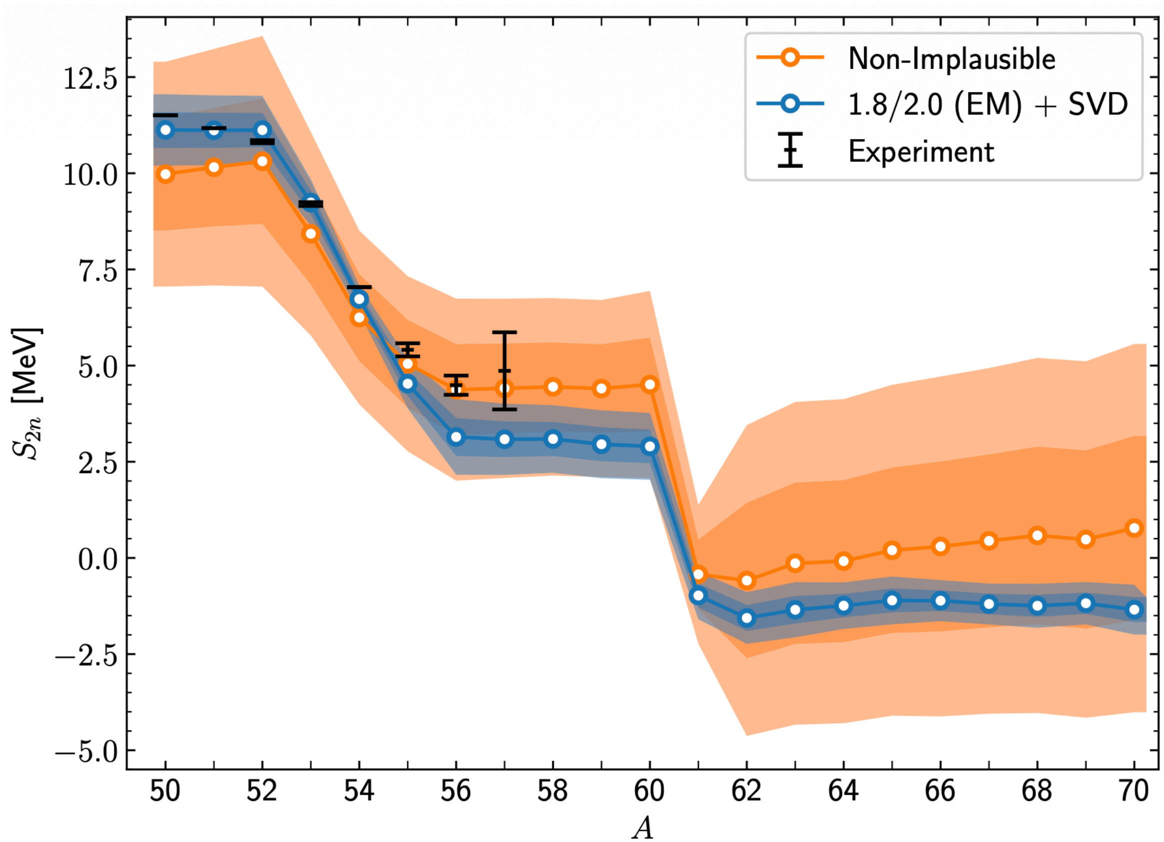
Cincar, Li, Plies, Vernik, Heinz, Miyagi, AS, in prep.

Goal: Build correlated ab-initio-based mass model for S_{2n} of Ca isotopes

Start from interaction distributions:

34 non-implausible interactions Hu et al., Nature Phys. (2022)

101 SVD variations for 1.8/2.0 (EM) Plies, Heinz, AS, arXiv:2509.24671



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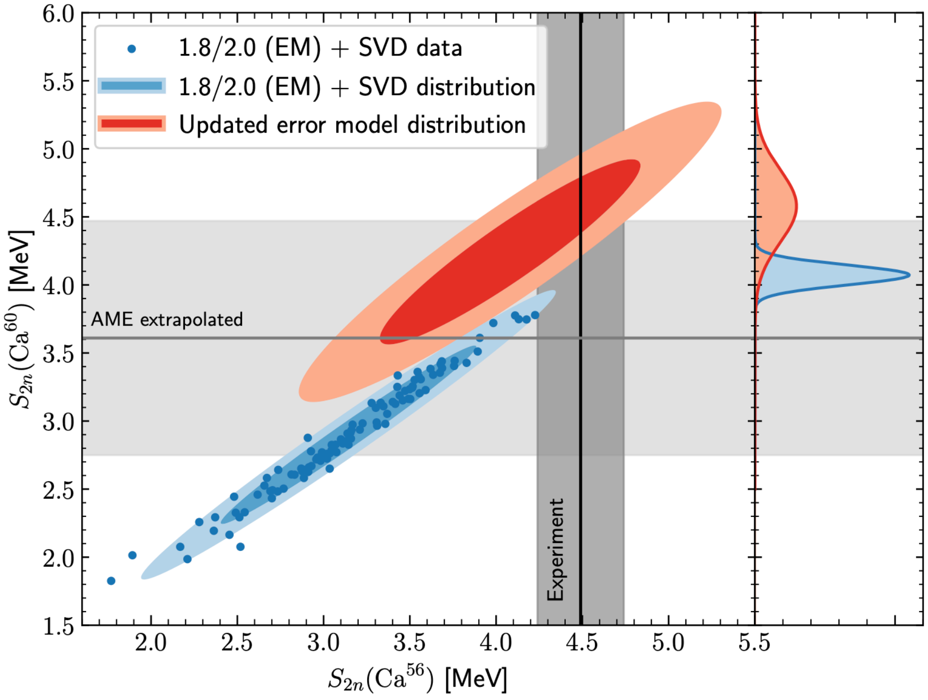
Start from interaction distributions: 34 NI, 101 SVD interactions

Include other uncertainties from:
- Many-body IMSRG(2, 3f2)
- Model space
- Systematic uncertainties



Condition on exp. $S_{2n}(^{50\text{-}56}\mathrm{Ca})$ uses correlations among S_{2n}

