Challenges for Nuclear Hamiltonians

Achim Schwenk

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EMMI

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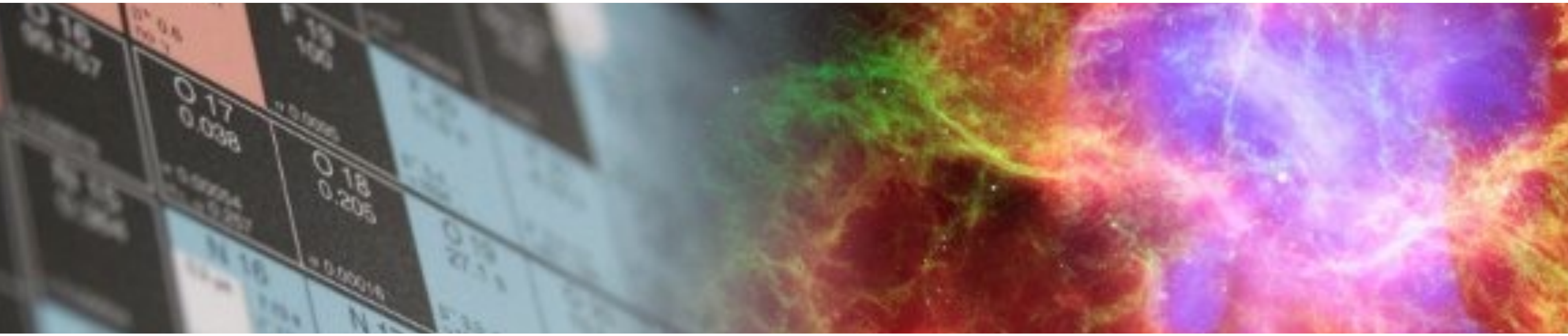

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Exzellente Forschung für Hessens Zukunft

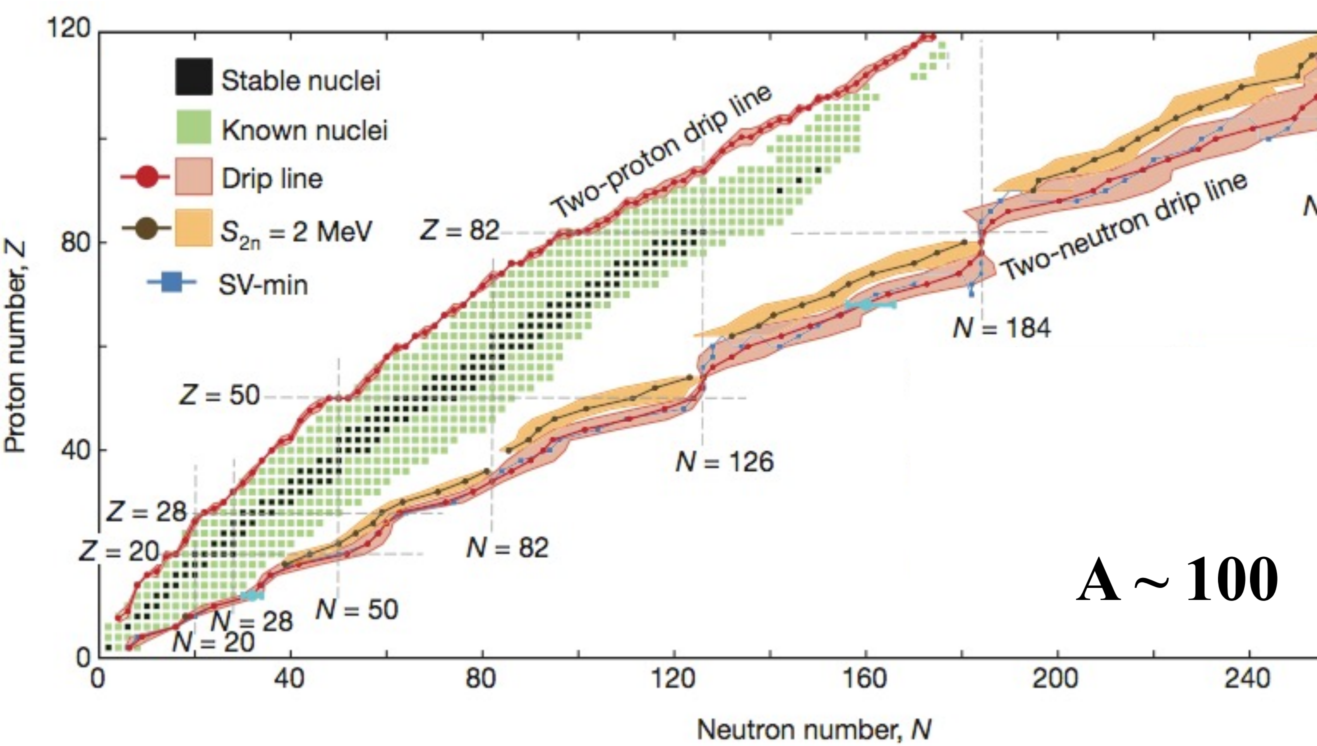
Structure of nuclei and dense matter in neutron stars

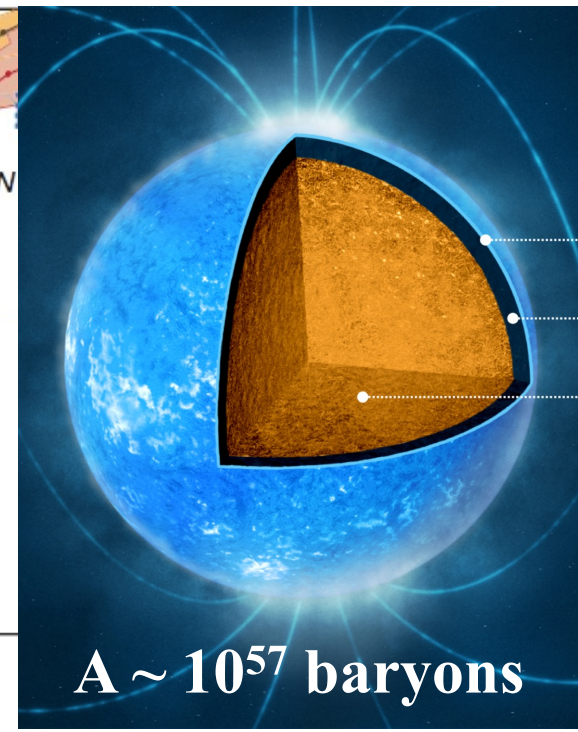
doi:10.1038/nature11188

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

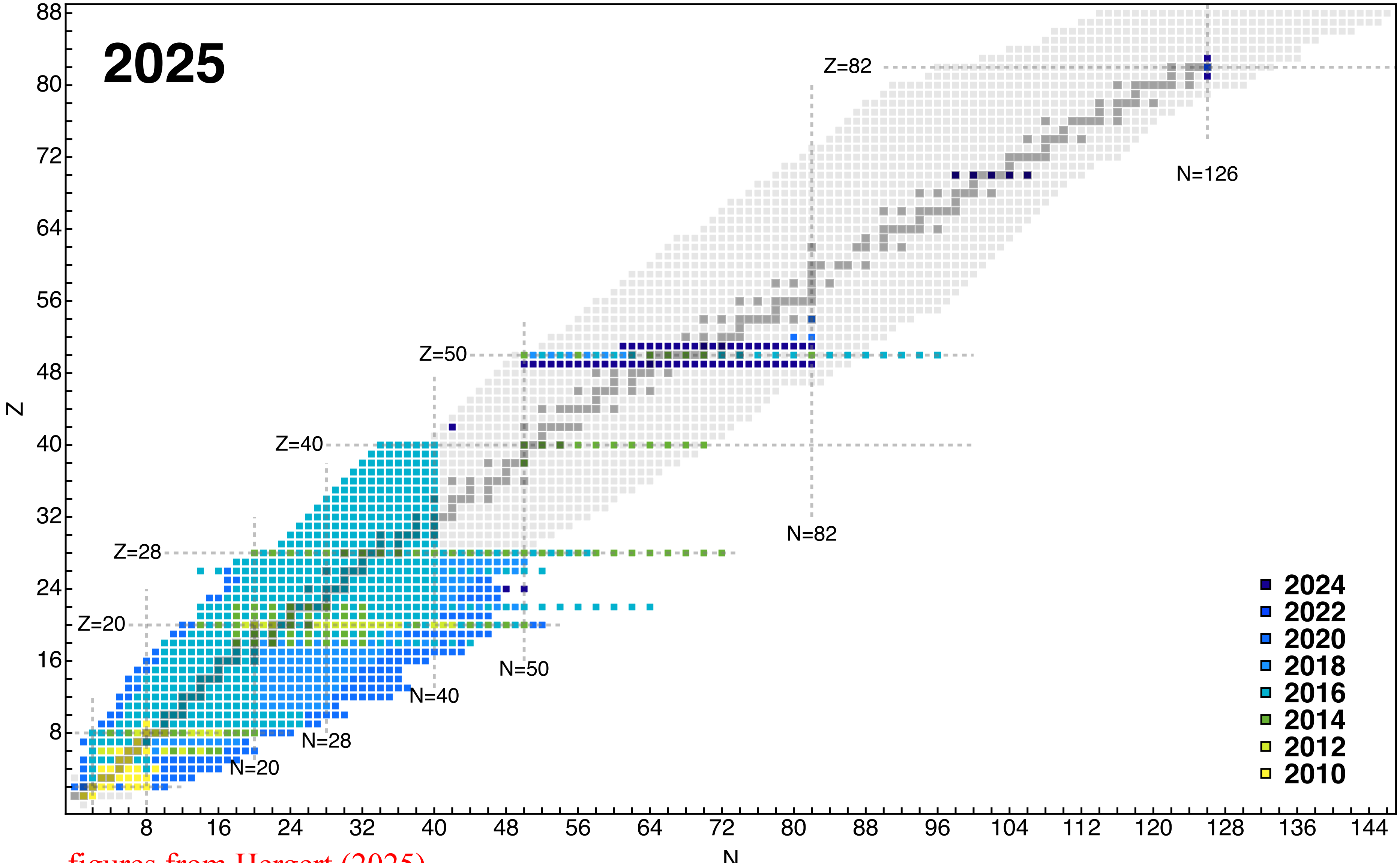




Extreme neutron-rich matter in neutron stars

Great progress in ab initio calculations of nuclei

systematic interaction expansion + systematic many-body expansion



figures from Hergert (2025)

Great progress in ab initio calculations of nuclei

systematic interaction expansion + systematic many-body expansion

ARTICLES
https://doi.org/10.1038/s41567-022-01715-8
nature physics
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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*
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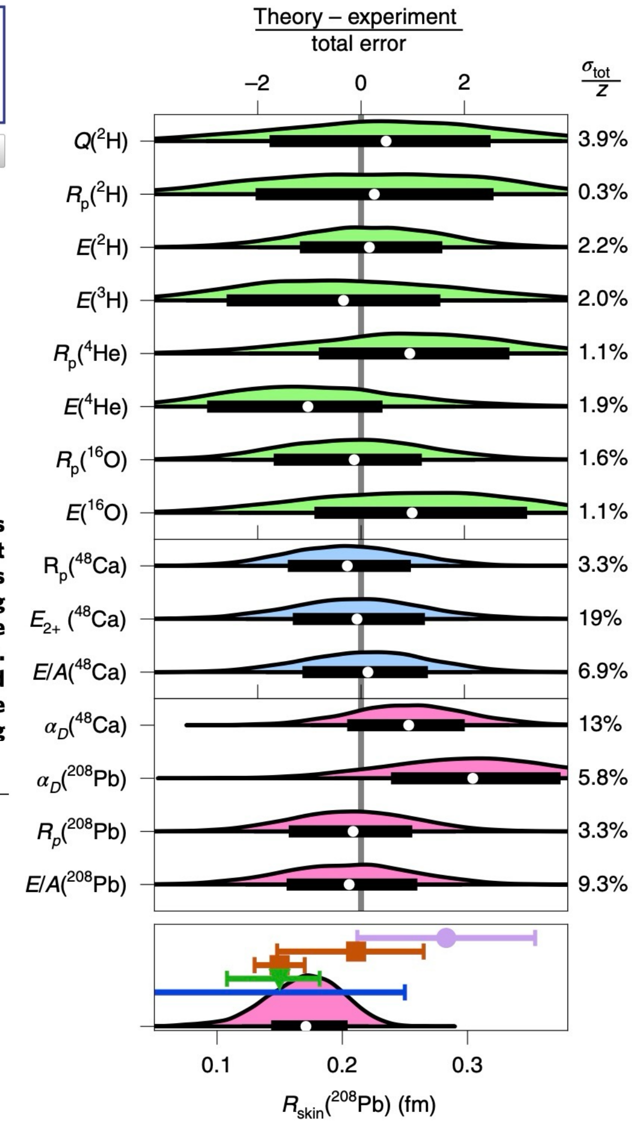
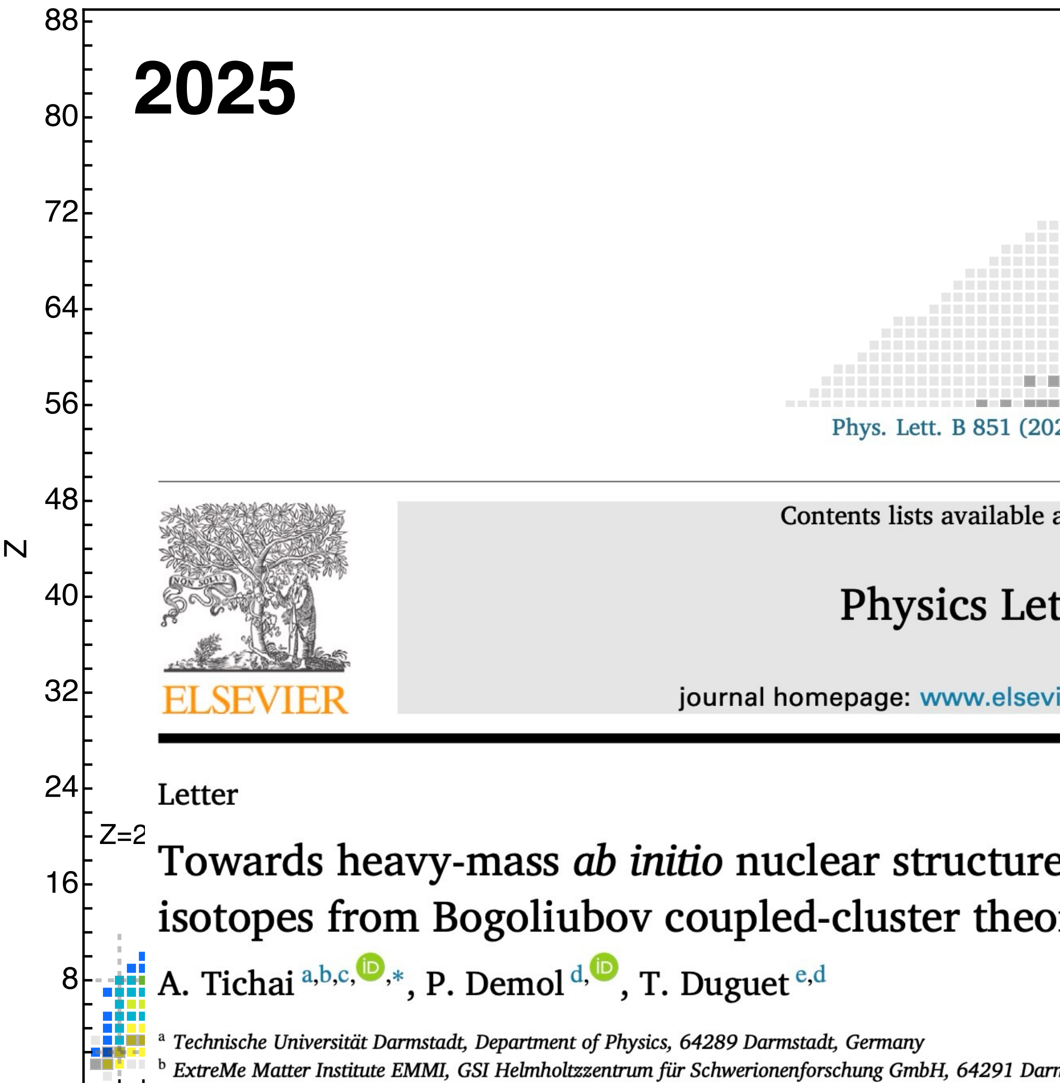
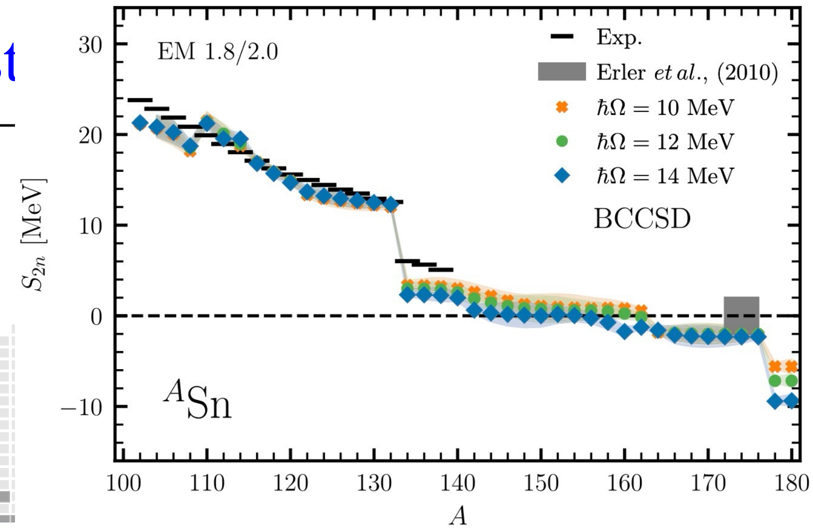
[6]*Department of Physics, McGill University, 3600 Rue University, Montréal, QC H3A 2T8, Canada*



Great progress in ab initio calculations of nuclei

systematic interaction expansion + syst





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Letter

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

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

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[e] *IRFU, CEA, Université Paris-Saclay, 91191 Gif-sur-Yvette, France*

Great progress in ab initio calculations of nuclei

systematic interaction expansion + systematic many-body expansion

PHYSICAL REVIEW LETTERS **132,** 232503 (2024)

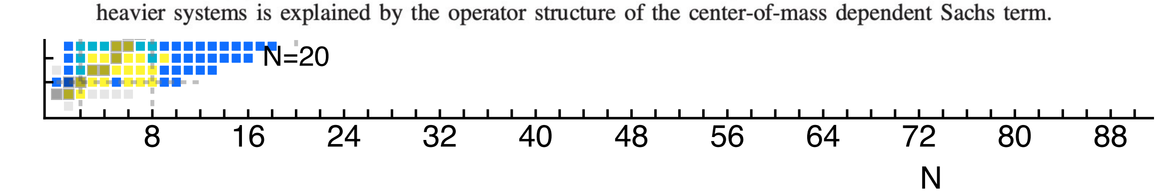
Impact of Two-Body Currents on Magnetic Dipole Moments of Nuclei

