Ab initio calculations of nuclei and nuclear matter

Achim Schwenk

TECHNISCHE UNIVERSITÄT DARMSTADT

EMMI

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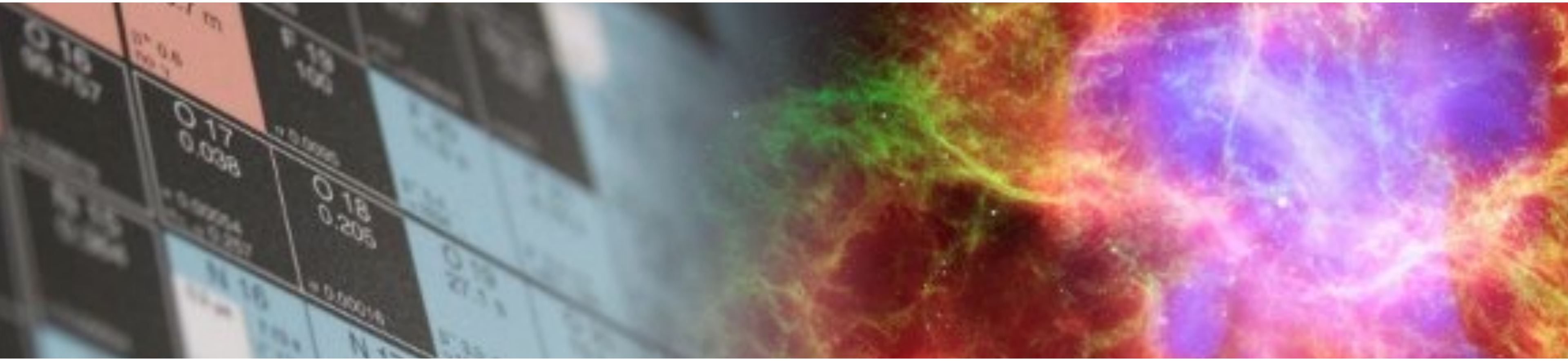

"Next generation ab initio nuclear theory", ECT*, July 16, 2025

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Hessens Zukunft

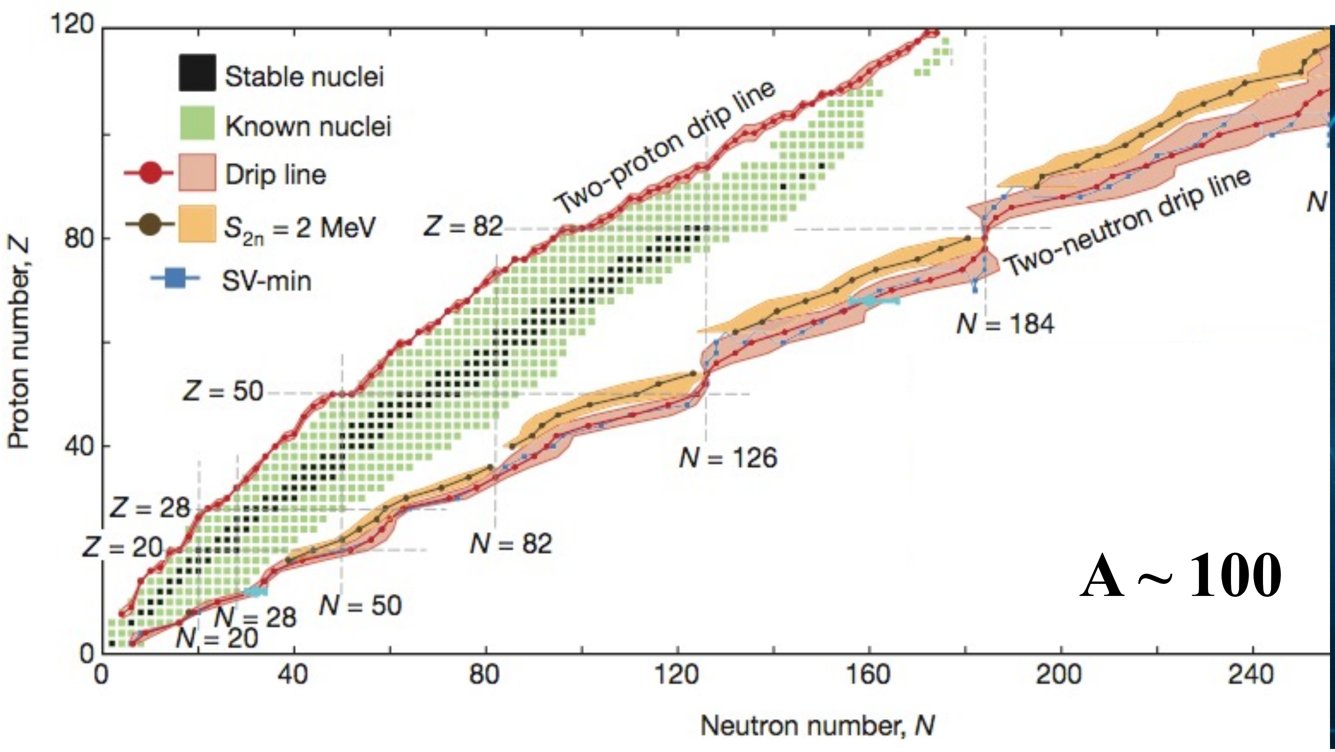
Structure of nuclei and dense matter in neutron stars