Correlated mass model for calcium isotopes

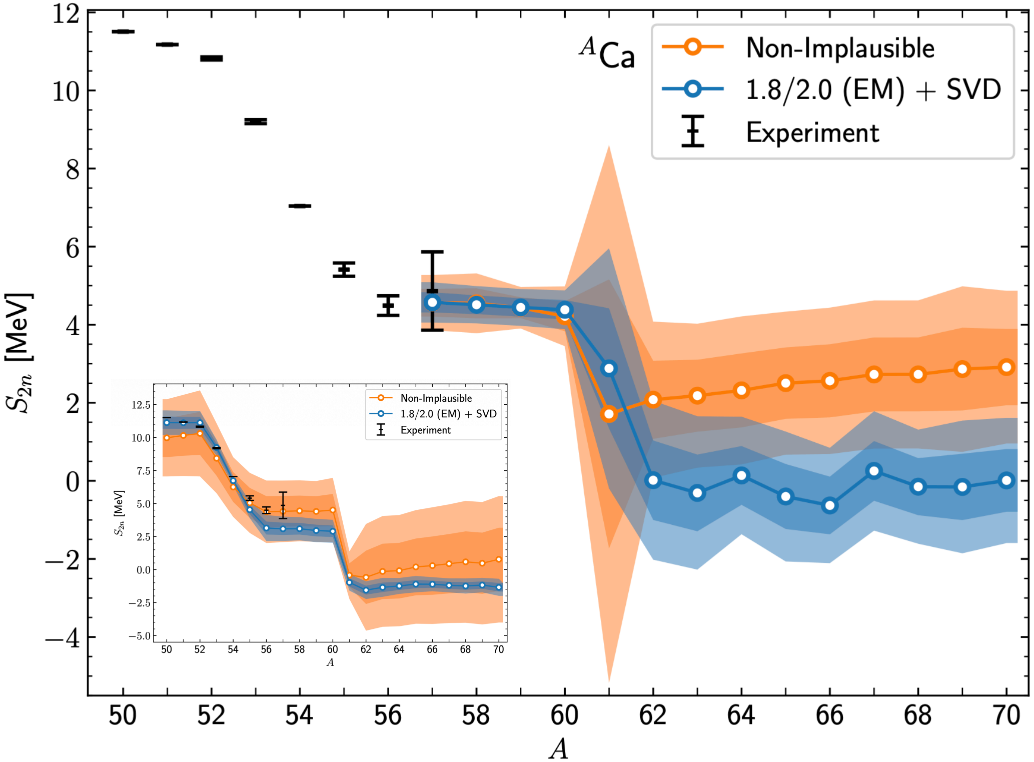
Cincar, Li, Plies, Vernik, Heinz, Miyagi, AS, in prep.

Goal: Build correlated ab-initio-based mass model for S_{2n} of Ca isotopes

Start from interaction distributions: 34 NI, 101 SVD interactions

Include other uncertainties: Many-body, model space, systematic

Leads to mass model with correlated uncertainties conditioned on data



large uncertainties for ^{61}Ca due to $s_{1/2}$ or $g_{9/2}$ uncertainty

difficult to predict dripline in Ca given theo. uncertainties

Recent developments

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Lellinger, Vazquez Rodríguez et al.

Nuclear masses around N=82 and r-process nucleosynthesis

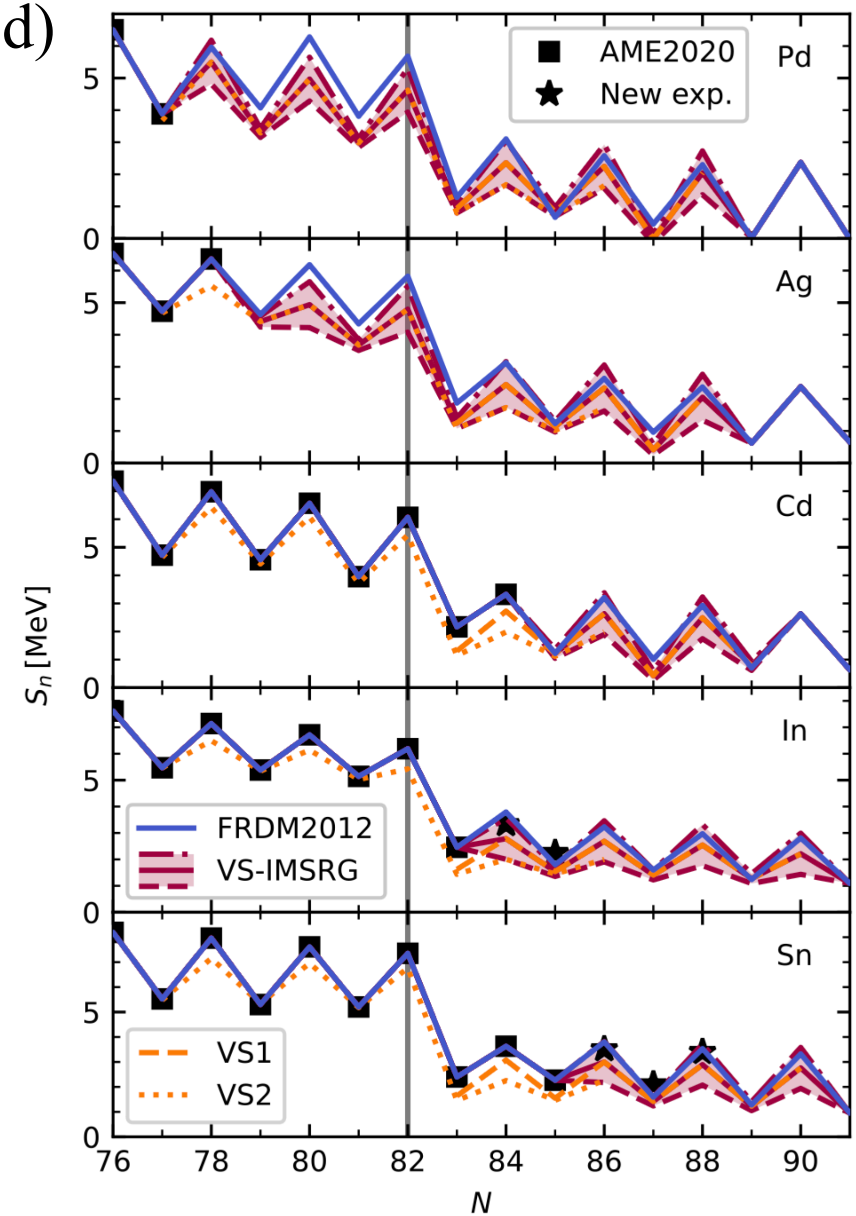
Kuske, Miyagi, Arcones, AS, arXiv:2509.19131

masses around N=82 (Sn, In, Cd, Ag, Pd)
→ interesting region at exp frontier

VS-IMSRG results with valence space
+ interaction uncertainties

separation energies have smaller
uncertainties due to correlations;
IMSRG(3f2) is within VS1, VS2

incorporate VS-IMSRG masses
with uncertainties (min/central/max)
in baseline AME2020 + FRDM2012