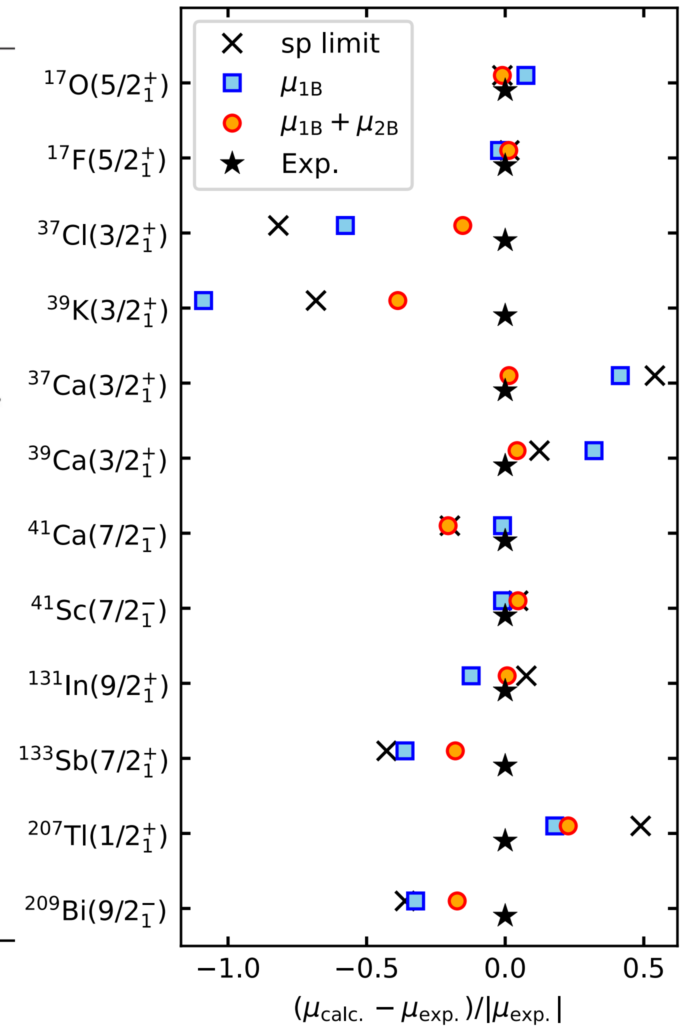
T. Miyagi,[1,2,3,*,‡‡] X. Cao,[4,†] R. Seutin,[3,1,2,‡] S. Bacca,[5,6,§] R. F. Garcia Ruiz,[7,∥] K. Hebeler,[1,2,3,¶] J. D. Holt,[8,9,**] and A. Schwenk[1,2,3,††]

[1]*Technische Universität Darmstadt, Department of Physics, 64289 Darmstadt, Germany*
[2]*ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*
[3]*Max-Planck-Institut für Kernphysik, Saupfercheckweg 1, 69117 Heidelberg, Germany*
[4]*Department of Physics and Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801-3080, USA*
[5]*Institute of Nuclear Physics, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany*
[6]*PRISMA+ Cluster of Excellence, Johannes Gutenberg-Universität Mainz, 55099 Mainz, Germany*
[7]*Department of Physics, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA*
[8]*TRIUMF, 4004 Wesbrook Mall, Vancouver British Columbia V6T 2A3, Canada*
[9]*Department of Physics, McGill University, Montréal, Quebec City H3A 2T8, Canada*

(Received 28 November 2023; revised 23 March 2024; accepted 25 April 2024; published 7 June 2024)

We investigate the effects of two-body currents on magnetic dipole moments of medium-mass and heavy nuclei using the valence-space in-medium similarity renormalization group with chiral effective field theory interactions and currents. Focusing on near doubly magic nuclei from oxygen to bismuth, we have found that the leading two-body currents globally improve the agreement with experimental magnetic moments. Moreover, our results show the importance of multishell effects for ^{41}Ca, which suggest that the $Z = N = 20$ gap in ^{40}Ca is not as robust as in ^{48}Ca. The increasing contribution of two-body currents in heavier systems is explained by the operator structure of the center-of-mass dependent Sachs term.

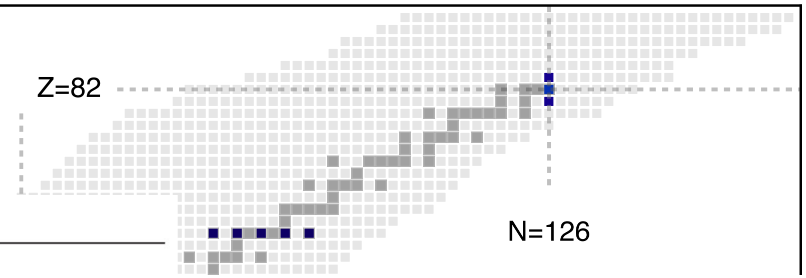




Great progress in ab initio calculations of nuclei

systematic interaction expansion + systematic many-body expansion

2025



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]

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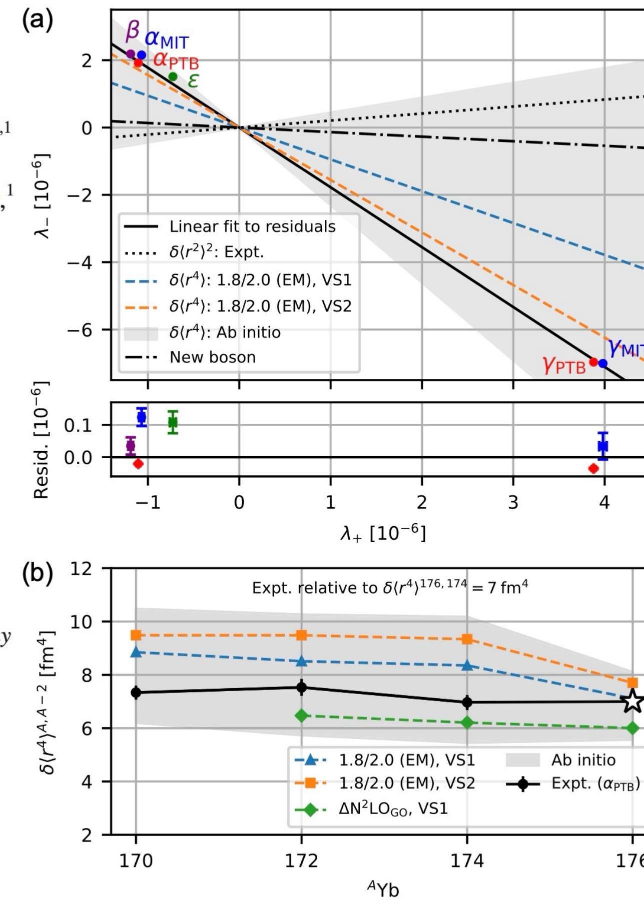
[2]*Heidelberg University, Grabengasse 1, 69117 Heidelberg, Germany*
[3]*Physikalisch-Technische Bundesanstalt, Bundesallee 100, 38116 Braunschweig, Germany*
[4]*Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany*
[5]*ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum 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*

(Received 23 June 2024; revised 6 November 2024; accepted 23 December 2024; published 11 February 2025)

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 $^2S_{1/2} \rightarrow {}^2D_{5/2}$ and $^2S_{1/2} \rightarrow {}^2F_{7/2}$ 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.

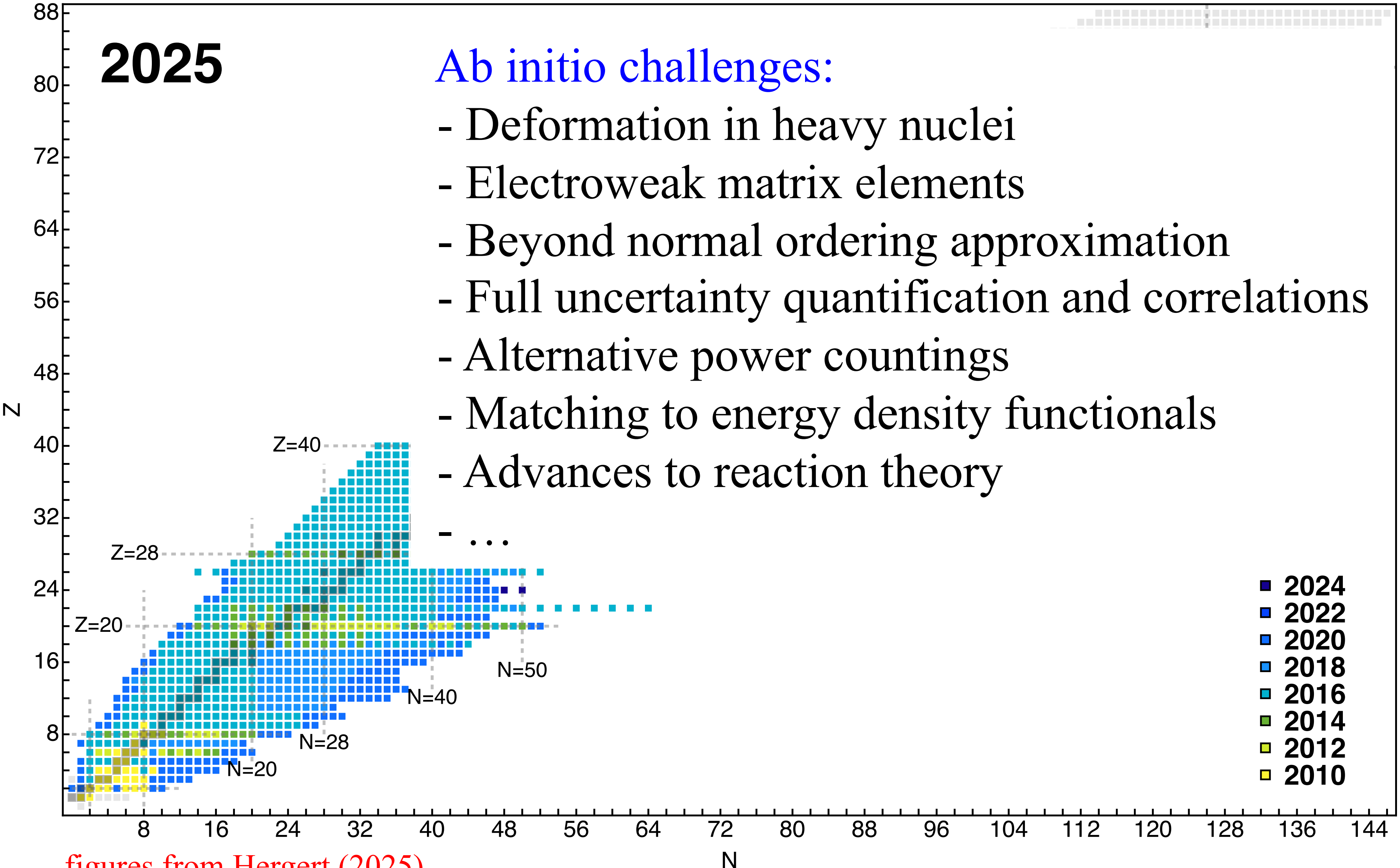


Great progress in ab initio calculations of nuclei

systematic interaction expansion + systematic many-body expansion

Ab initio challenges:

- Deformation in heavy nuclei
- Electroweak matrix elements
- Beyond normal ordering approximation
- Full uncertainty quantification and correlations
- Alternative power countings
- Matching to energy density functionals
- Advances to reaction theory
- …



figures from Hergert (2025)

Outline

Chiral EFT interaction uncertainties and challenges

with P. Arthuis, M. Companys, K. Hebeler, A. Tichai, U. Vernik

Next generation NN+3N interactions: Wish list

with F. Alp, Y. Dietz, K. Hebeler

Ab initio nuclear masses for r-process nucleosynthesis

with J. Kuske, T. Miyagi, A. Arcones

Uncertainty quantification and correlated mass model for calcium isotopes

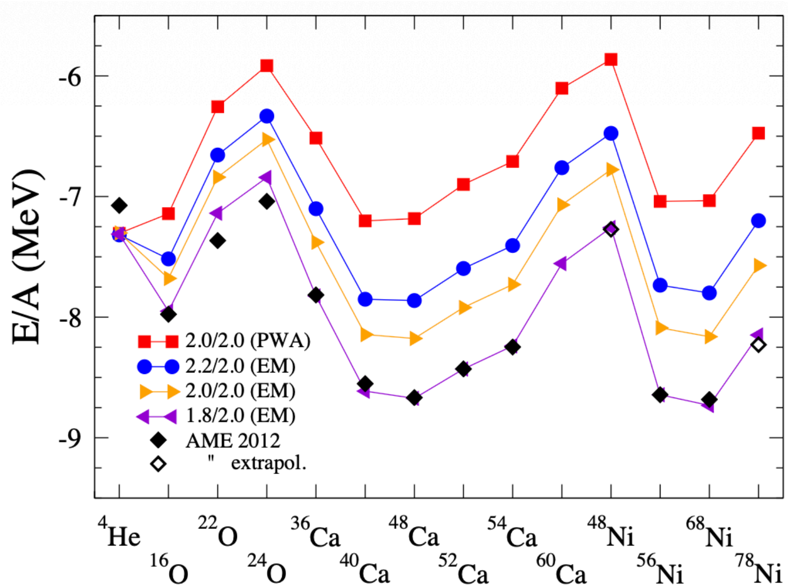
with M. Cincar, Z. Li, T. Plies, U. Vernik, M. Heinz, T. Miyagi,
I. Svensson, A. Tichai, K. Hebeler

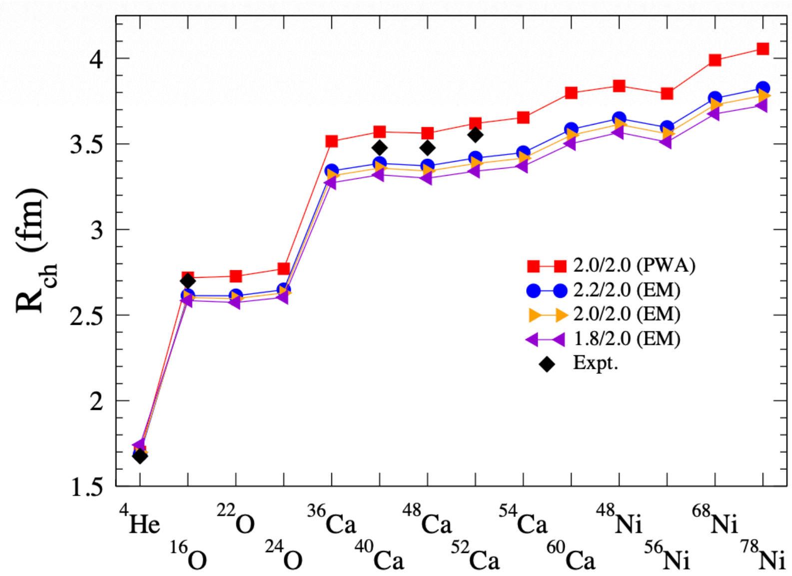
Chiral NN+3N interactions up to ^{208}Pb

Optimization strategies for NN+3N interactions

1.8/2.0 (EM) interaction Hebeler et al., PRC (2011), Simonis et al., PRC (2017)

NN N^{3}LO (SRG evolved) + 3N N^{2}LO fit to ^{3}H energy and ^{4}He radius





+ SRG preserves high-quality NN scattering

− mixed N^{3}LO + N^{2}LO, SRG evolution not consistent,…

Chiral NN+3N interactions up to ^{208}Pb

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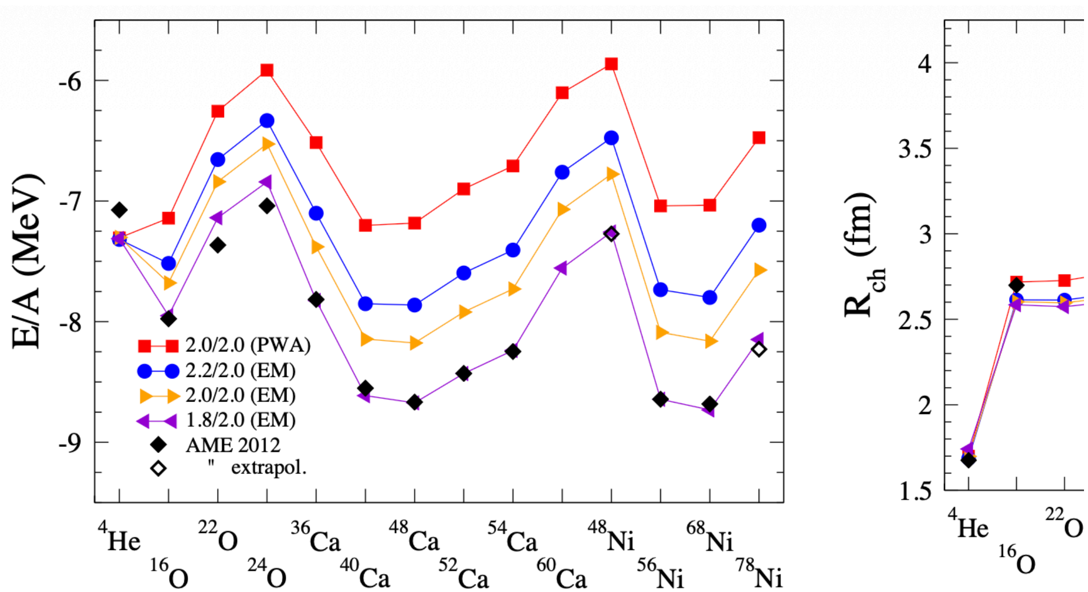