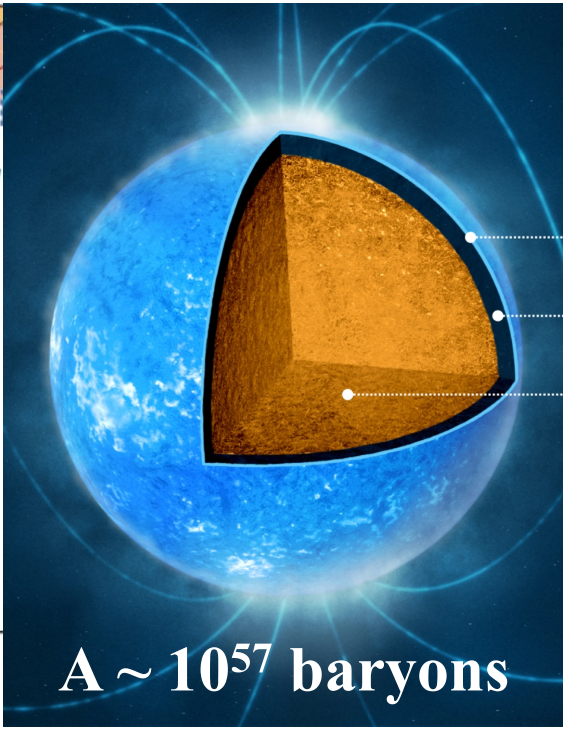
doi:10.1038/nature11188

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

Challenges

Next generation NN+3N interactions up to heavy nuclei: status and wish list P. Arthuis, K. Hebeler, T. Plies, I. Svensson, U. Vernik

Uncertainty quantification for medium-mass nuclei
M. Companys, M. Heinz, T. Plies, I. Svensson, A. Tichai, K. Hebeler

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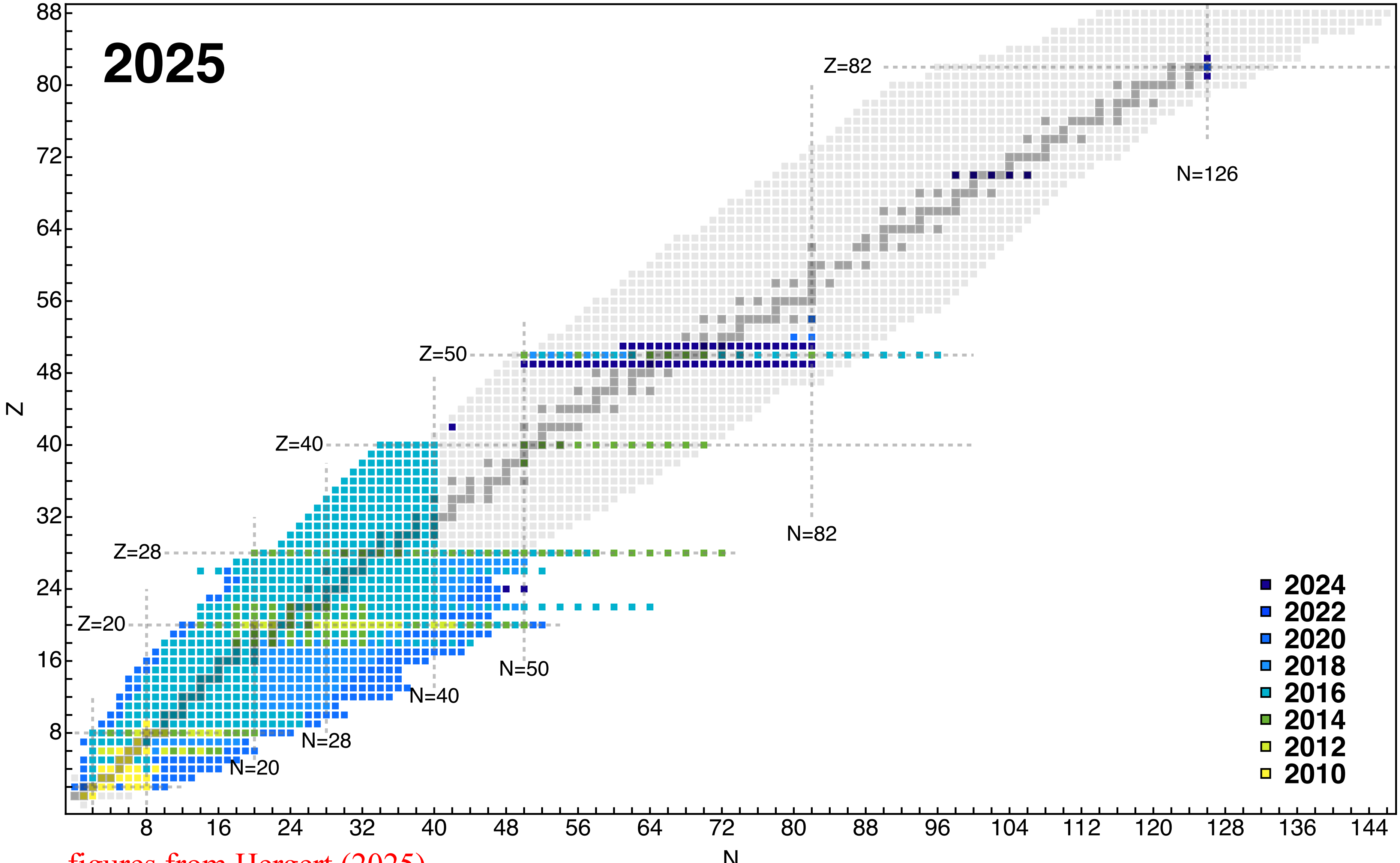
Great progress in ab initio calculations of nuclei