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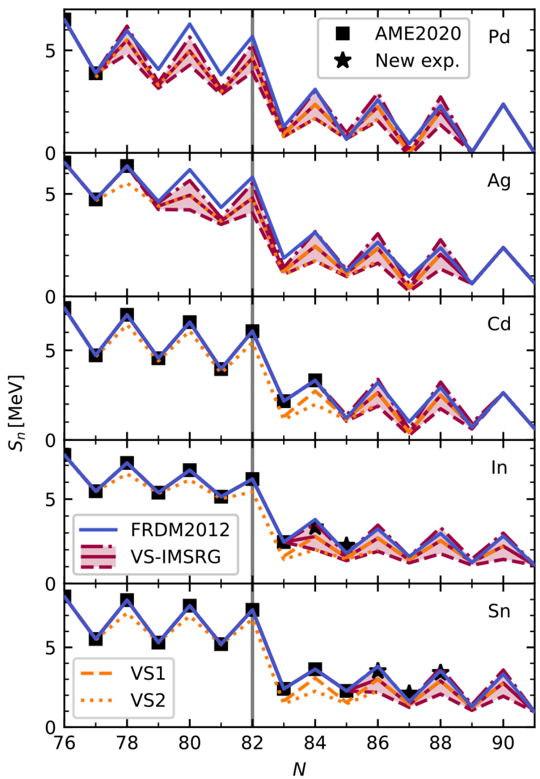
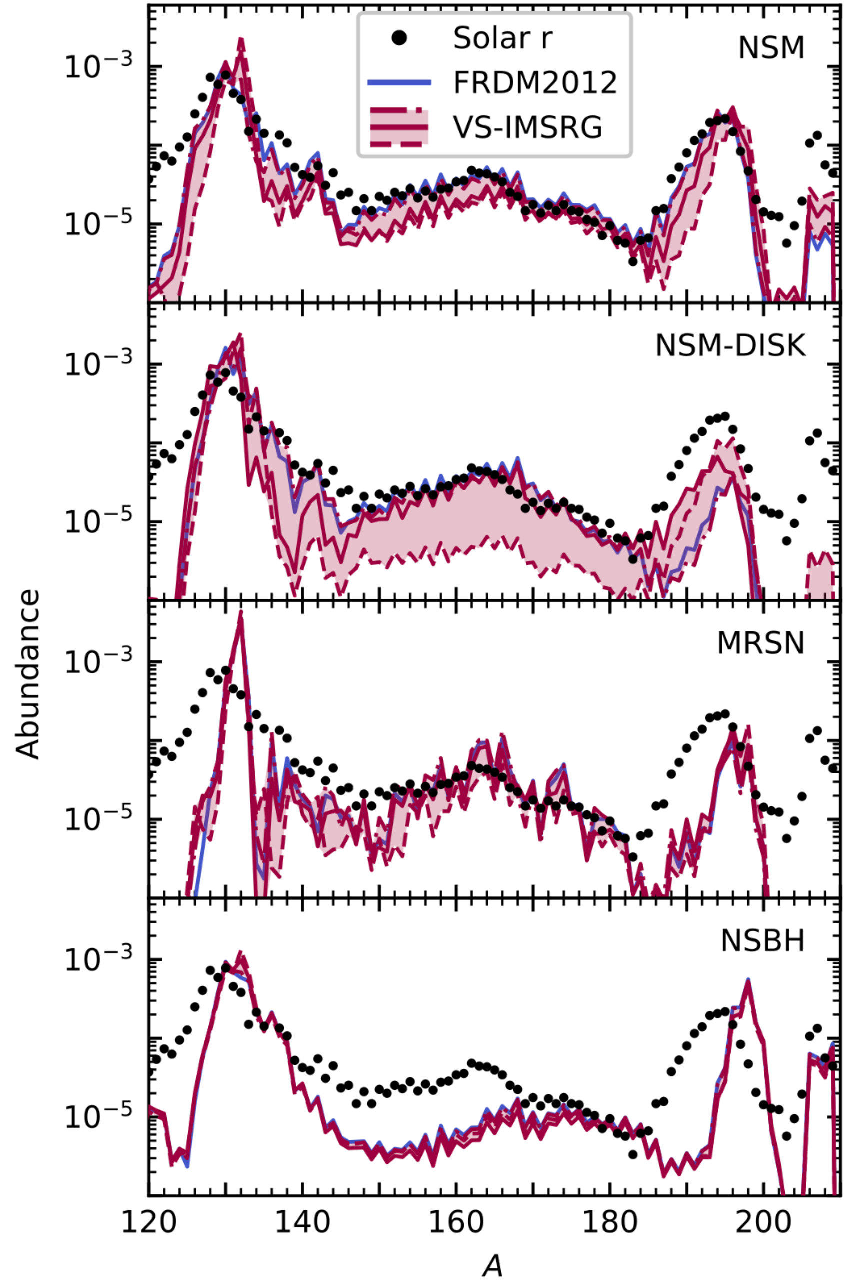
VS-IMSRG masses (min/central/max)