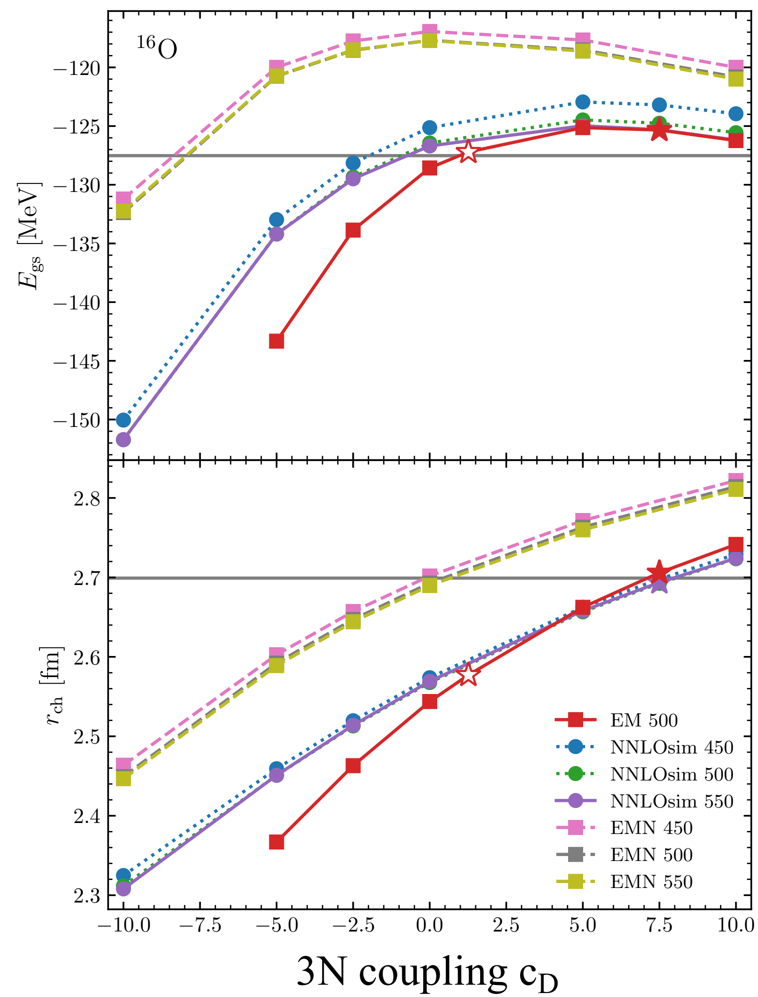

3N fit to ^3H energy and ^{16}O energy/radius

Arthuis, Hebeler, AS, arXiv:2401.06675

with large $c_D = 7.5$

Chiral NN+3N interactions up to ^{208}Pb

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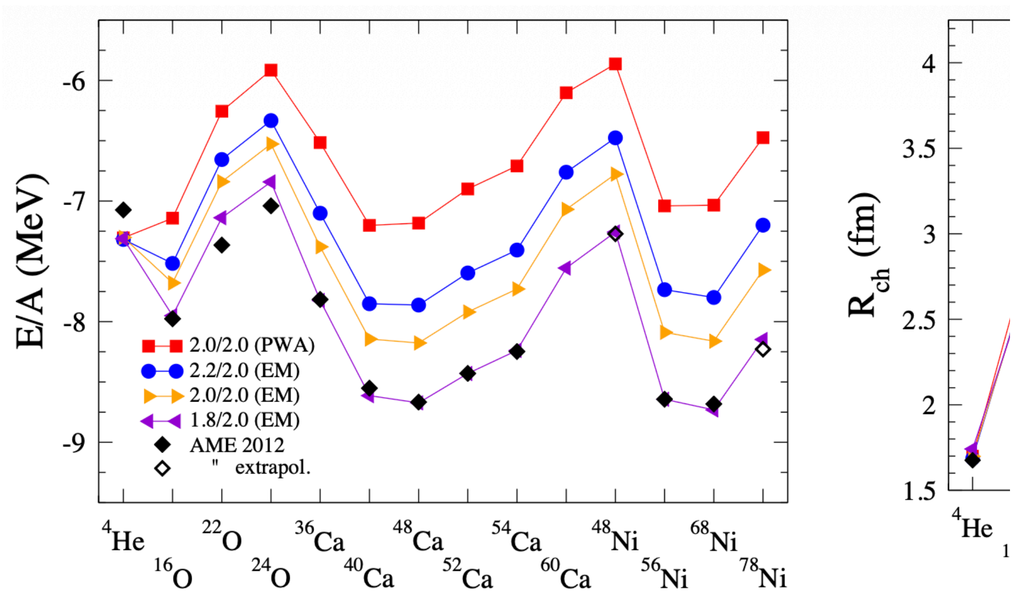

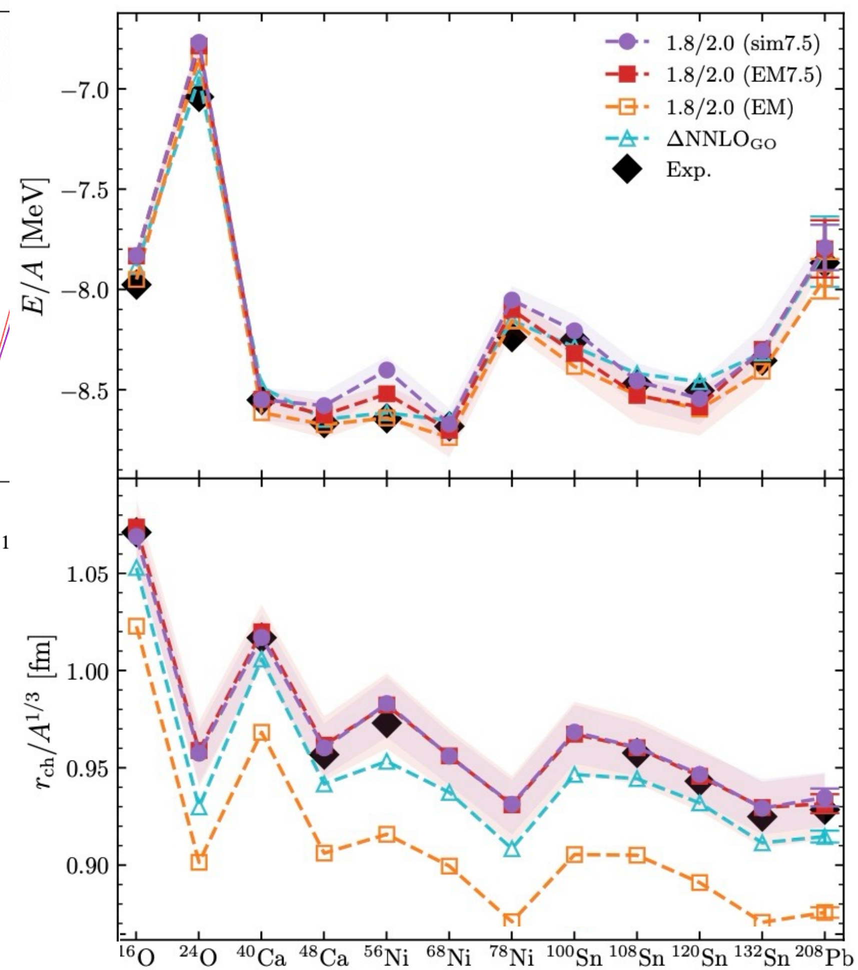

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Arthuis, Hebeler, AS, arXiv:2401.06675

with large $c_D = 7.5$

Chiral NN+3N interactions up to ^{208}Pb

other NN+3N interactions for global ab initio calcs see Gaute's talk

- Δ-full interactions ΔN^2LO_{GO} Jiang et al., PRC (2020)
  fit to very low-energy NN scattering and A=3,4,
  optimized to nuclear matter/medium-mass nuclei

- nonimplausible ΔN^2LO interactions Hu et al., Nat. Phys. (2024)
  similar strategy plus conservative uncertainty quantification

- N^3LO_{Texas} mixed NN N^3LO + 3N N^2LO Hu et al., arXiv:2512.11723
  similar fitting strategy, including also higher energy NN scattering

- Lattice EFT: NN N^3LO + 3N N^2LO Elhatisari et al., Nature (2024)
  + 6 additional 3N parameters adjusted to selected nuclei

- order-by-order LO…N^3LO Hüther et al., PLB (2020)
  based on EMN NN with consistent 3N SRG evolved,
  but for unevolved interactions 3N fits to ^{16}O not possible with EMN

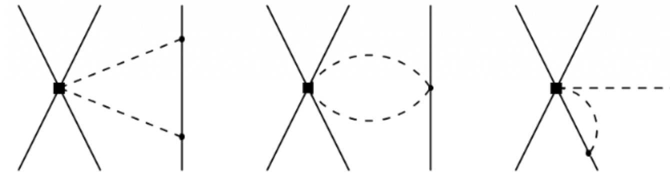
Quark mass dependent 3N forces

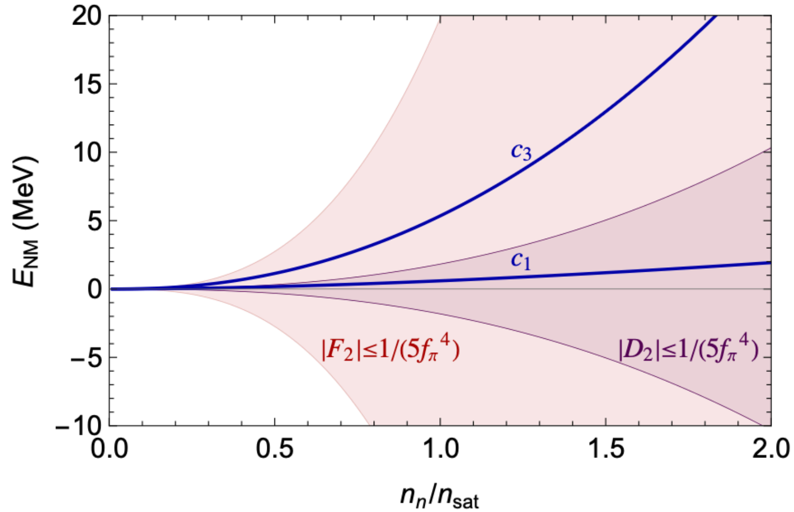
Cirigliano, Dawid, Dekens, Reddy, PRL (2025)

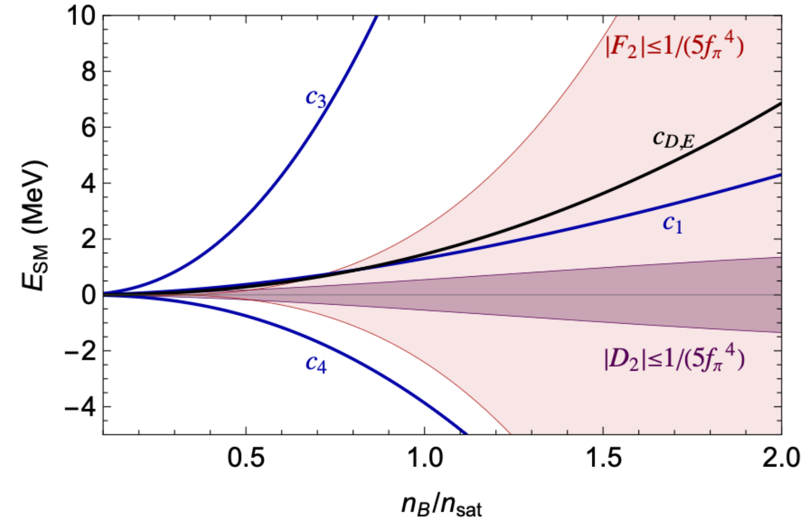
suggested class of N^4LO 3N forces

may be as large as $N^{2 \text{ or } 3}LO$

see Hartree-Fock calcs for nuclear matter







explore dominant F_2 interaction in medium-mass nuclei

Vernik, Hebeler, AS, arXiv:2512.20454

define F_2 in units F_π^{-4}, so range above is ± 0.2

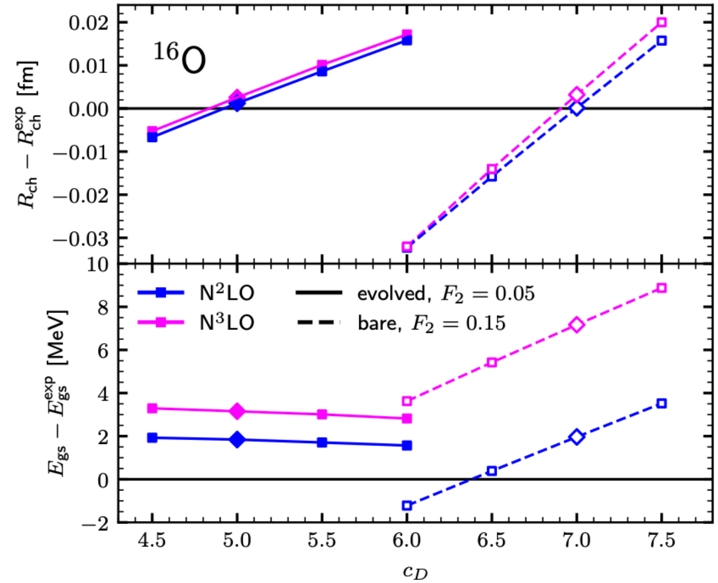
3N fits to ^{3}H energy and ^{16}O energy/radius

(also studied fits to ^{3}H energy and half-life, not as promising for nuclei)

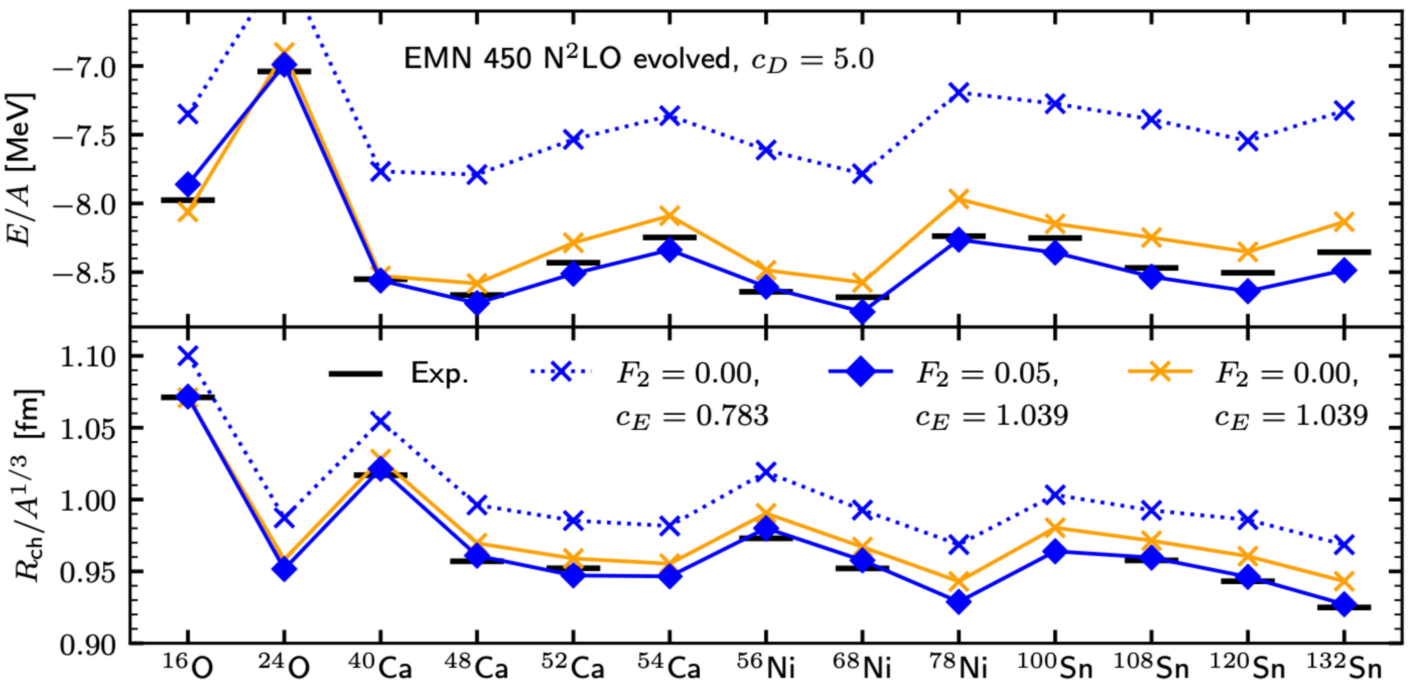
Quark mass dependent 3N forces

Vernik, Hebeler, AS, arXiv:2512.20454

3N fits to ^{3}H energy and ^{16}O energy/radius possible for unevolved and evolved NN



good reproduction of energies/radii up to ^{132}Sn at NN+3N N^{2}LO and N^{3}LO both large $c_D = 5$



Quark mass dependent 3N forces

Vernik, Hebeler, AS, arXiv:2512.20454

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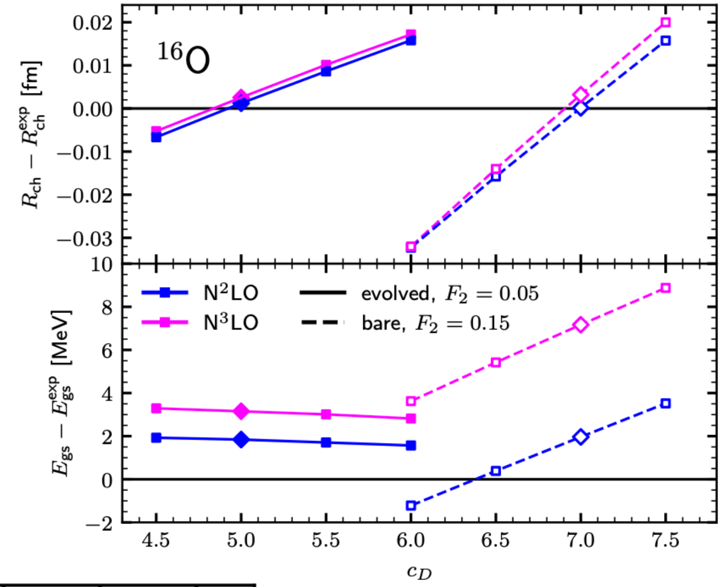

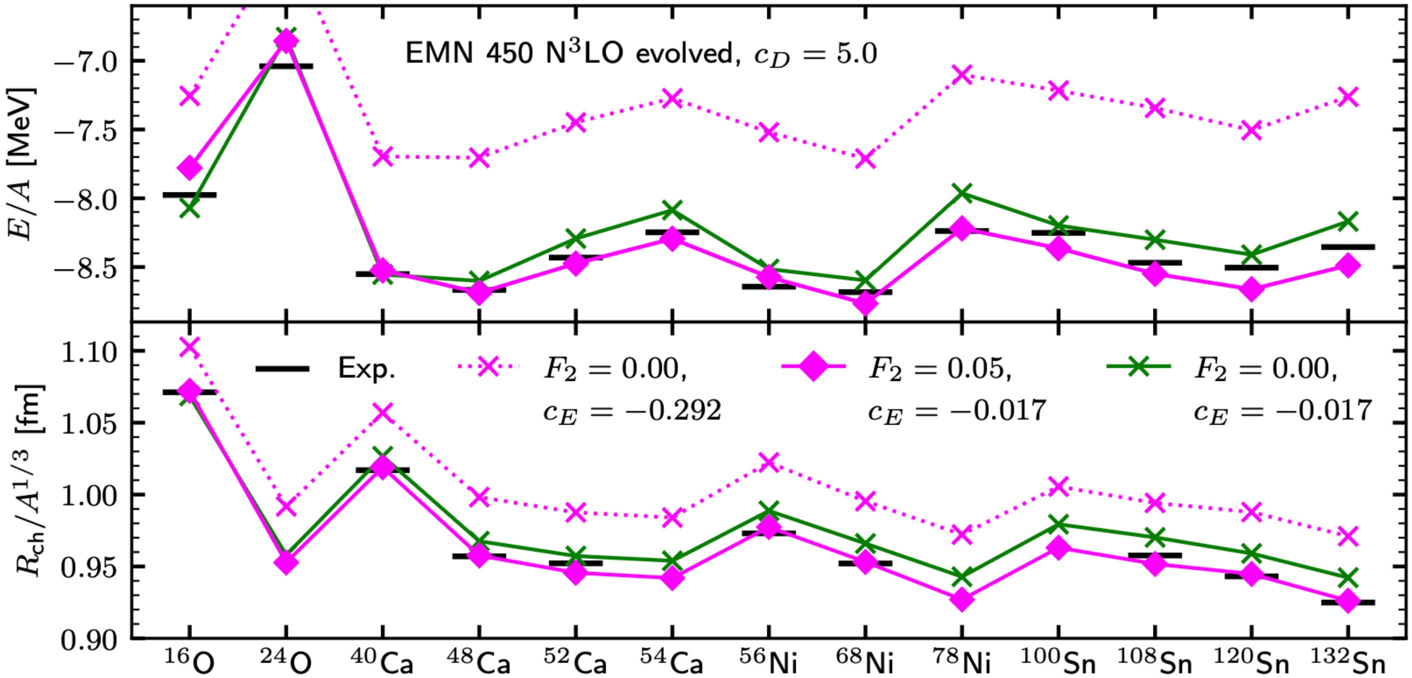

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Vernik, Hebeler, AS, arXiv:2512.20454

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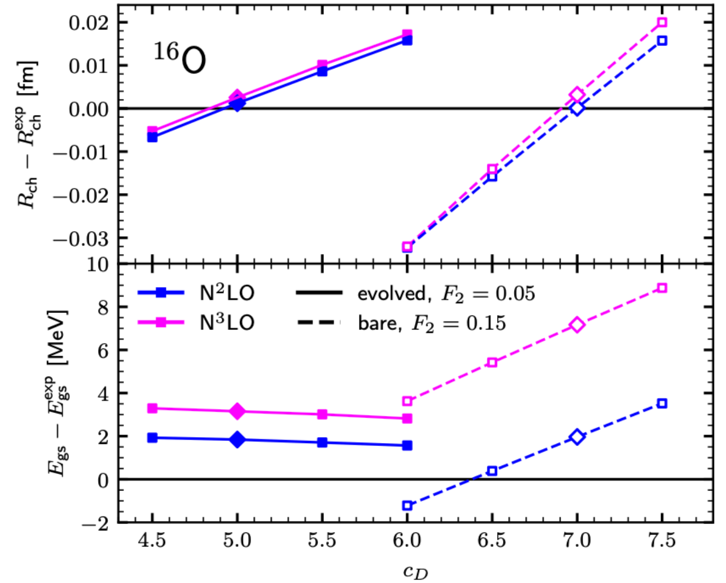
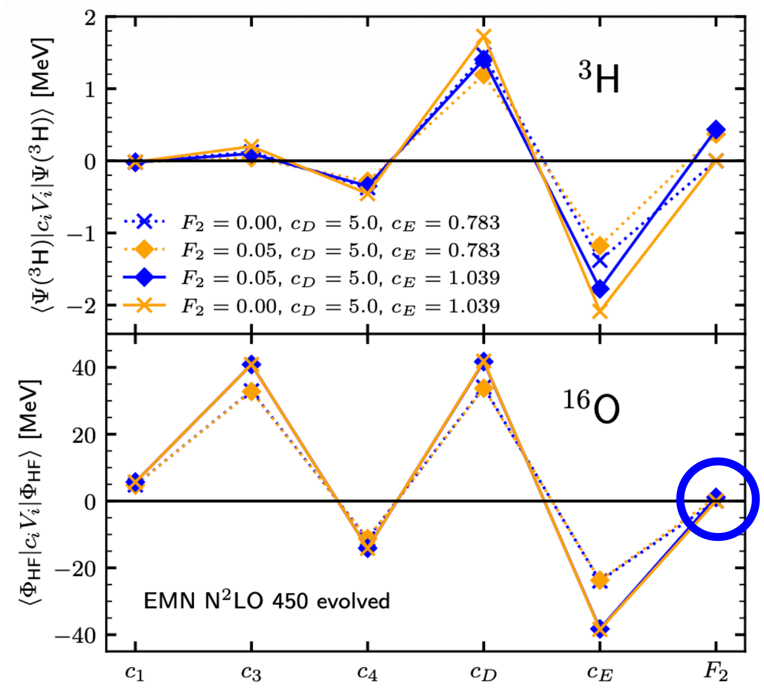
good reproduction of energies/radii up to ^{132}Sn at NN+3N N^{2}LO and N^{3}LO both large $c_D = 5$

however: main effect of F_2 is to shift short-range 3N c_E

F_2 itself has very small impact on energies of nuclei

seems more natural to include F_2 with other small short-range 3N terms at N^{4}LO





Next generation NN+3N interactions: Wish list

- Low resolution enough for converged calculations up to ^{208}Pb

- Order-by-order interactions amenable to UQ,
  at least two orders with 3N

- Interactions for different cutoffs/schemes

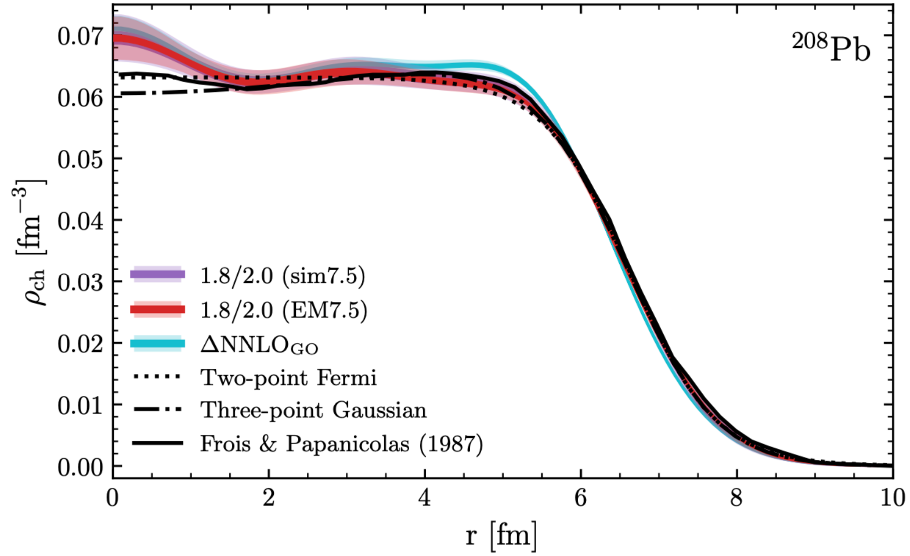
- Good description of NN scattering and A=3,4 systems

- Pion-full: leading two-body currents are parameter-free,
  3-neutron interactions parameter-free up to N^3LO

Density distributions in nuclei

Arthuis, Hebeler, AS, arXiv:2401.06675, see also Matthias' talk

good agreement for density distributions up to ^{208}Pb



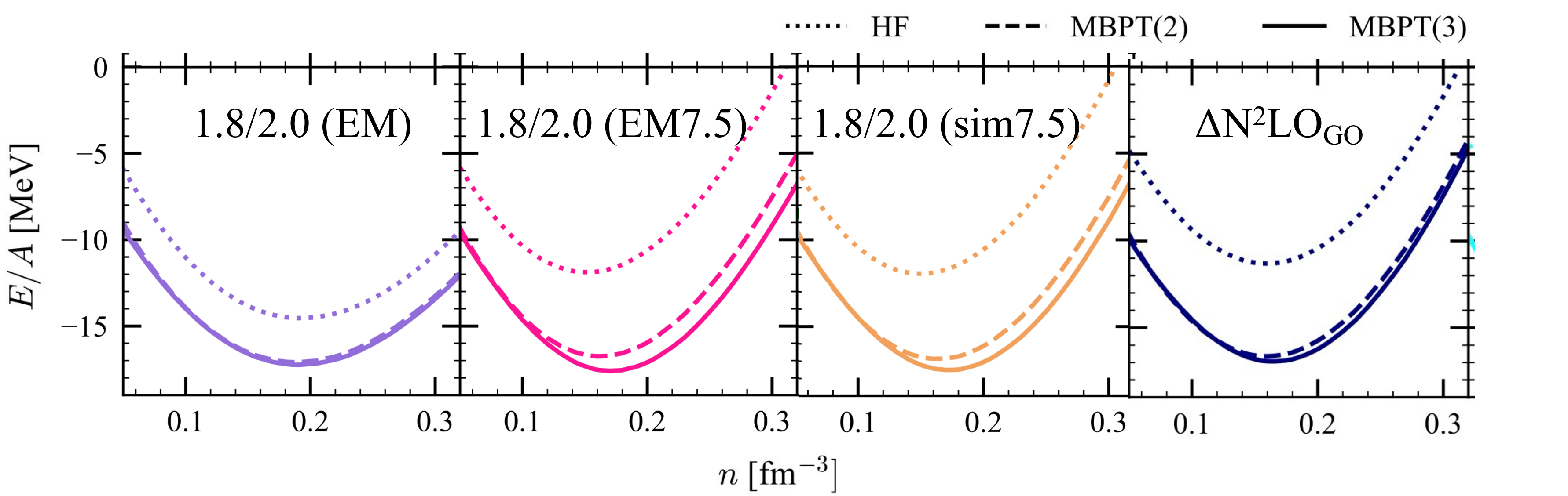
for these interactions

reasonable radii and densities

at Hartree-Fock level

compare with nuclear matter results

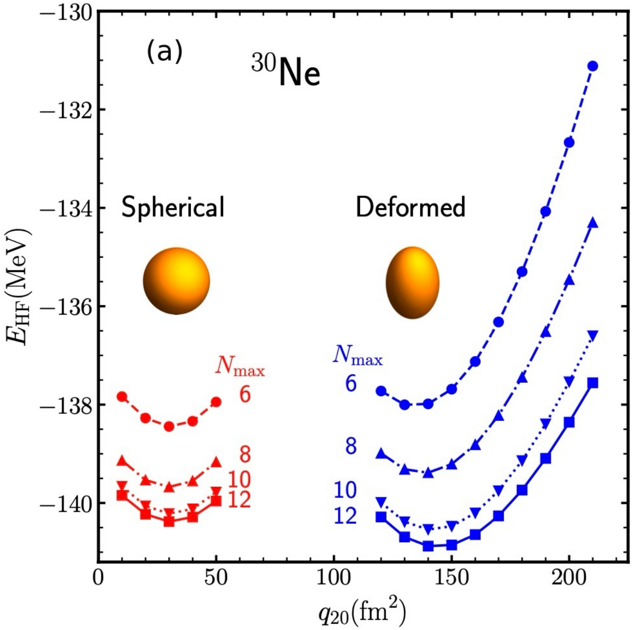
Alp, Dietz, Hebeler, AS, PRC (2025)



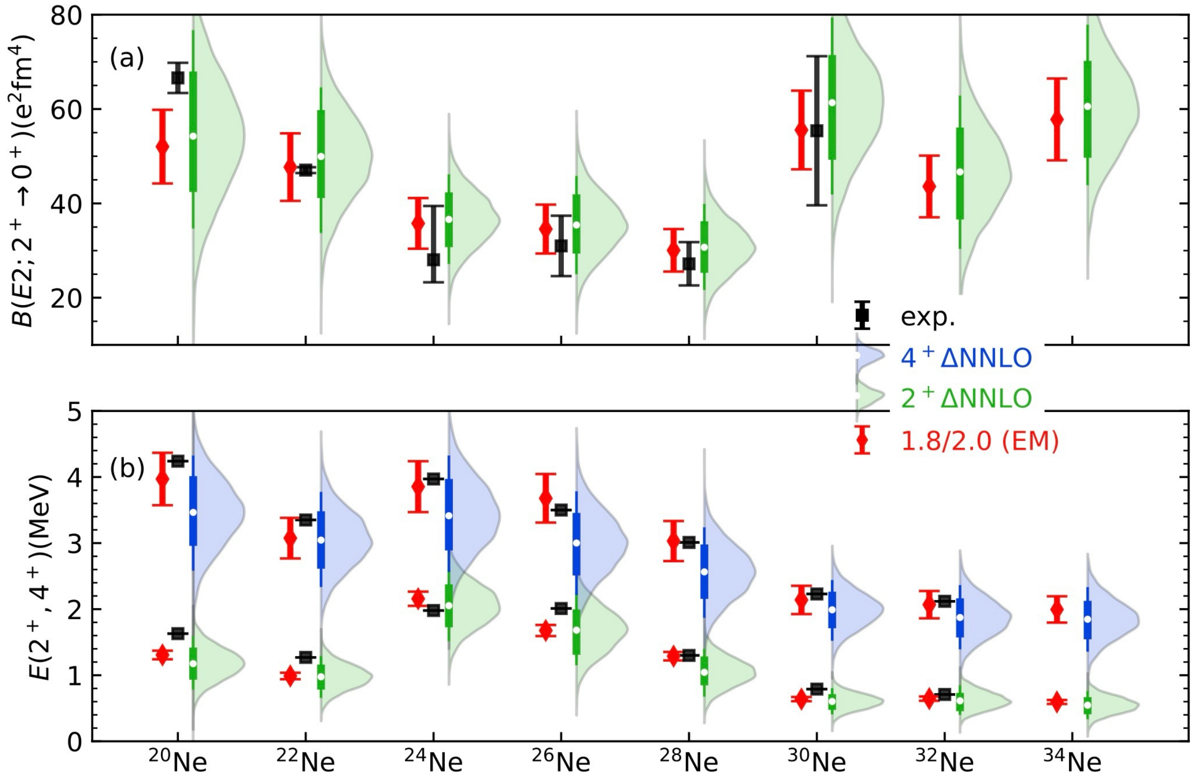
Ab initio calculations of deformed nuclei

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 normal ordering challenges to go beyond A~100

Next generation NN+3N interactions: Wish list

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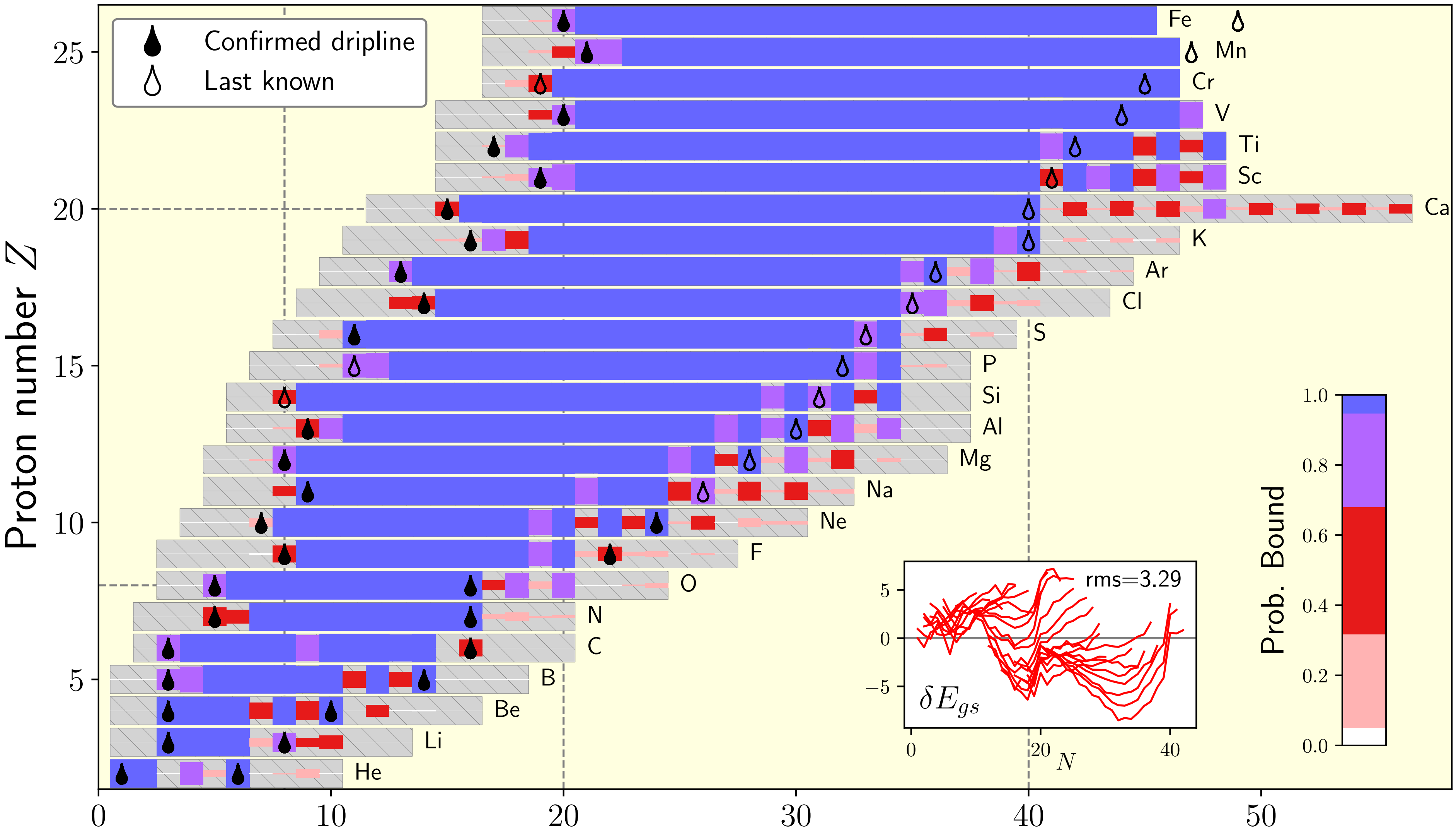
- Order-by-order interactions amenable to UQ,
  at least two orders with 3N
- Interactions for different cutoffs/schemes
- Good description of NN and A=3,4 systems
- Pion-full: leading two-body currents are parameter-free,
  3-neutron interactions parameter-free up to N^3LO
- Reasonable saturation properties (informed by matter/nuclei),
  reasonable saturation density at HF level?