in baseline AME2020 + FRDM2012

explore r-process predictions for different astrophysics scenarios





Nuclear masses around N=82 and r-process nucleosynthesis

Kuske, Miyagi, Arcones, AS, arXiv:2509.19131

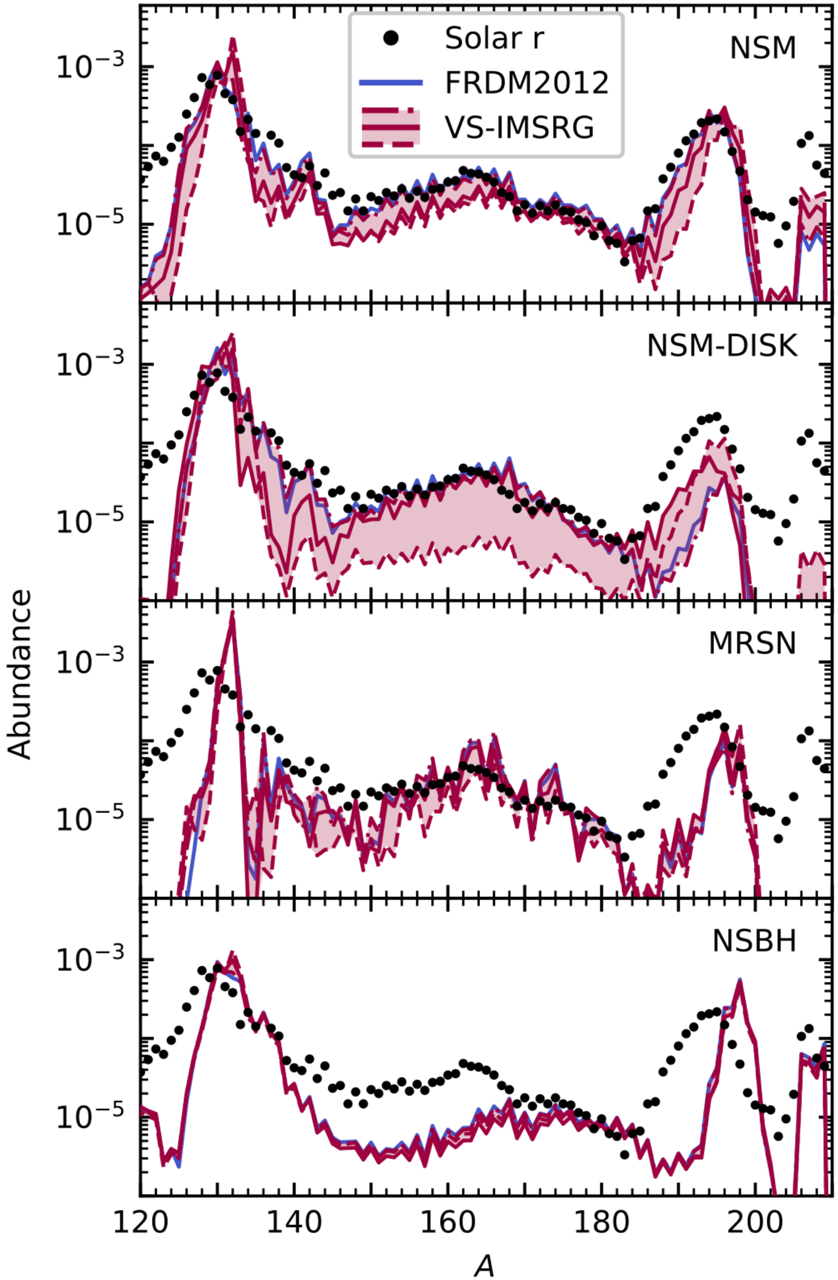
VS-IMSRG masses (min/central/max)
in baseline AME2020 + FRDM2012

explore r-process predictions for different astrophysics scenarios

largest effects for n-star mergers (NSM and NSM-DISK)

ab initio masses strengthen waiting point of 2nd peak, leading to slower nucleosynthesis flow, and important impact on 3rd peak

future: use correlated ab-initio-based mass model conditioned on data



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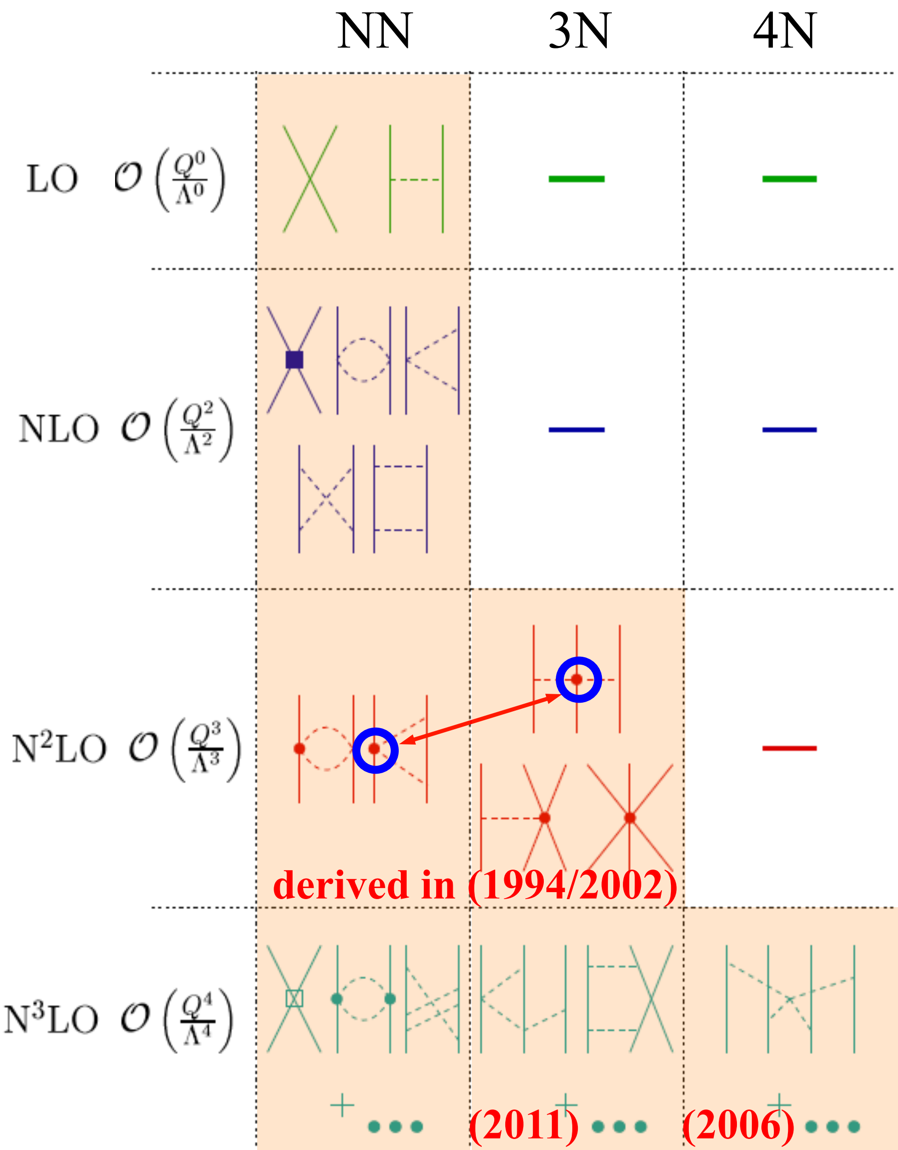
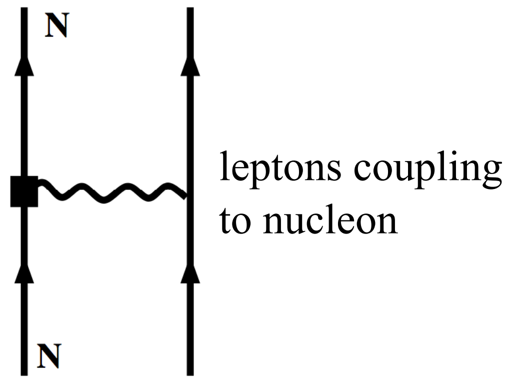
Miyagi, Cao, Seutin, Bacca, Garcia Ruiz, Hebeler, Holt, AS, PRL (2024)
Lellinger, Vazquez Rodríguez et al.