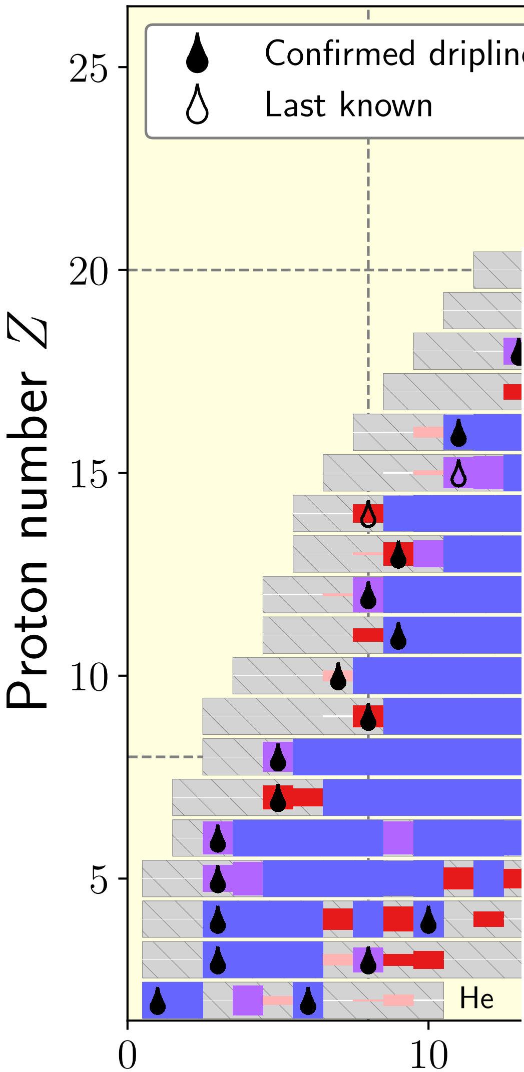
Nuclear landscape based on a chiral NN+3N interaction



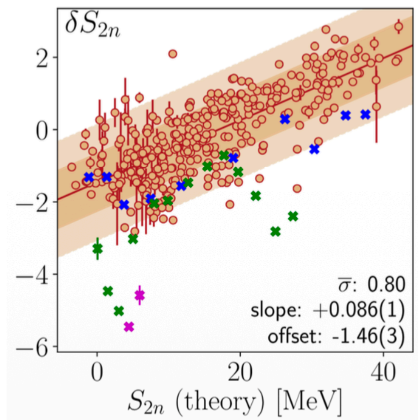
Stroberg, Holt, AS, Simonis, PRL (2021)

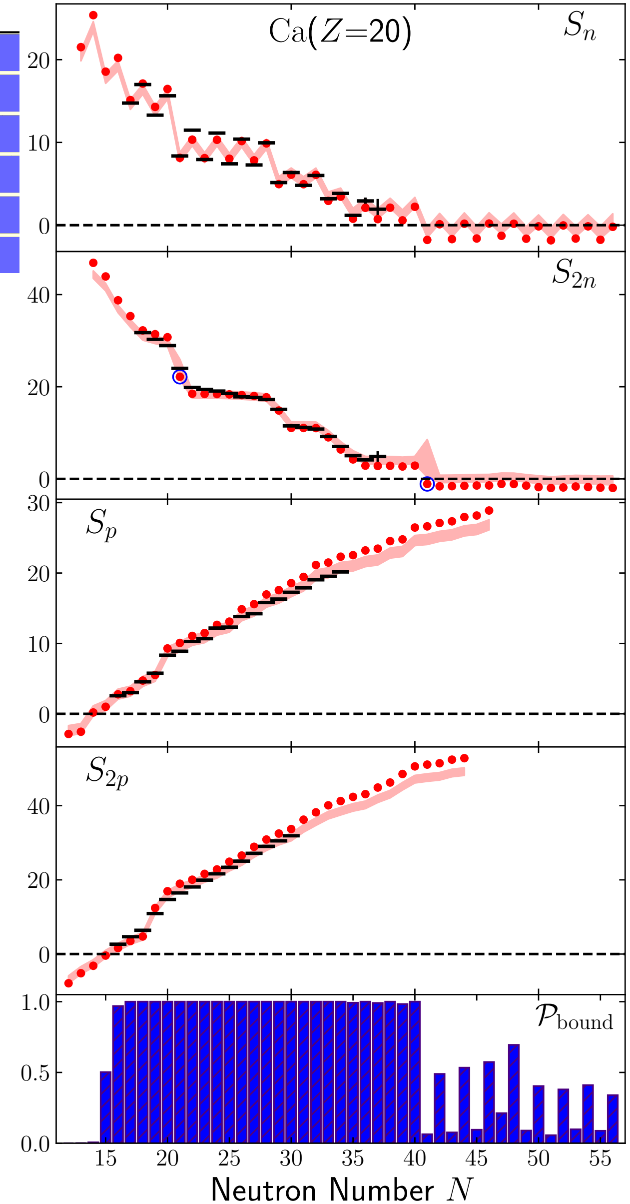
global ab initio calculations, but limited uncertainty estimate for NN+3N

Nuclear landscape based on a chiral NN+3N interaction



Final predictions include systematic uncertainty from residuals to known masses





Stroberg, Holt, AS, Simonis,

incl. syst. uncertainties: dripline at ^{61}Ca or beyond

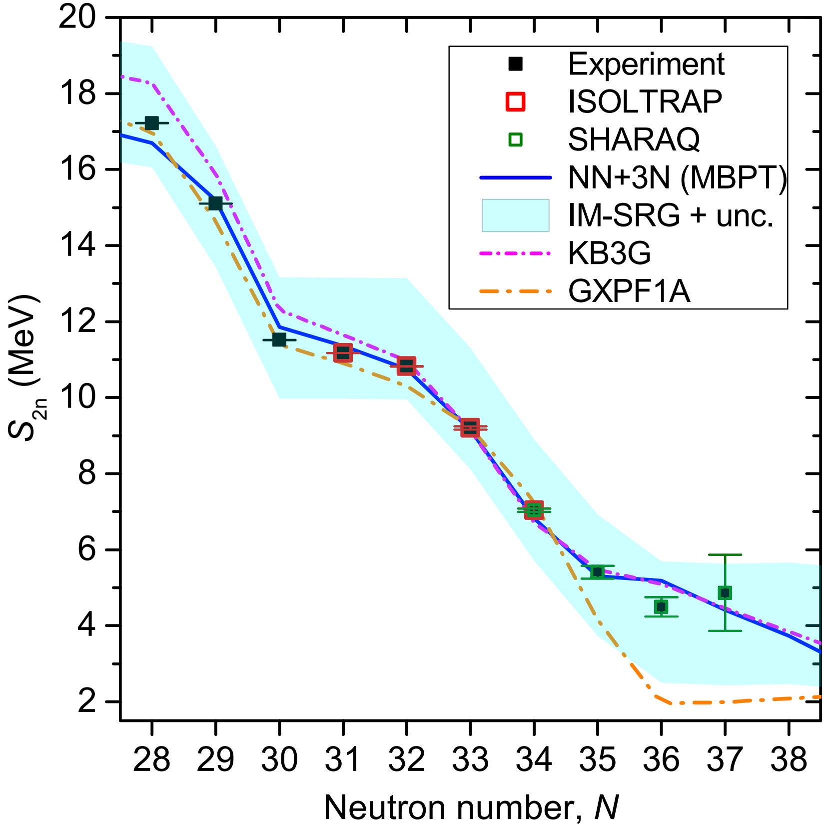
global ab initio calculations, but limited uncertainty estimate for NN+3N

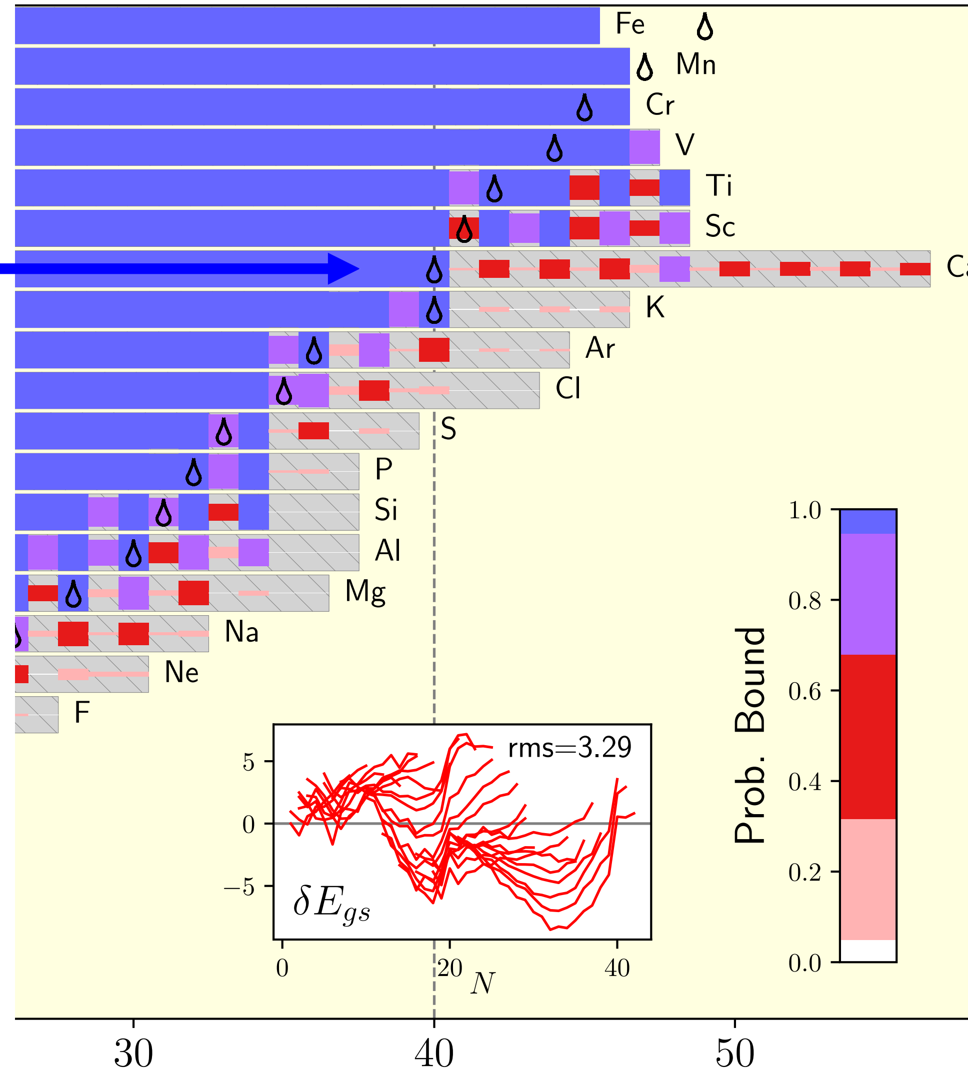
Neutron-rich calcium masses

active exp-theory collaborations for rare isotopes

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

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



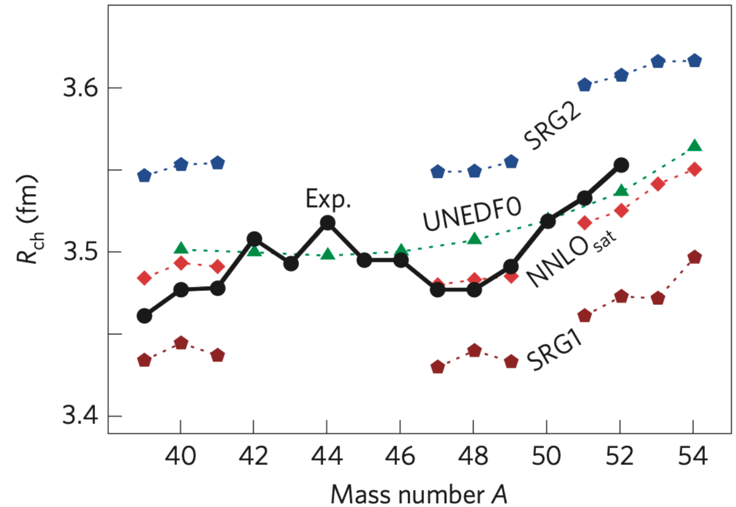


^{52}Ca-^{48}Ca radius puzzle

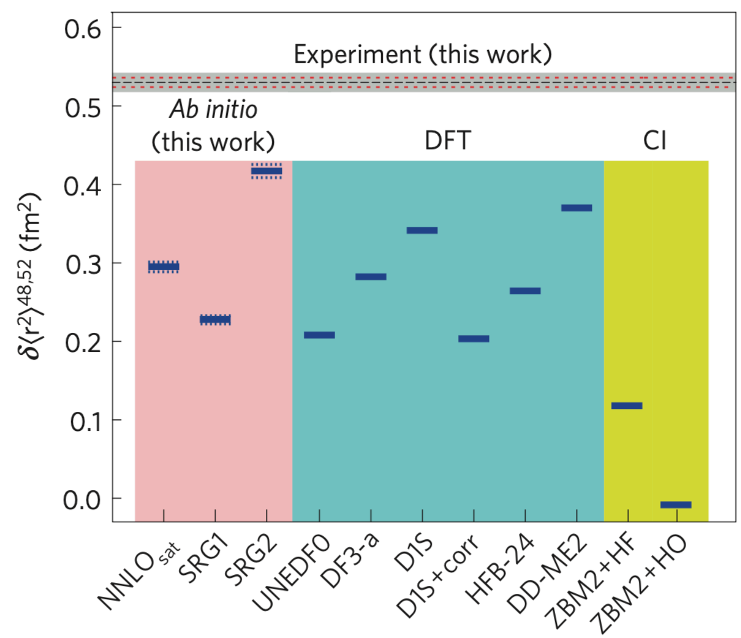
nature physics | ARTICLES
PUBLISHED ONLINE: 8 FEBRUARY 2016 | DOI: 10.1038/NPHYS3645

Unexpectedly large charge radii of neutron-rich calcium isotopes

R. F. Garcia Ruiz[1]*, M. L. Bissell[1,2], K. Blaum[3], A. Ekström[4,5], N. Frömmgen[6], G. Hagen[4], M. Hammen[6], K. Hebeler[7,8], J. D. Holt[9], G. R. Jansen[4,5], M. Kowalska[10], K. Kreim[3], W. Nazarewicz[4,11,12], R. Neugart[3,6], G. Neyens[1], W. Nörtershäuser[6,7], T. Papenbrock[4,5], J. Papuga[1], A. Schwenk[3,7,8], J. Simonis[7,8], K. A. Wendt[4,5] and D. T. Yordanov[3,13]



Challenging to reproduce large charge radius increase from ^{48}Ca to ^{52}Ca with ab initio calculations



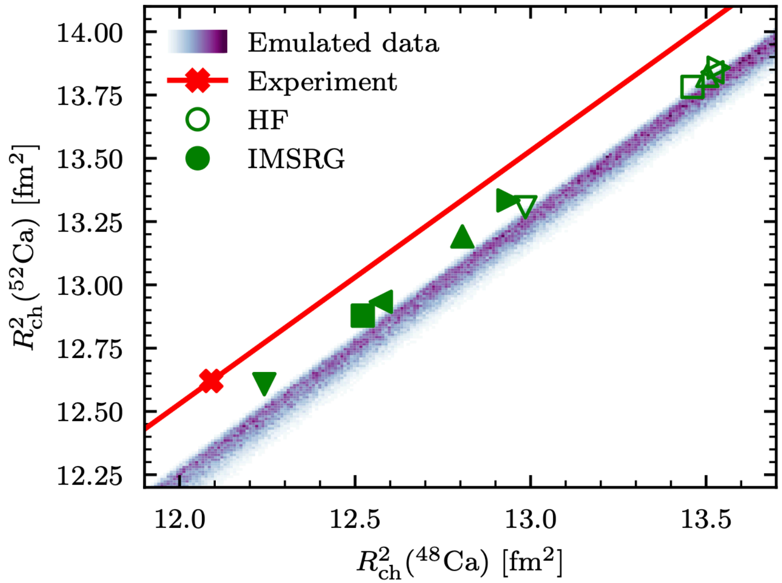
Challenge: Uncertainties greatly reduced in differential, correlated quantities

Possible solutions to the ^{52}Ca-^{48}Ca radius puzzle?

Due to 3N variations?

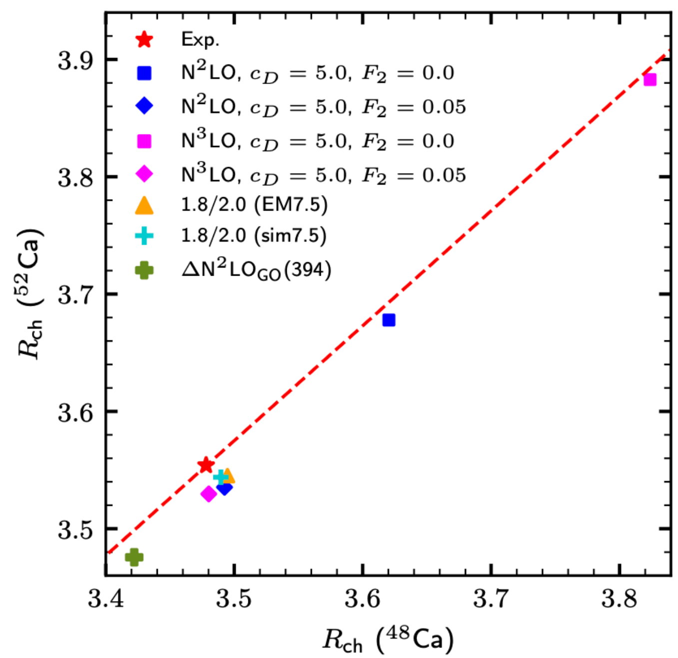
Companys Franzke, Tichai, Hebeler, AS, arXiv:2510.08362

broad variations of c_3, c_4, c_D, c_E also highly correlated, do not solve puzzle



Due to quark mass dependent 3N forces?

Vernik, Hebeler, AS, arXiv:2512.20454

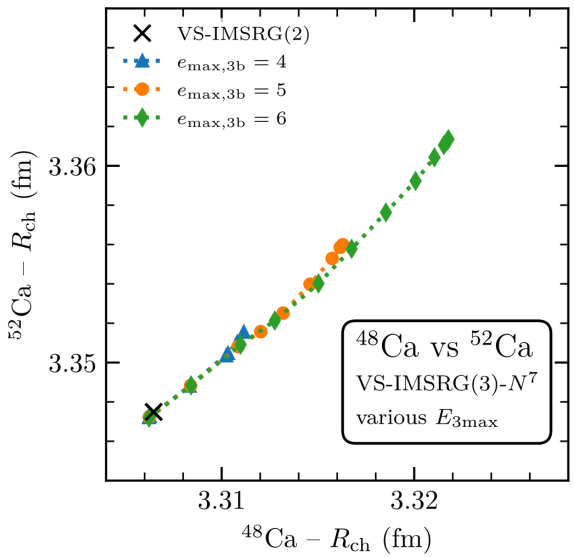


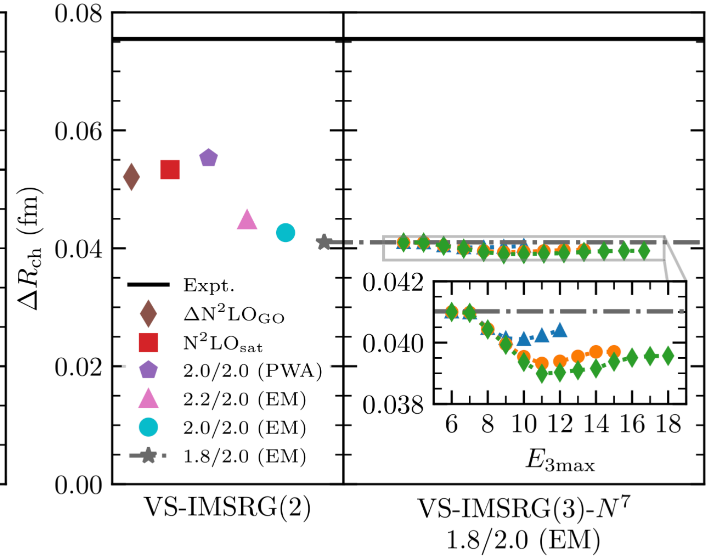
Other NN interactions have so far not solved puzzle either…

Possible solutions to the ^{52}Ca-^{48}Ca radius puzzle?

Due to many-body uncertainties? Heinz et al., PRC (2025)

many-body truncations highly correlated, so change IMSRG(2→3) is very small for radius increase





Remaining many-body possibilities:

- collective many-body correlations beyond IMSRG(3)
- approximations related to reference state
- normal ordering approximation
- …

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Ab initio nuclear masses for r-process nucleosynthesis
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with M. Cincar, Z. Li, T. Plies, U. Vernik, M. Heinz, T. Miyagi, I. Svensson, A. Tichai, K. Hebeler

Nuclear masses around N=82 and r-process nucleosynthesis

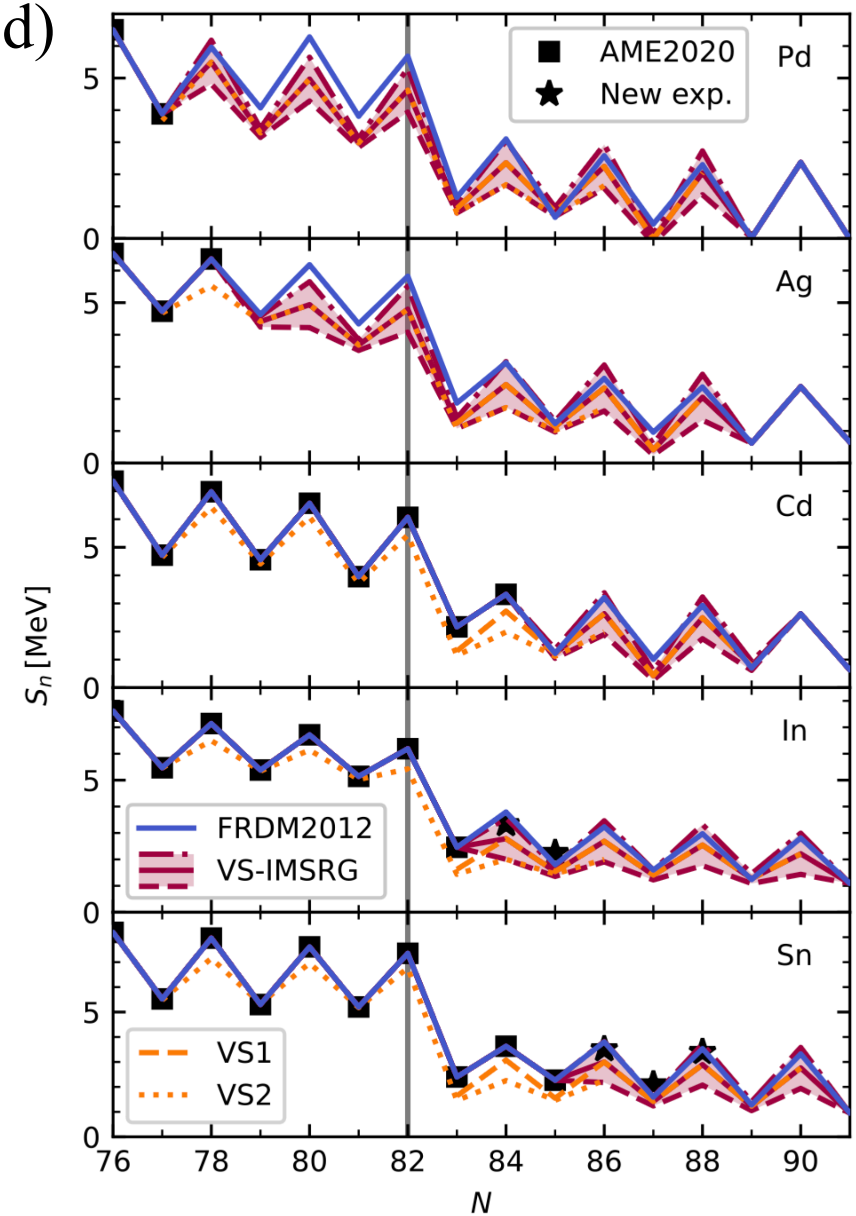
Kuske, Miyagi, Arcones, AS, arXiv:2509.19131

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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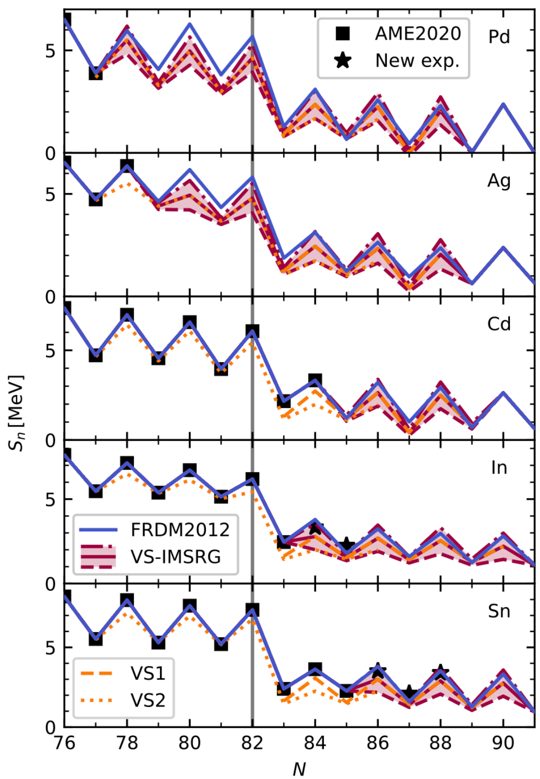
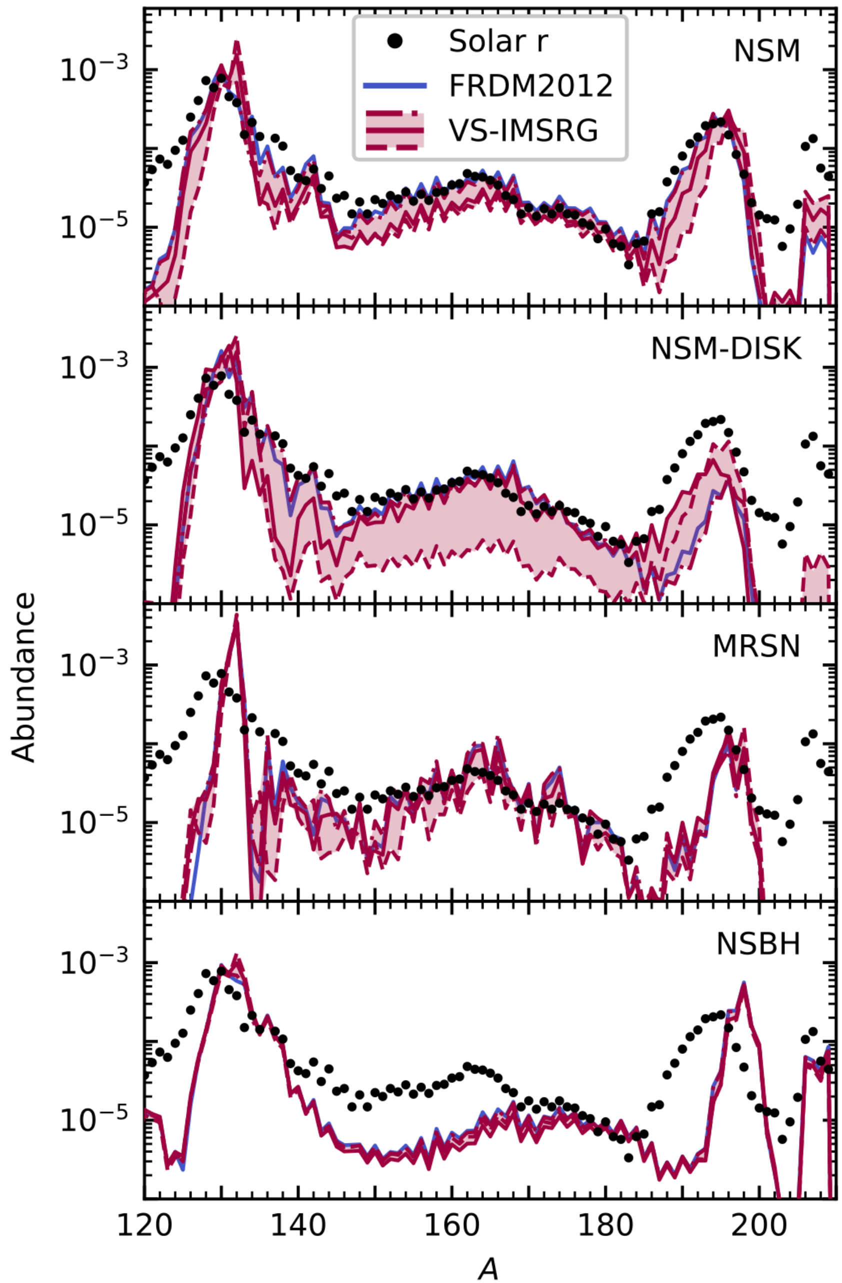
VS-IMSRG masses (min/central/max)

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

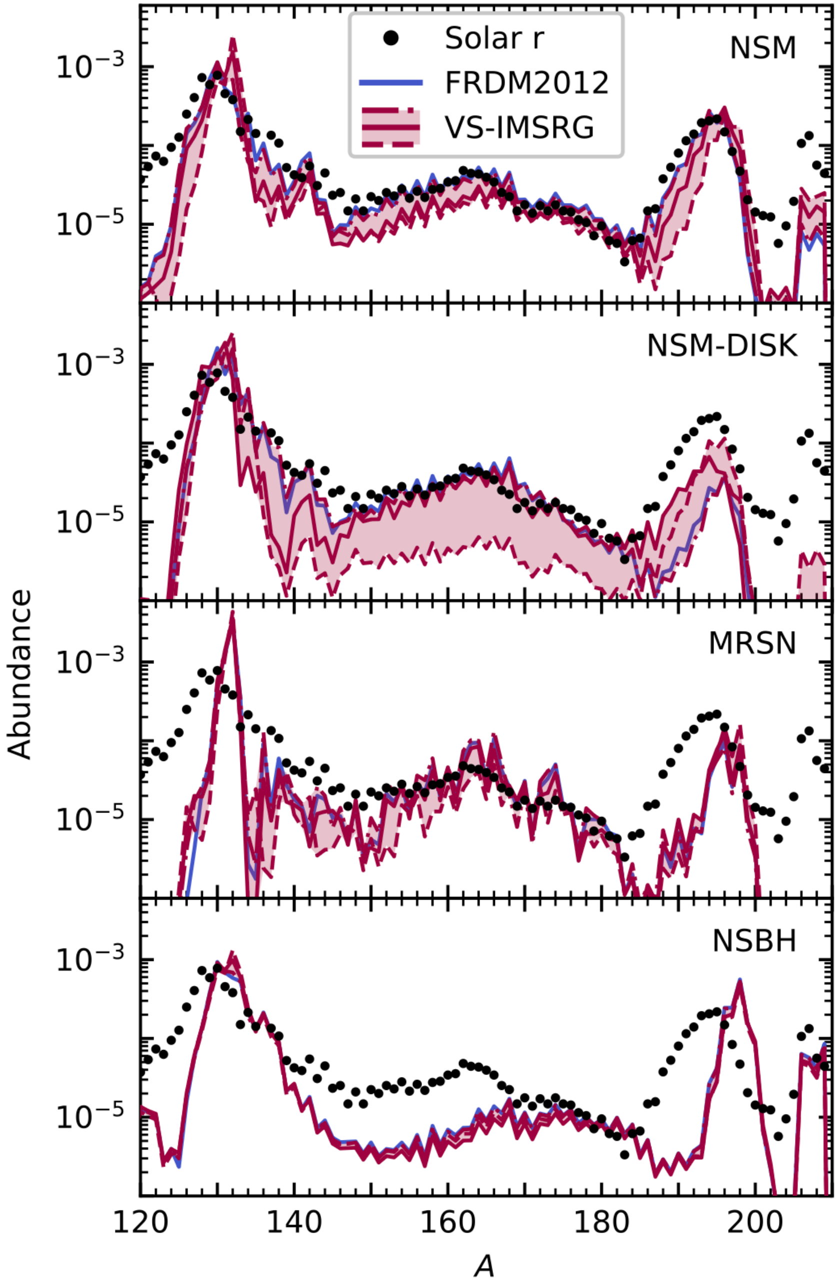
VS-IMSRG masses (min/central/max)
in baseline AME2020 + FRDM2012

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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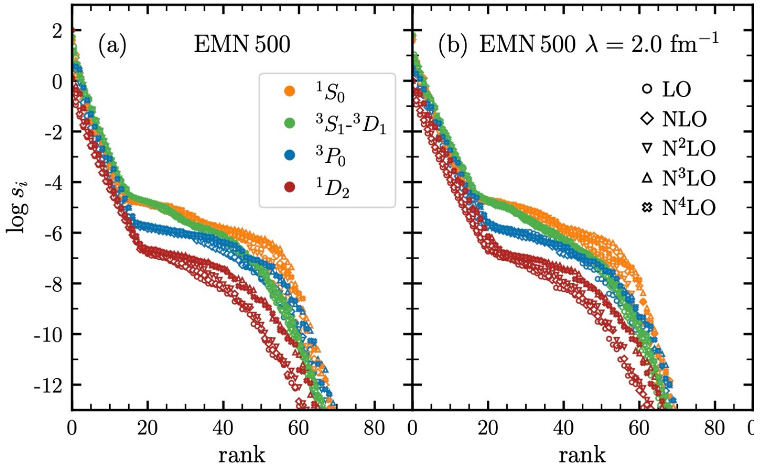
Uncertainty estimates for SRG-evolved interactions

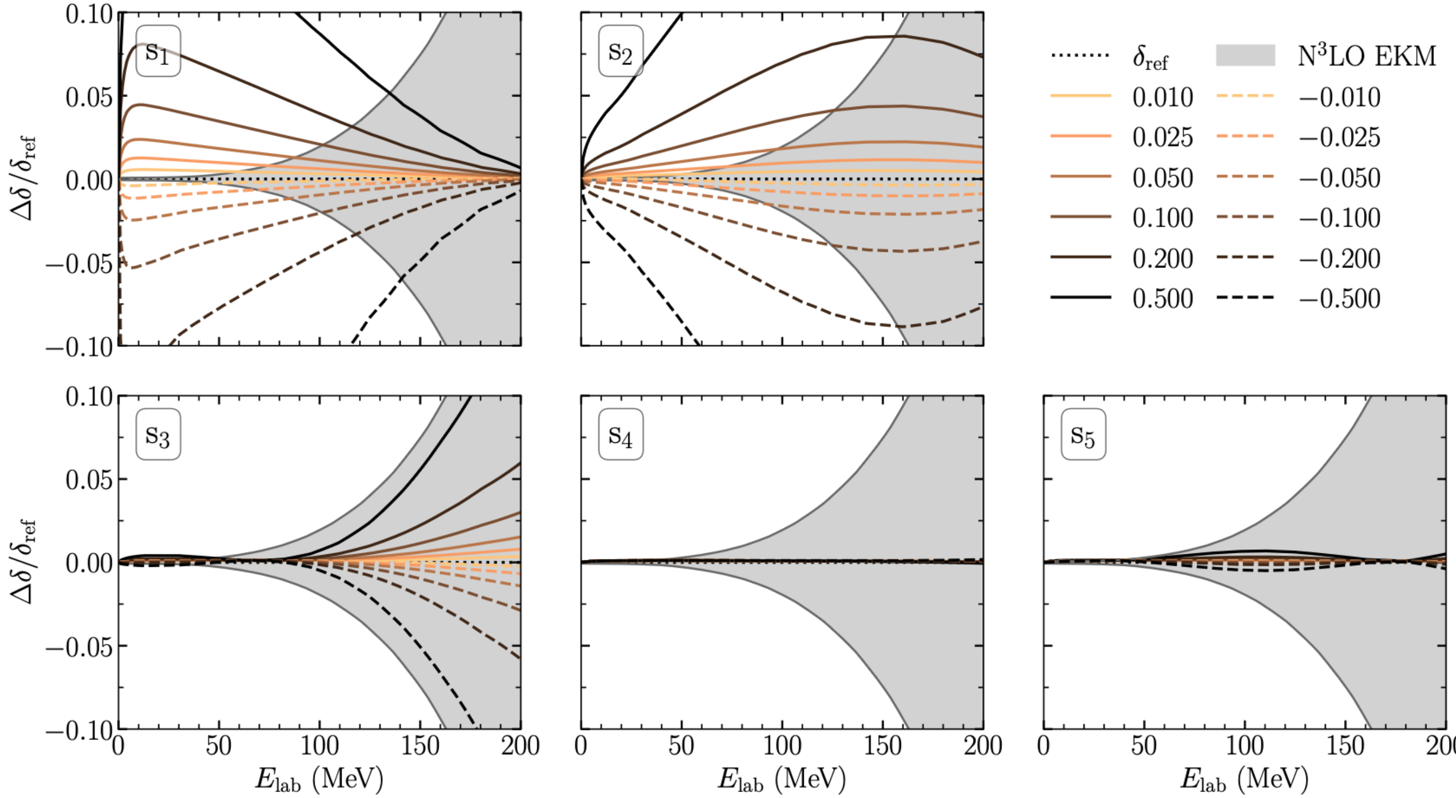
Plies, Heinz, AS, arXiv:2509.24671, see Matthias' talk

use singular value decomposition (SVD) as operator basis see Tichai et al., PLB (2021)