Chiral EFT for coupling to electroweak interactions

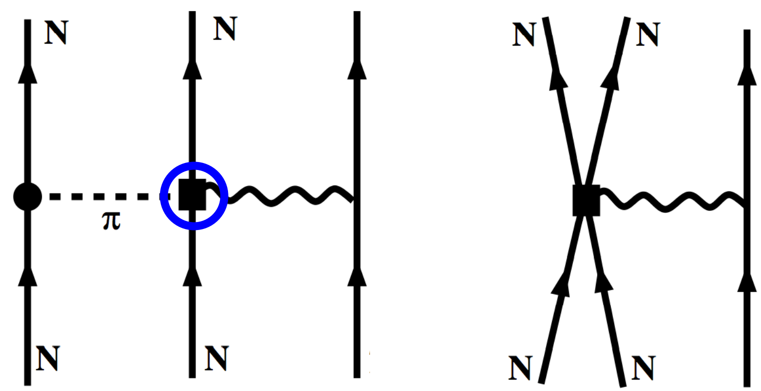


axial-vector currents (beta decays)

one-body currents at Q^0 and Q^2



+ two-body currents at Q^3



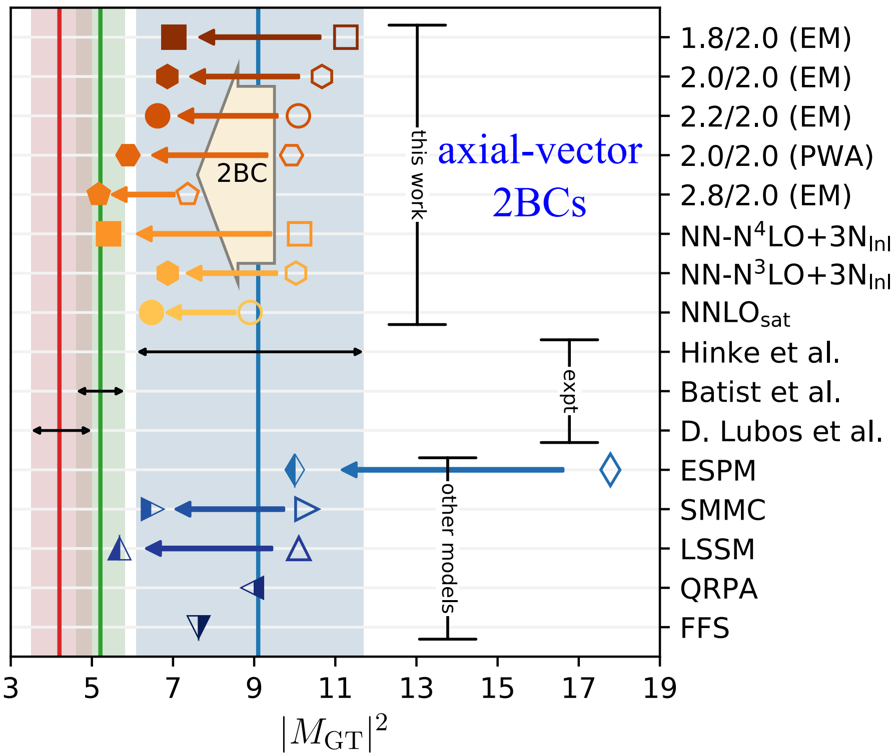
same couplings in forces and currents

Chiral EFT for coupling to electroweak interactions

important contributions from consistent two-body currents (2BCs)

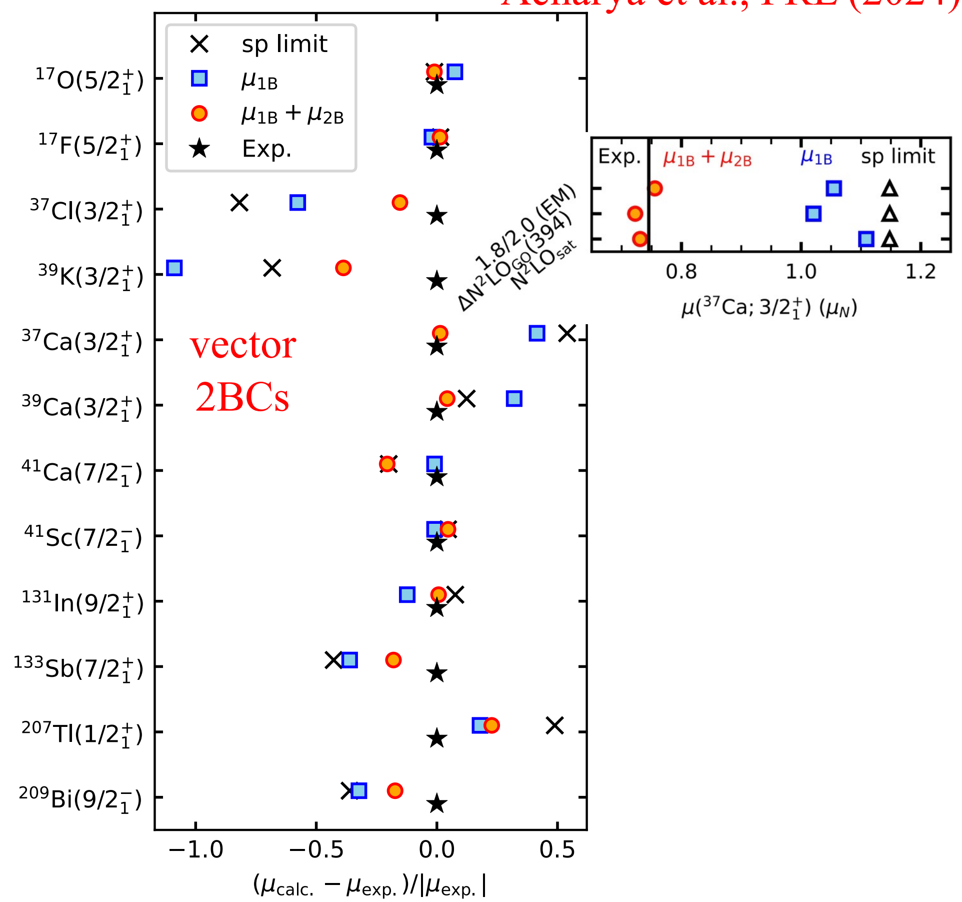
Gamow-Teller beta decay of ^{100}Sn

Gysbers et al., Nature Phys. (2019)



Magnetic moments of nuclei

Pastore et al. (2012-) Miyagi et al., PRL (2024)
Acharya et al., PRL (2024)



two-body currents key for quenching puzzle of beta decays + improve magnetic moments

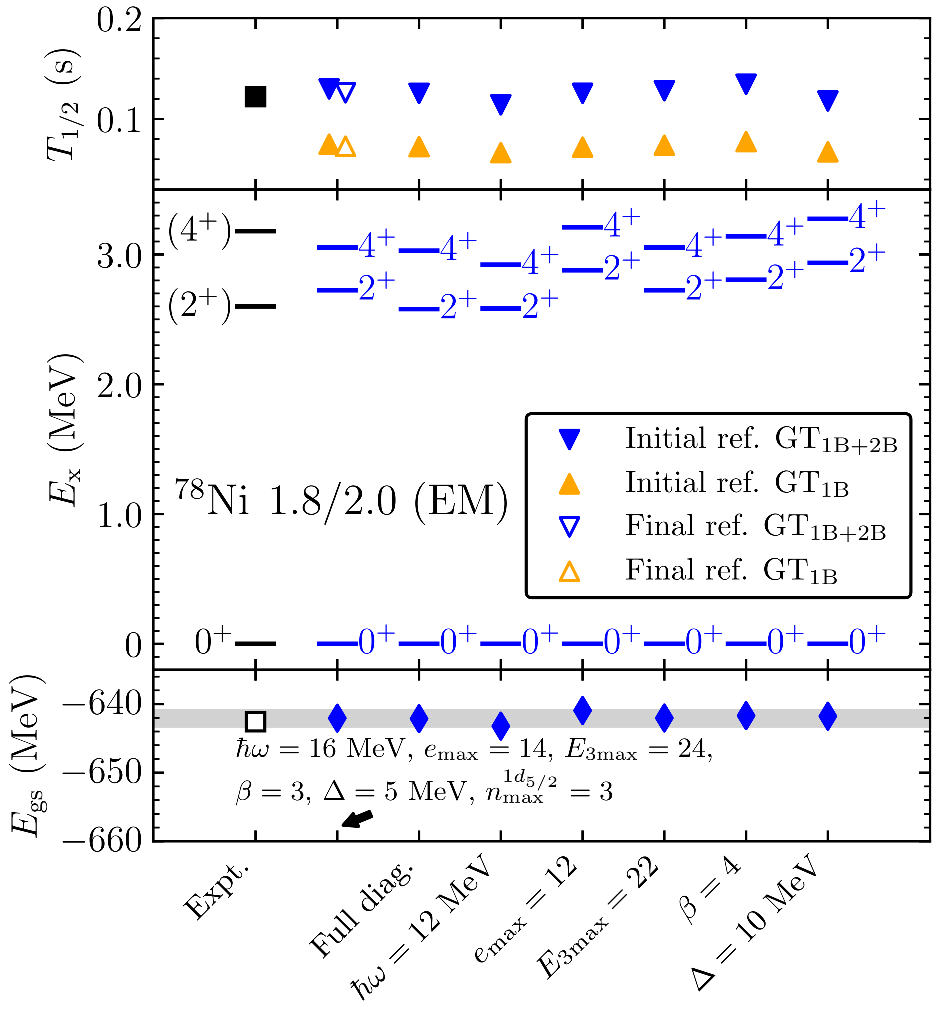
Gamow-Teller beta decays for N=50 nuclei

Zhen Li, Miyagi, AS, arXiv:2509.19131, PRL in press

VS-IMSRG calculations for valence space on top of ^{48}Ca core

1.8/2.0 (EM) interaction with 1B + 2B currents,

test sensitivities to IMSRG + model space choices



very good agreement with exp with 2B currents included, weak sensitivities to theo. choices

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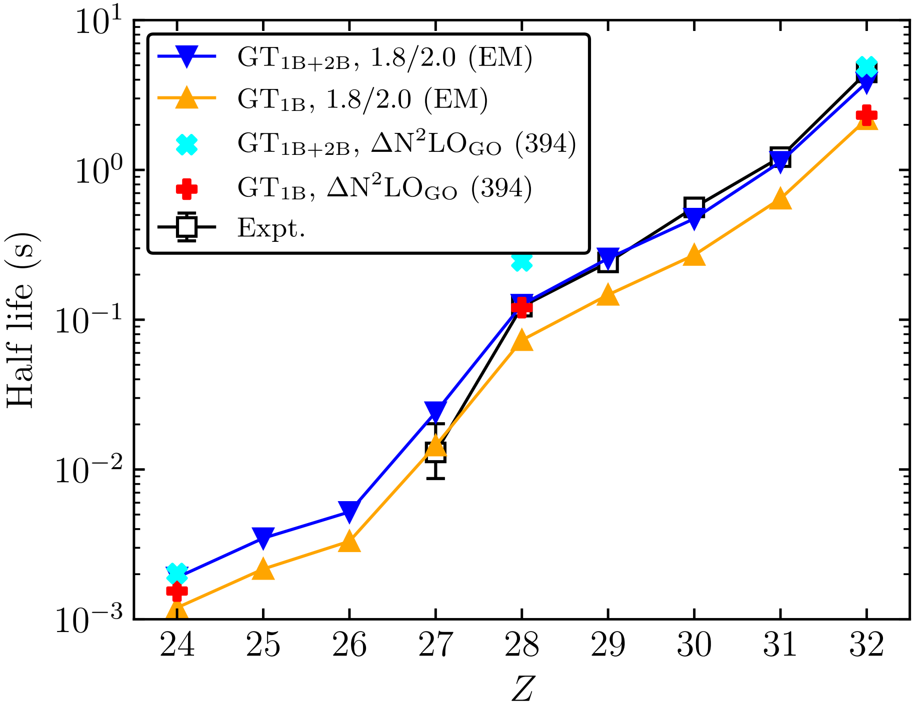
for N=50 nuclei, explore in addition ΔN^2LO_{GO} interaction