consider largest 5 singular values/operators

effectively 3 generate phase shift variation





Uncertainty estimates for SRG-evolved interactions

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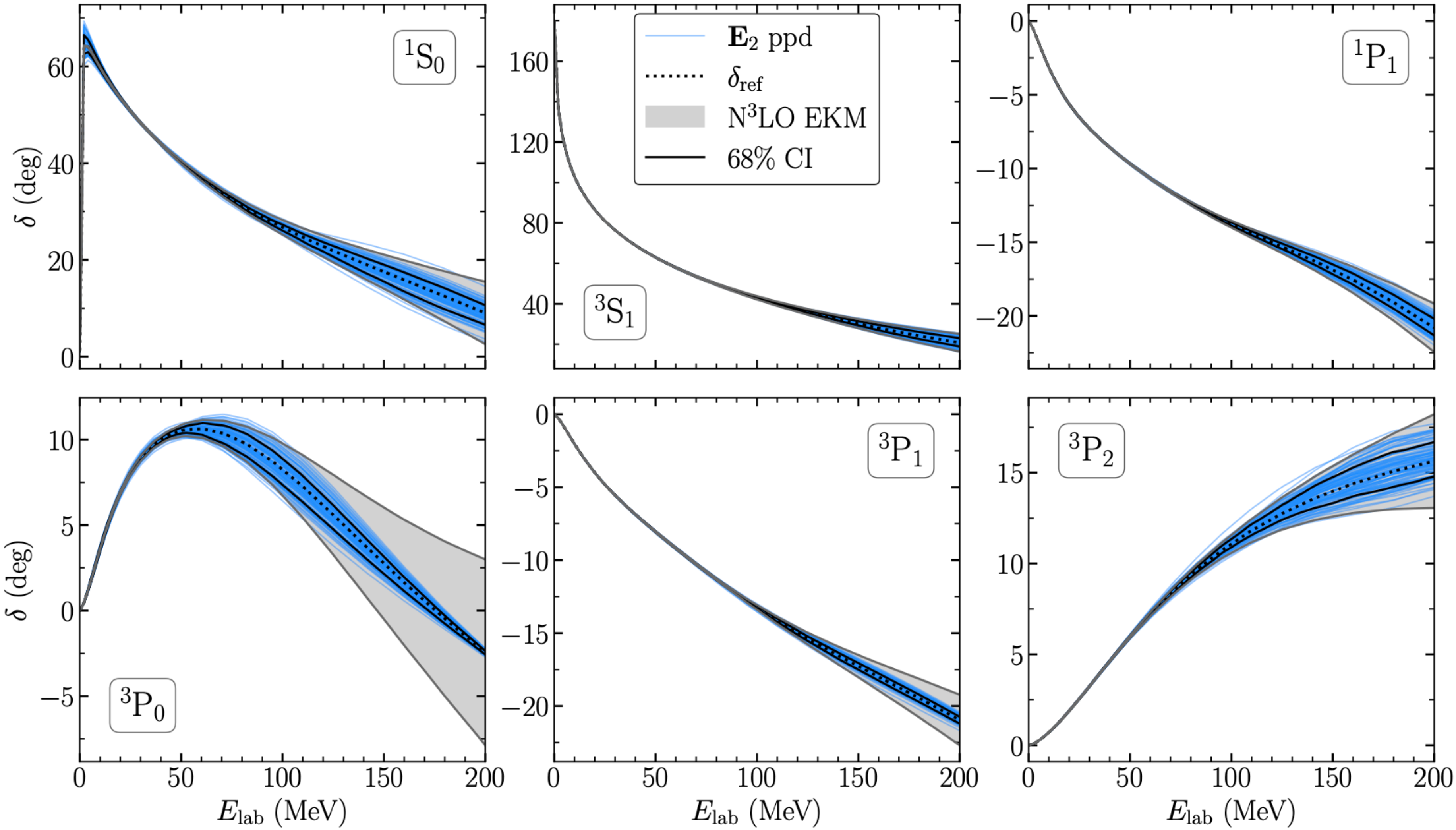
generate range of low-resolution NN interactions from random draws among 3 singular values with likelihood given by EFT uncertainties



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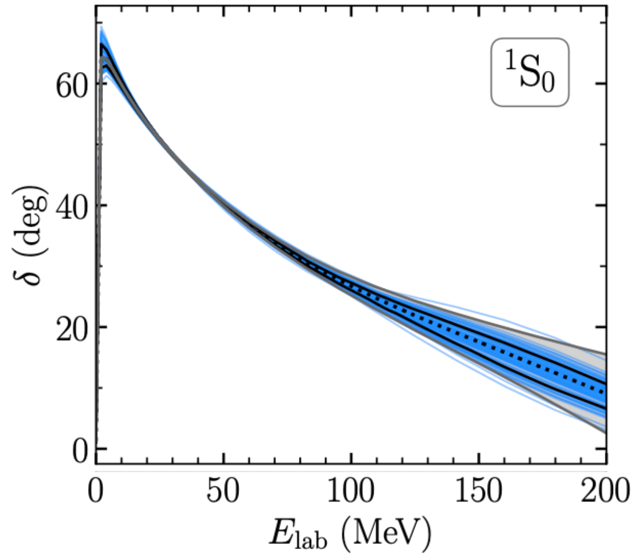
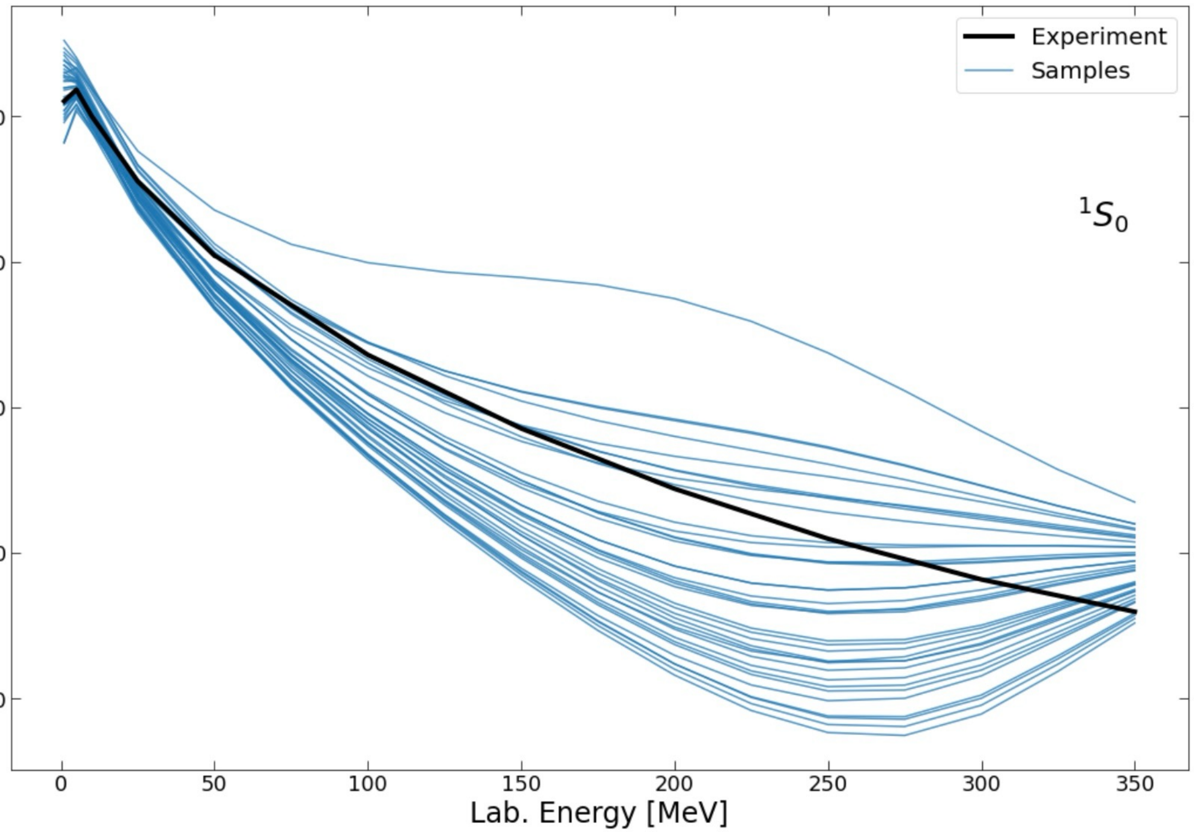




comparison to nonimplausible ΔN^2LO interactions Ekström, Forssen et al.

Uncertainty estimates for SRG-evolved interactions

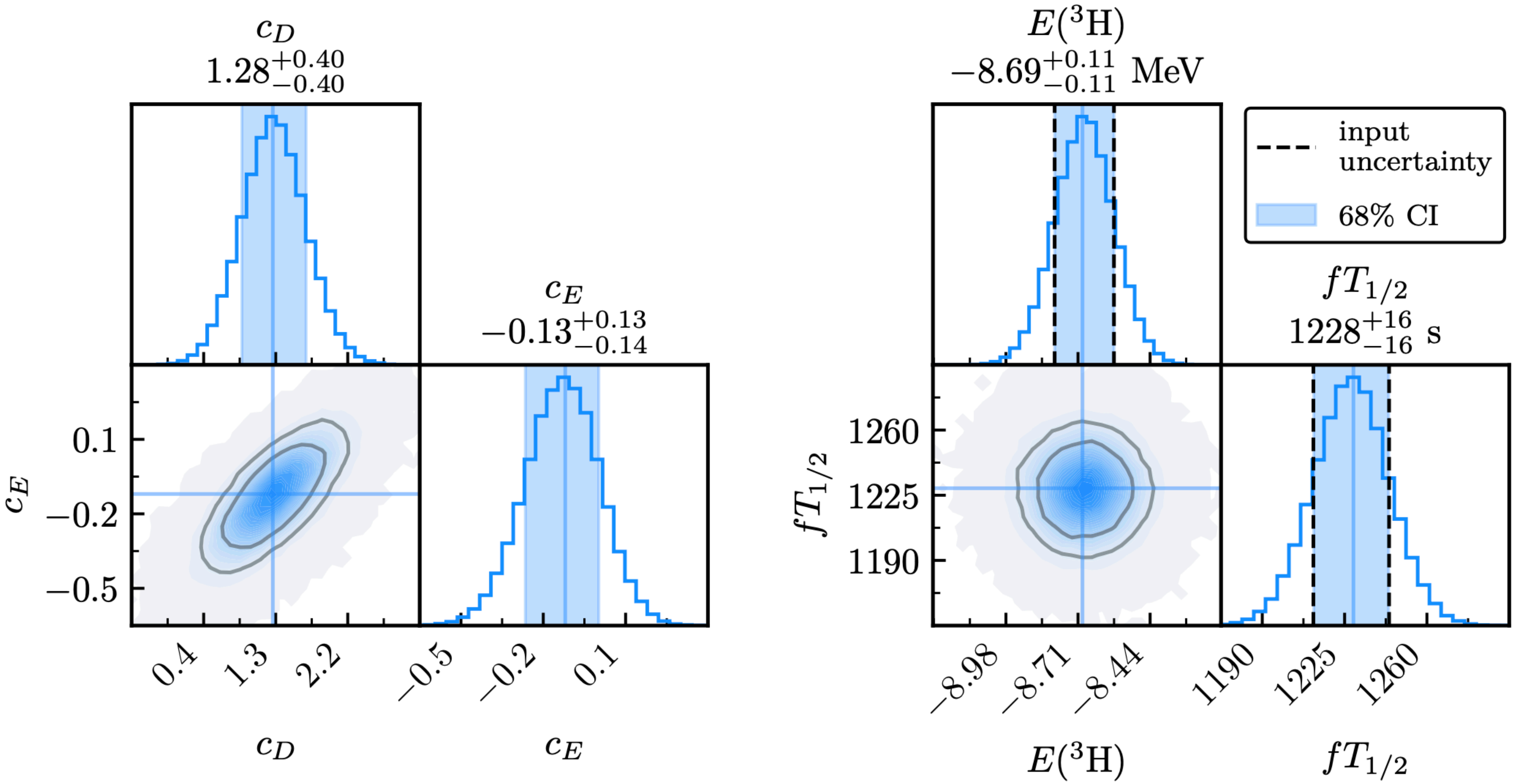
Plies, Heinz, AS, arXiv:2509.24671, see Matthias' talk

generate range of low-resolution NN+3N interactions

NN: S and P waves, higher partial waves unvaried

3N uncertainties from ^{3}H energy and half-life

following Wesolowski, Svensson et al., PRC (2021)



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generate range of low-resolution NN+3N interactions

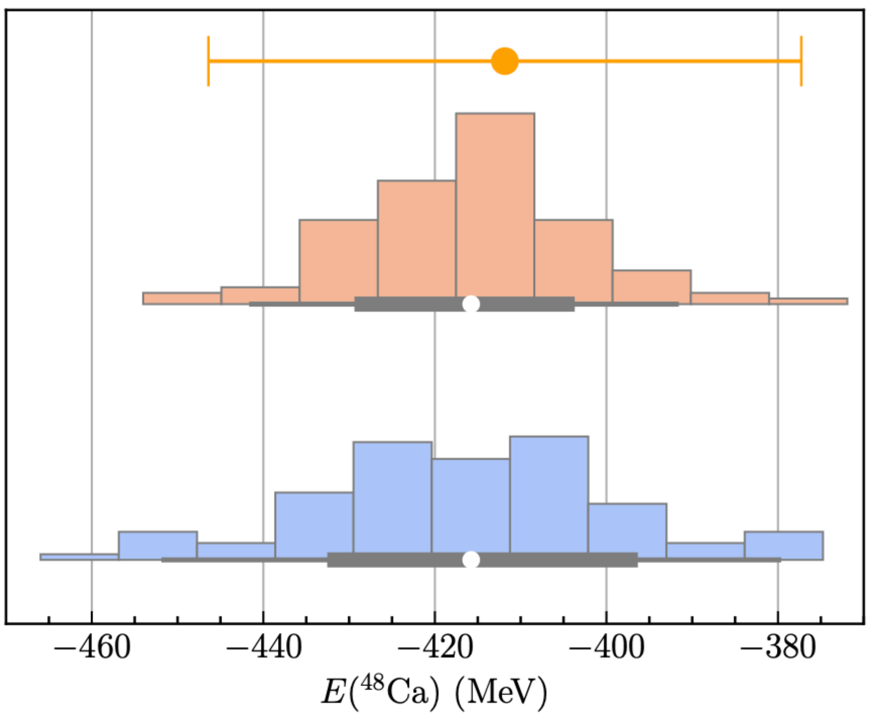
NN: S and P waves, higher partial waves unvaried

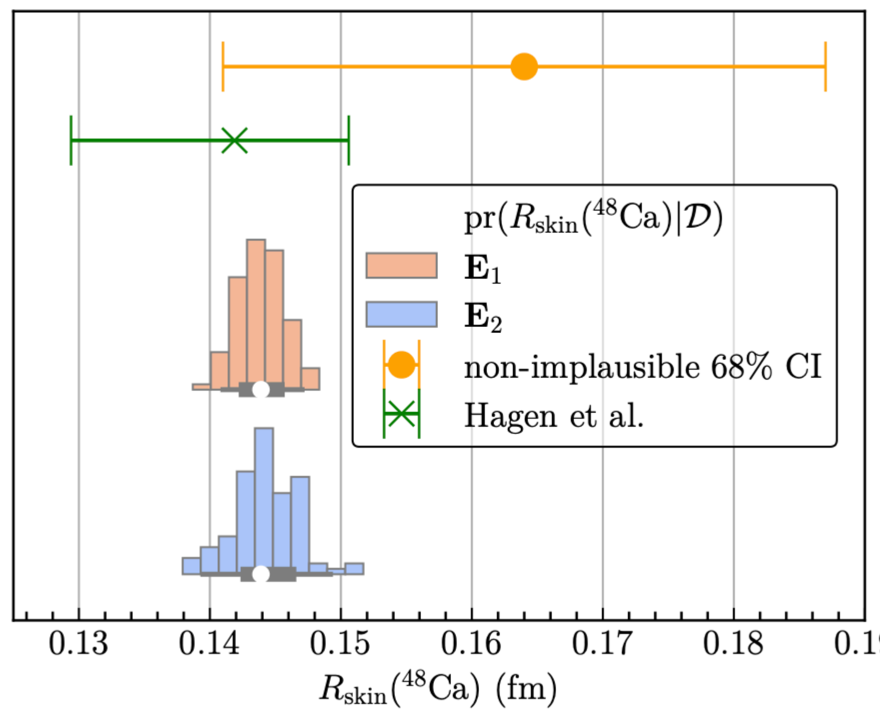
3N uncertainties from ^{3}H energy and half-life

following Wesolowski, Svensson et al., PRC (2021)

resulting posterior distributions for ^{48}Ca energy and neutron skin

Note: no explicit statistical model for truncation uncertainties included





Correlated mass model for calcium isotopes

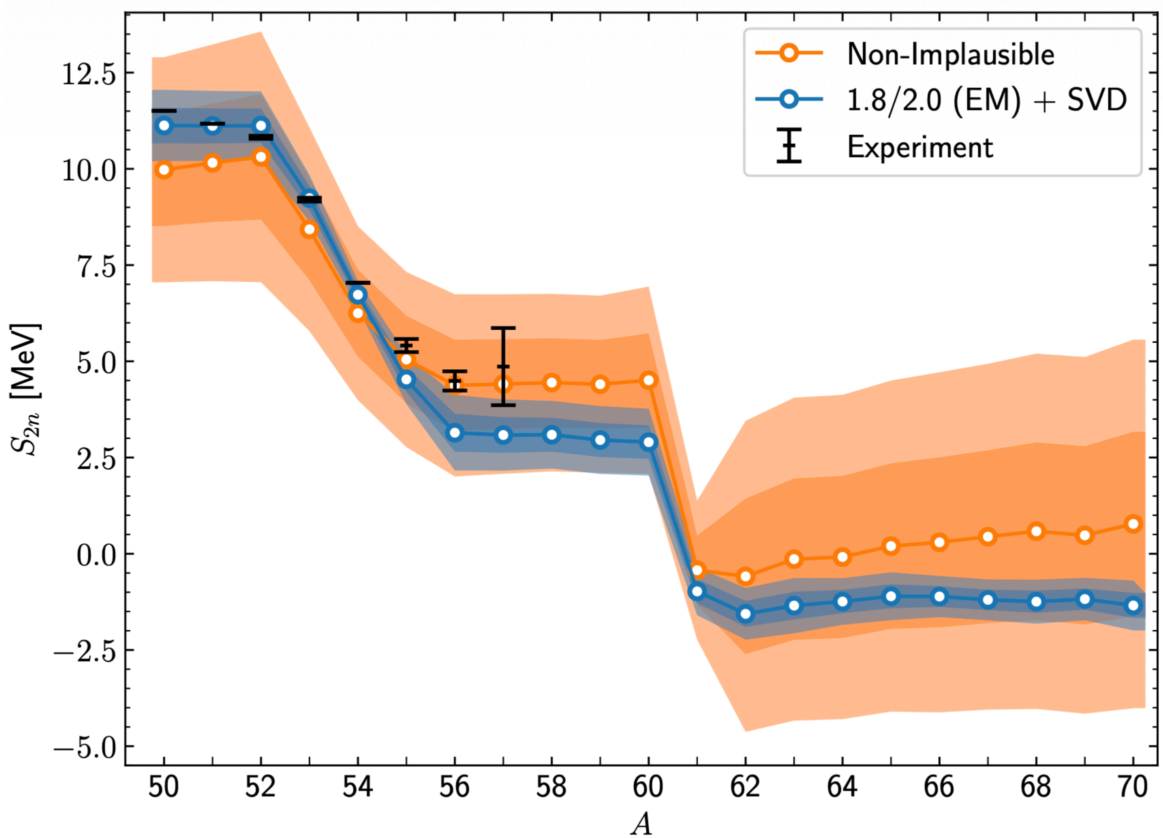
Cincar, Li, Plies, Vernik, Heinz, Miyagi, AS, in prep.