overall good agreement with exp, without adjustments

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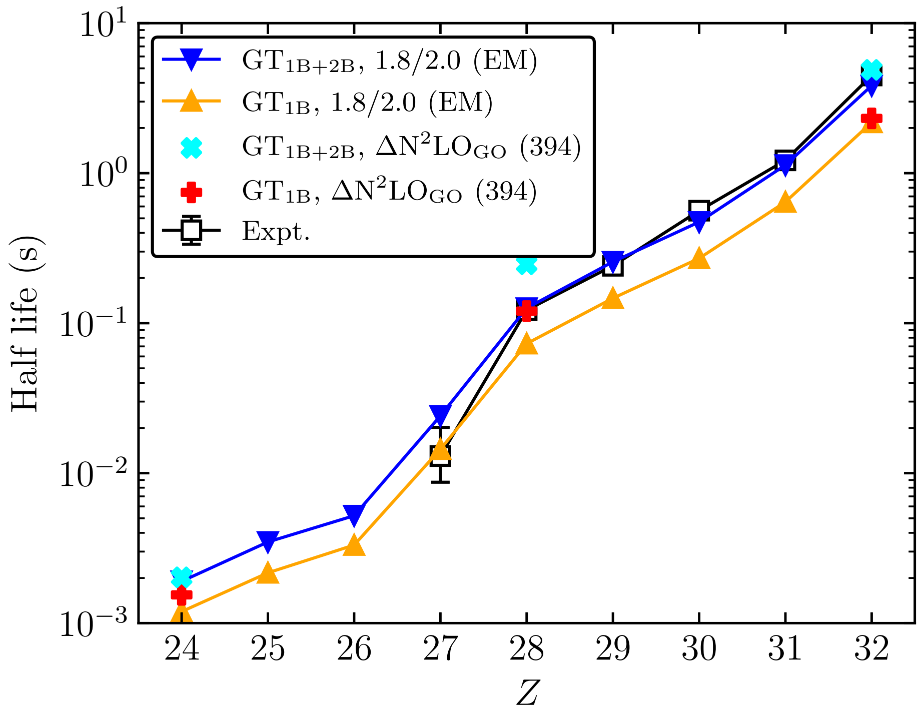
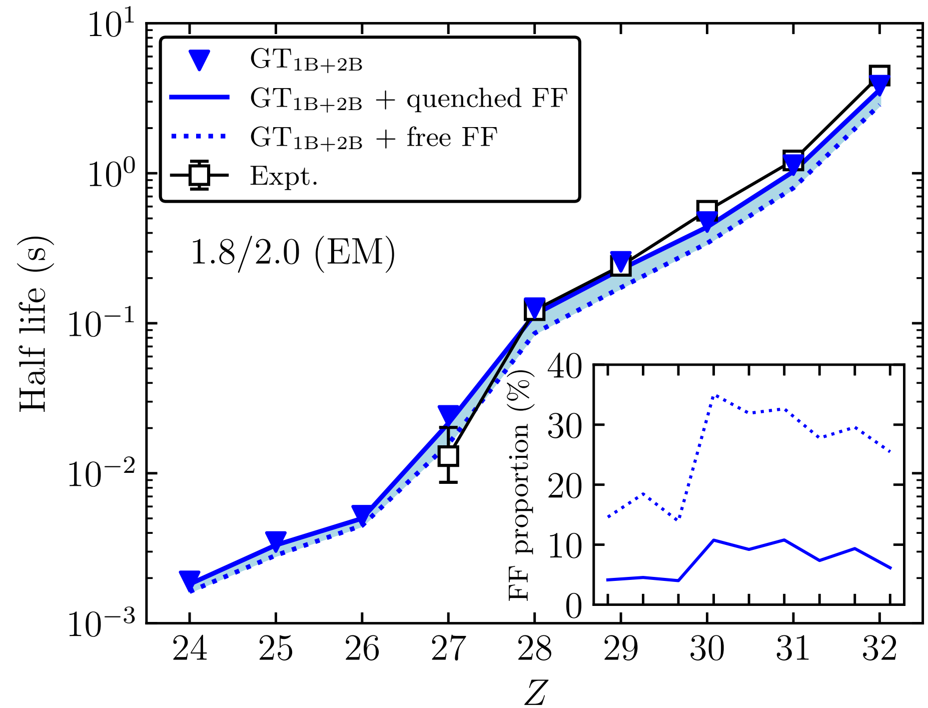


overall good agreement with exp, without adjustments



+ contributions from first-forbidden (FF) transitions

Recent developments

Correlated mass model for calcium isotopes

Cincar, Li, Plies, Vernik, Heinz, Miyagi, AS, in prep.

Ab initio nuclear masses for r-process nucleosynthesis

across N=82: Kuske, Miyagi, Arcones, AS, arXiv:2509.19131
work on N=126: Lariviere, Vassh, Holt, et al.

Beta decays and electromagnetic moments

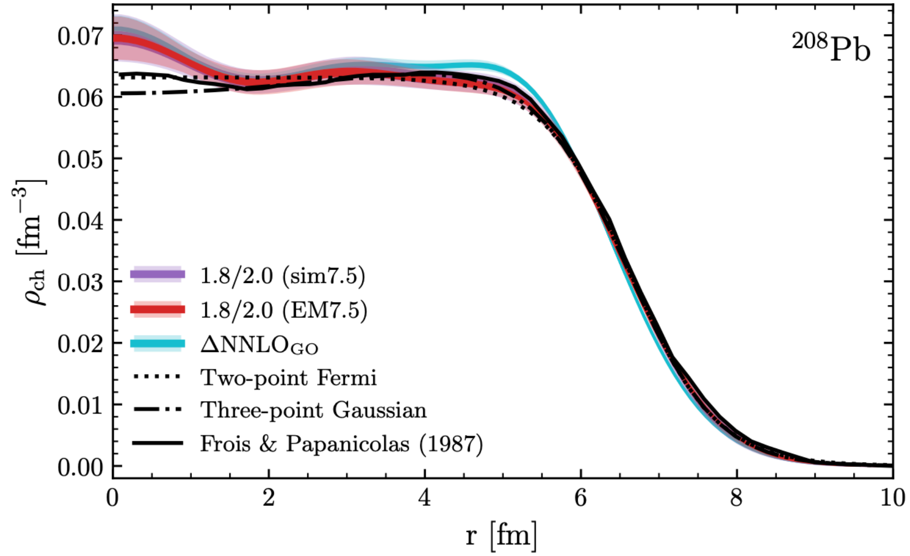
Li, Miyagi, AS, arXiv:2509.19131, PRL in press
Miyagi, Cao, Seutin, Bacca, Garcia Ruiz, Hebeler, Holt, AS, PRL (2024)
Lellinger, Vazquez Rodríguez et al.

Thanks to great group and collaborators!

Nuclear interactions with good saturation properties

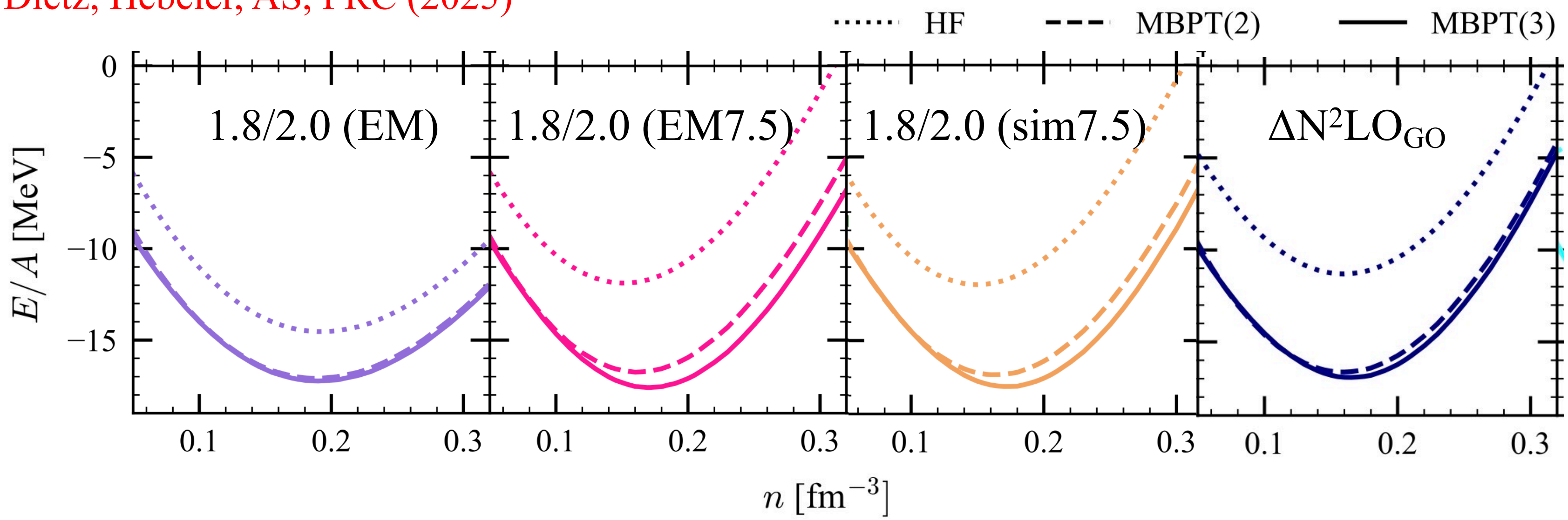
several NN+3N interactions give accurate energies and radii up to ^{208}Pb

see, e.g., Jiang et al., PRC (2020),
Arthuis, Hebeler, AS, arXiv:2401.06675



for these interactions
reasonable radii and densities
at Hartree-Fock level

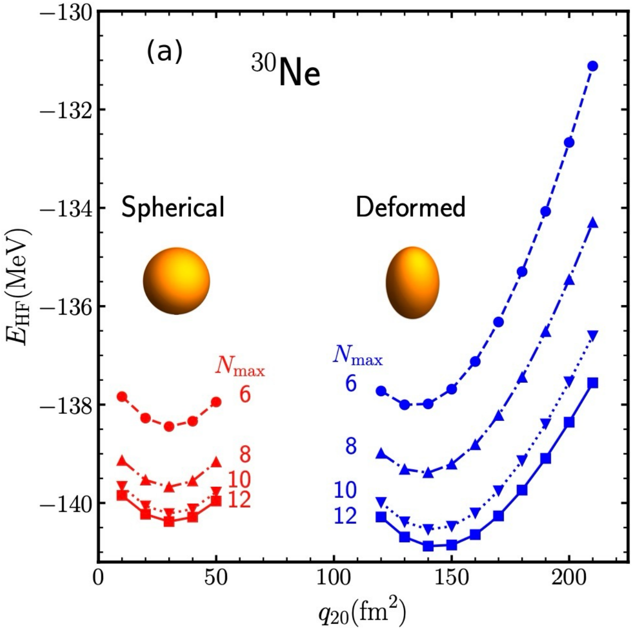
compare with nuclear matter results
Alp, Dietz, Hebeler, AS, PRC (2025)



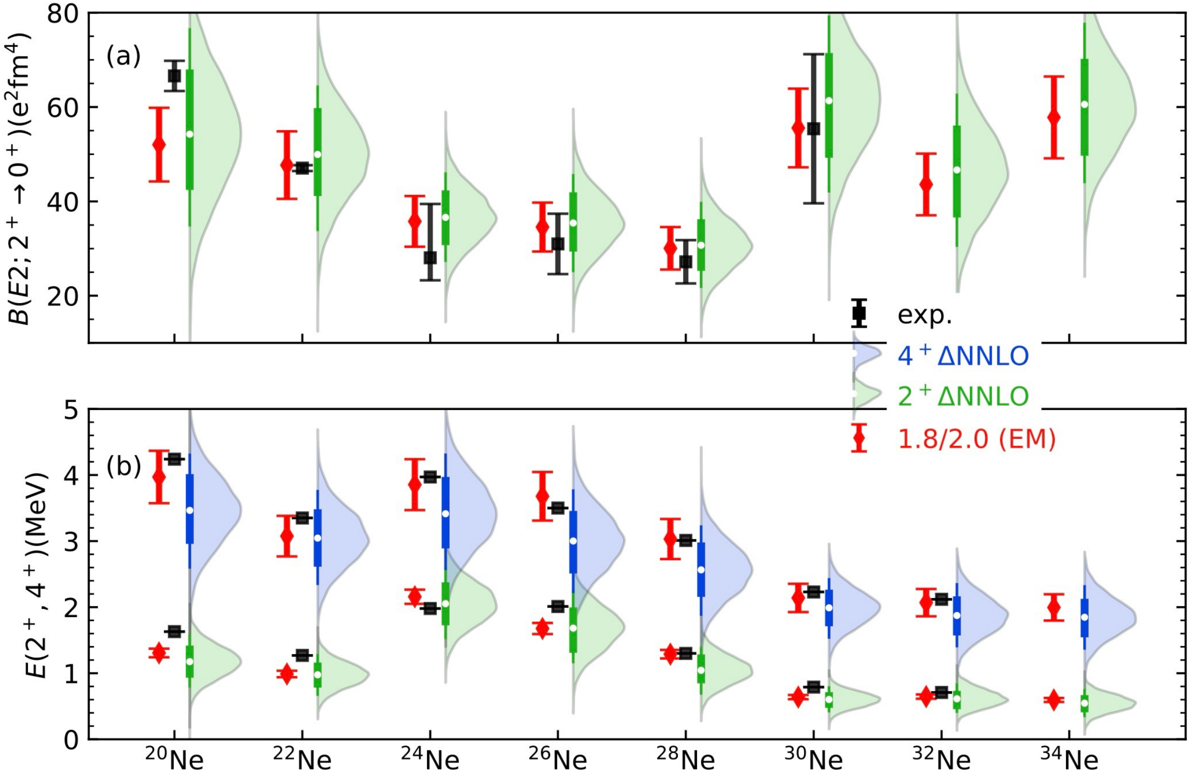
Ab initio calculations of deformed nuclei

Sun et al., PRX (2025)

can explore shapes at the Hartree-Fock level



deformed coupled-cluster theory to include correlations on top of Hartree-Fock shape



Need to overcome 3N challenges to go beyond A~100