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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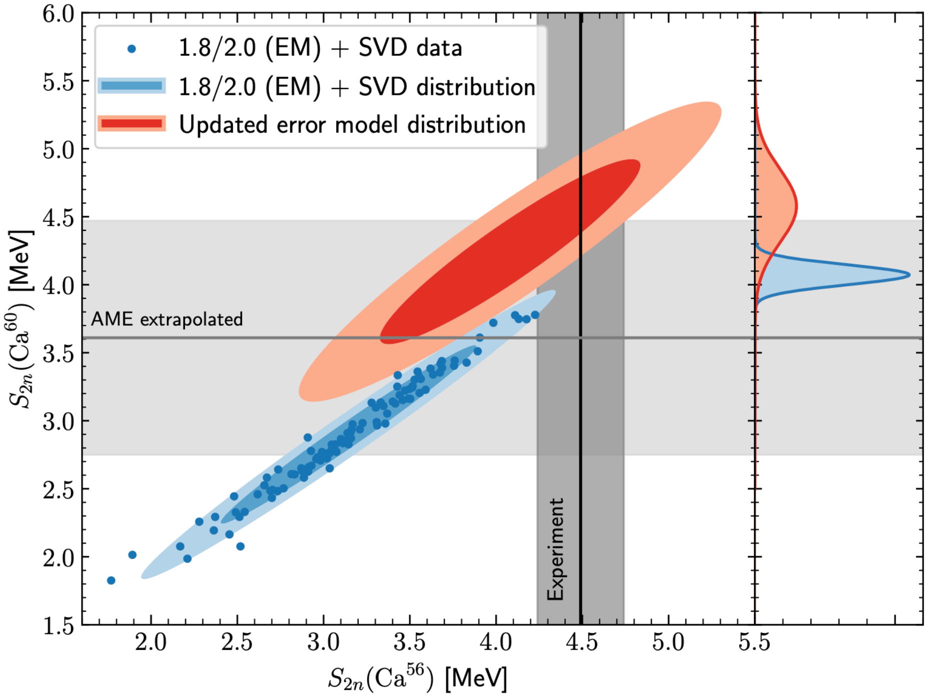
Start from interaction distributions: 34 NI, 101 SVD interactions

Include other uncertainties from:
(assume ind. normally distr.)

- Many-body IMSRG(2, 3f2)
- Model space
- Systematic uncertainties



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

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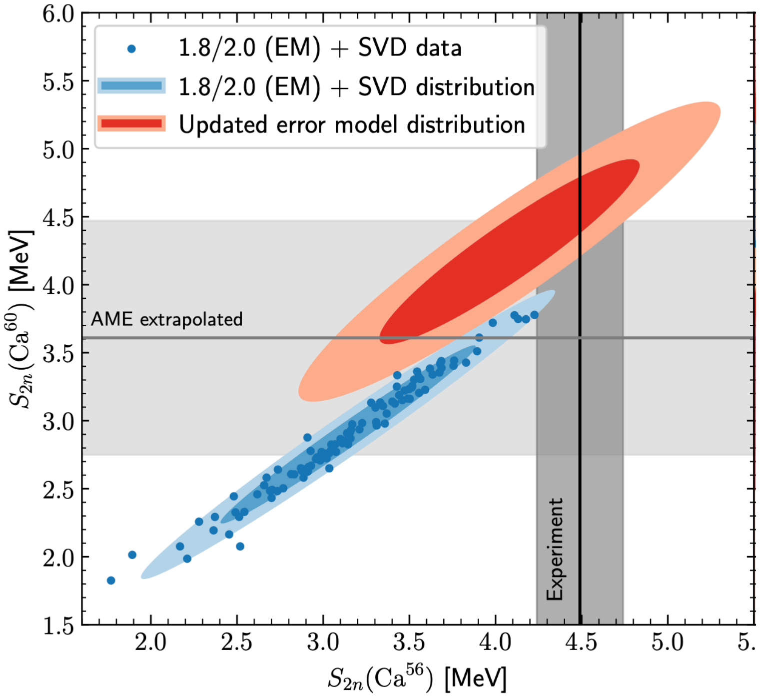
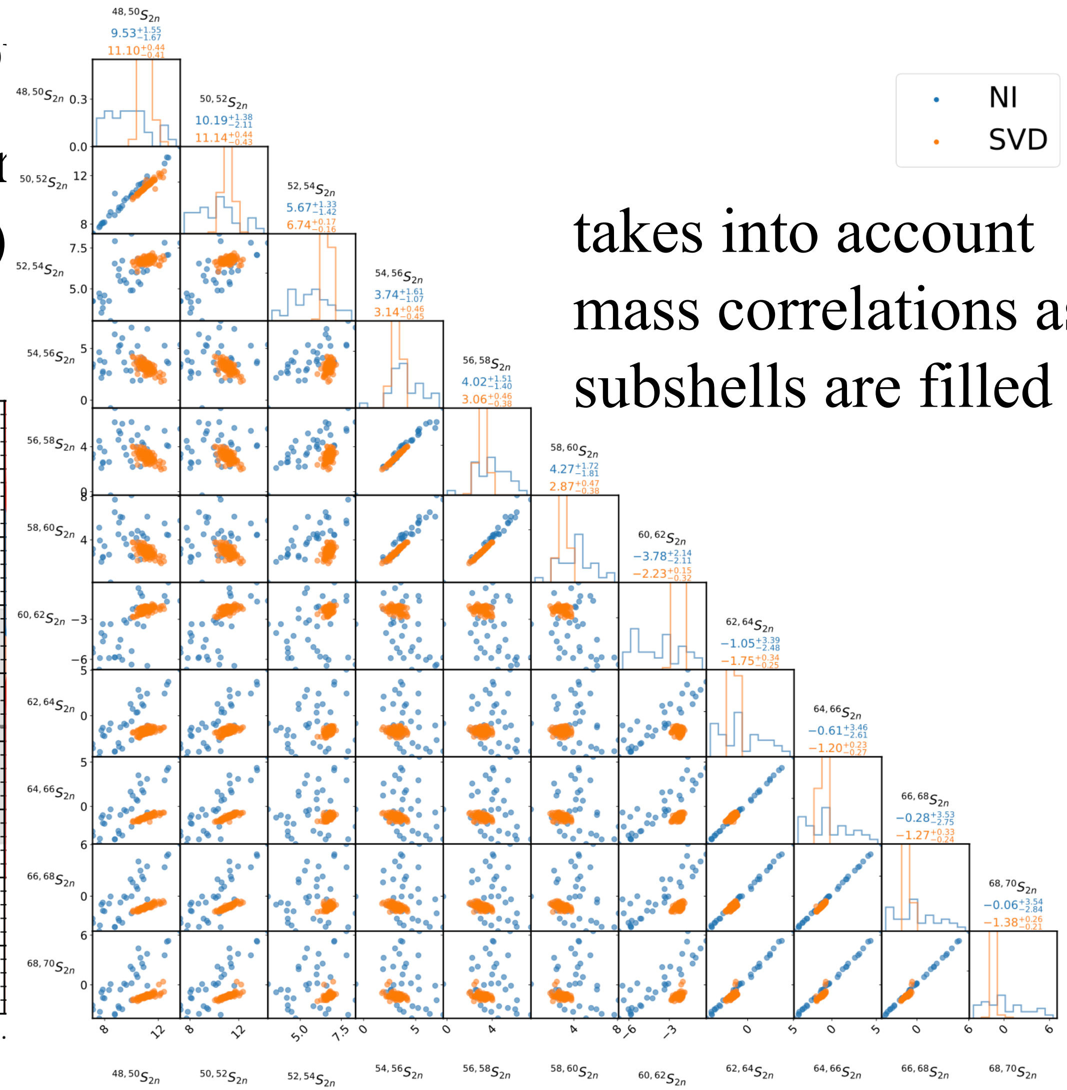




takes into account mass correlations as subshells are filled

Correlated mass model for calcium isotopes

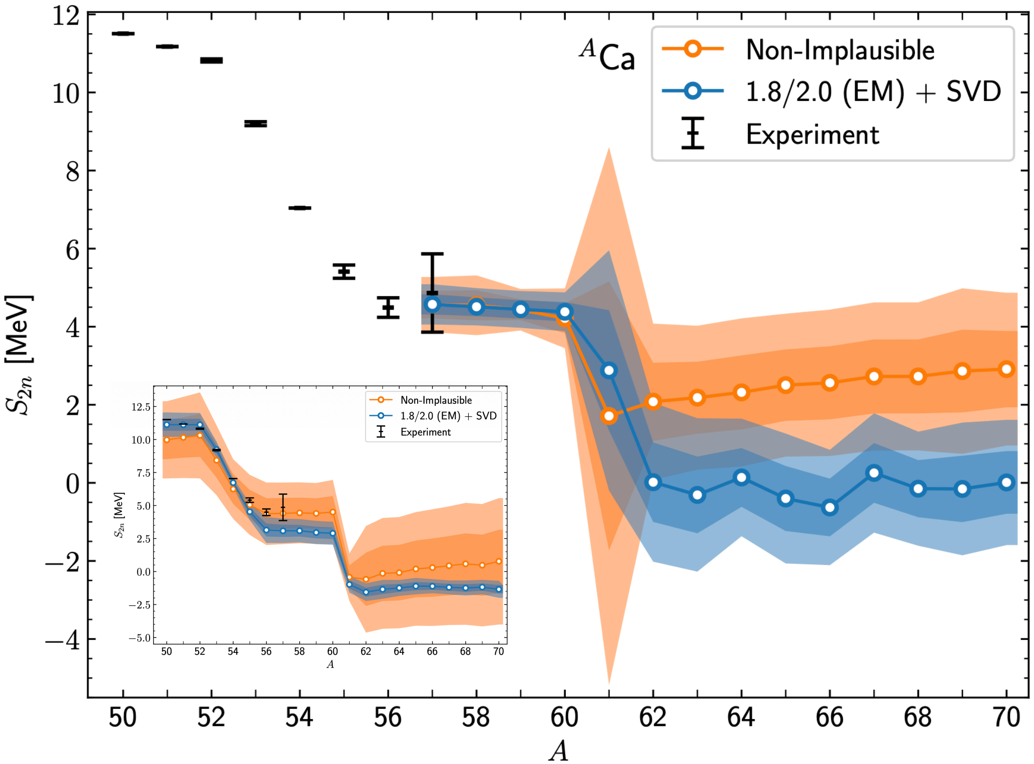
Cincar, Li, Plies, Vernik, Heinz, Miyagi, AS, in prep.

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

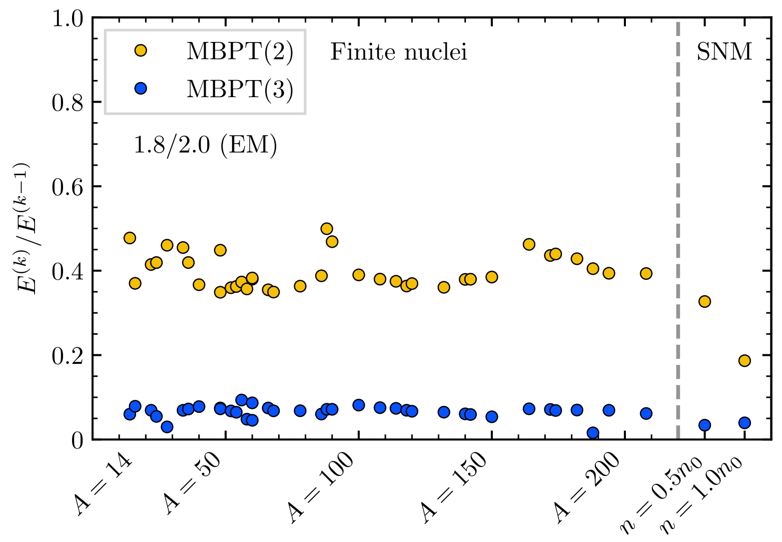
Many-body truncation uncertainties

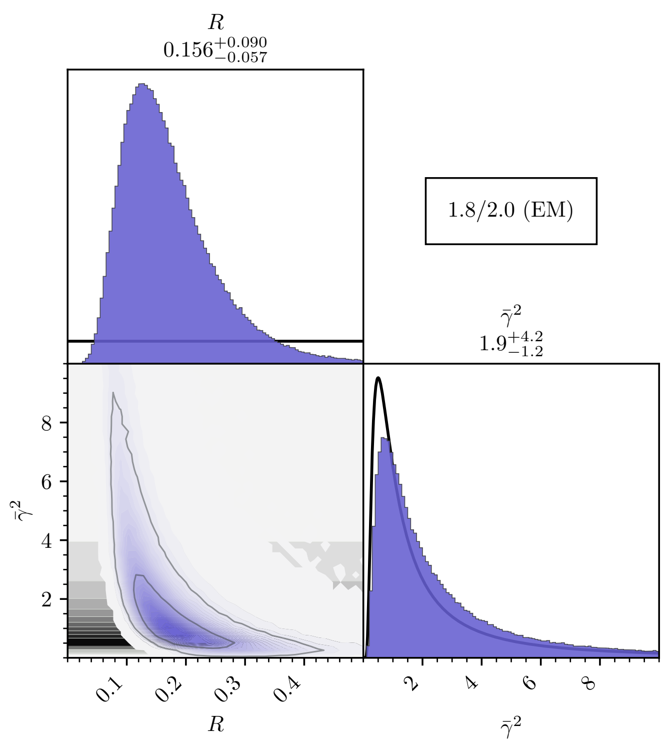
Svensson, Tichai, Hebeler, AS, PRC (2025)

idea: use BUQEYE error model for MBPT expansion

$$E_0 = \underbrace{E_{\text{ref}}\gamma_0}_{E_{\text{HF}}} + \underbrace{E_{\text{ref}}\gamma_1 R^1}_{\text{MBPT(2)}} + \underbrace{E_{\text{ref}}\gamma_2 R^2}_{\text{MBPT(3)}} + \ldots$$

Bayesian inference of ratio R and variance of γ_i from 3 nuclei





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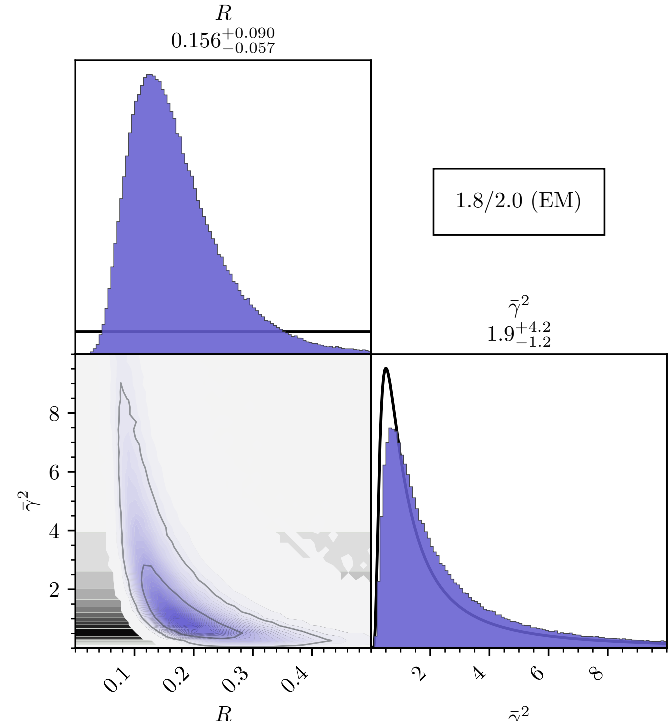
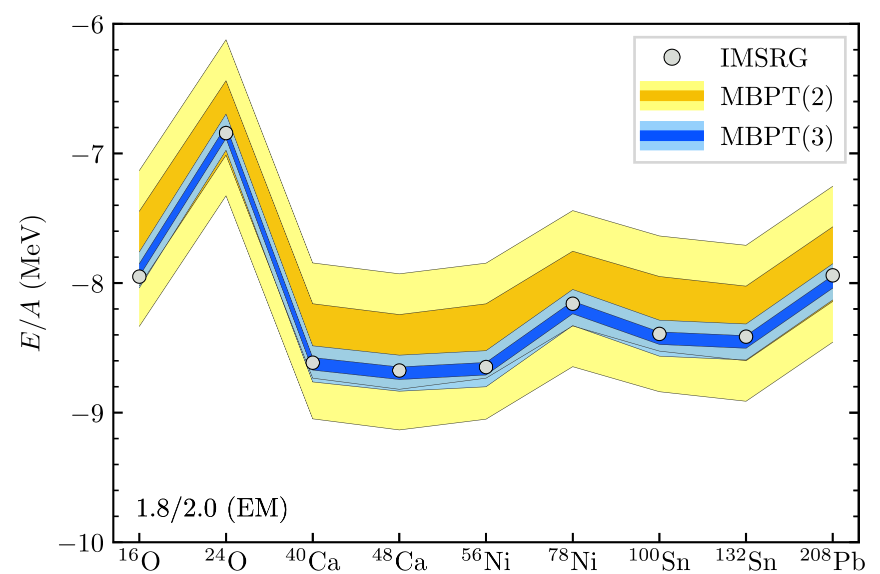


Bayesian inference of ratio R and variance of γ_i from 3 nuclei

posterior distributions at different orders

good agreement with IMSRG(2)

enables many-body uncertainty estimates beyond expert assessment



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I. Svensson, A. Tichai, K. Hebeler

Next generation NN+3N interactions: Wish list

- Low resolution enough for converged calculations up to ^{208}Pb
- Order-by-order interactions amenable to UQ,
at least two orders with 3N
- Interactions for different cutoffs/schemes
- Good description of NN and A=3,4 systems
- Pion-full: leading two-body currents are parameter-free,
3-neutron interactions parameter-free up to N^3LO
- Reasonable saturation properties (informed by matter/nuclei),
reasonable saturation density at HF level?