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,‖]
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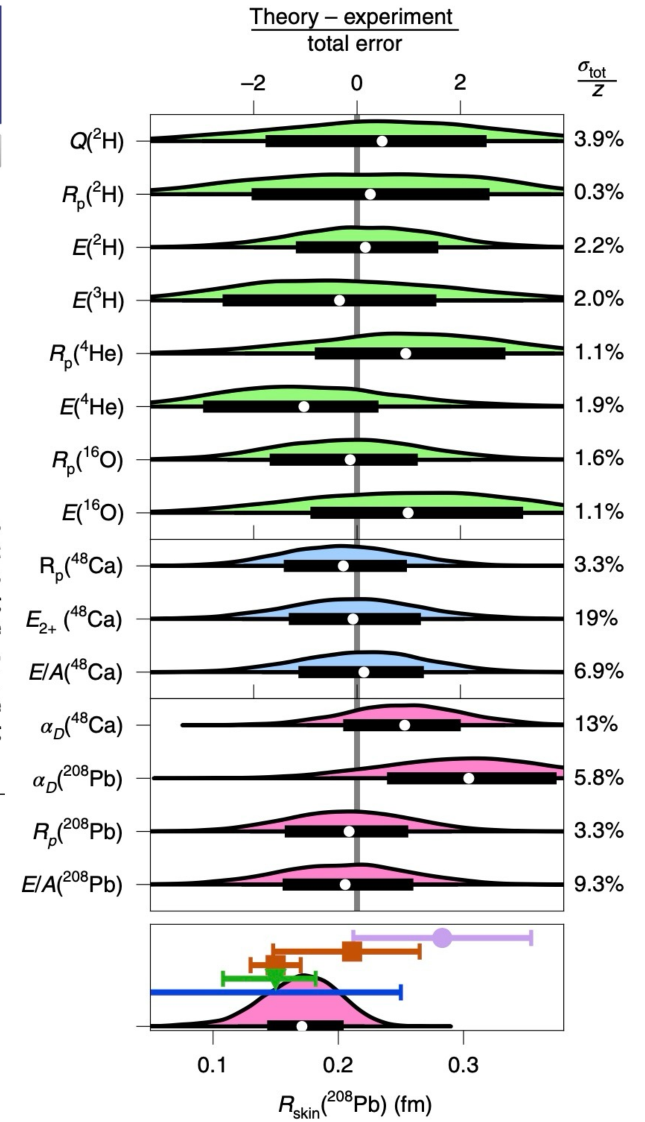
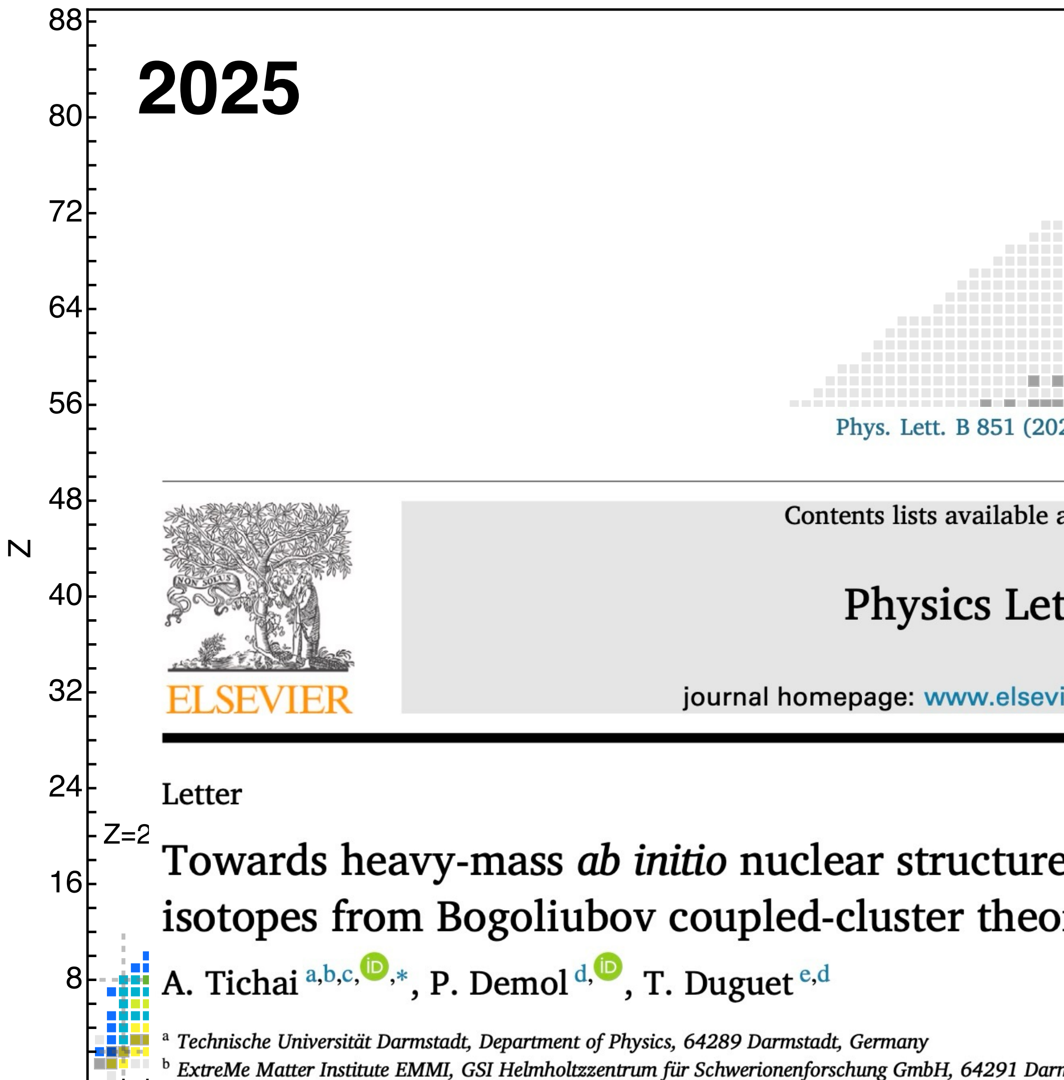
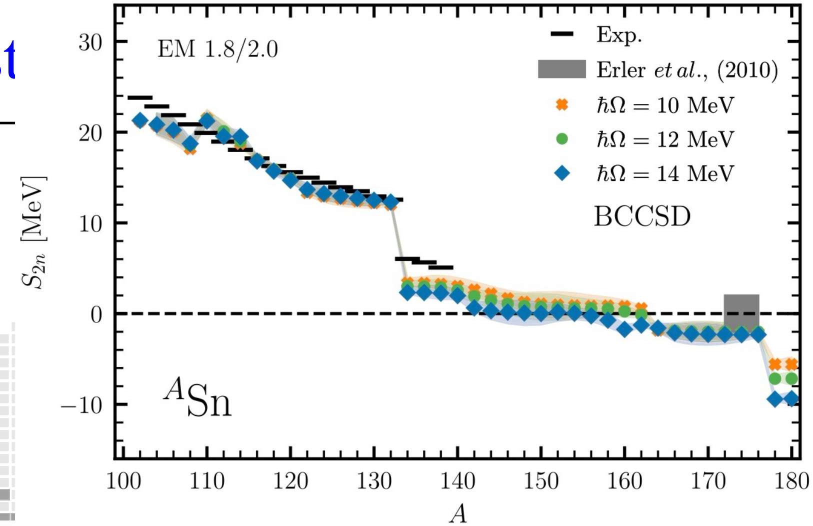
[2]*Department of Physics, University of Washington, Seattle, Washington 98195, USA*
[3]*Technische Universität Darmstadt, 64289 Darmstadt, Germany*
[4]*ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*
[5]*Max-Planck-Institut für Kernphysik, 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

systematic interaction expansion + syst





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Letter

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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[b] *ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*
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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,††]

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[2]*ExtreMe Matter Institute EMMI, GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany*
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[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*
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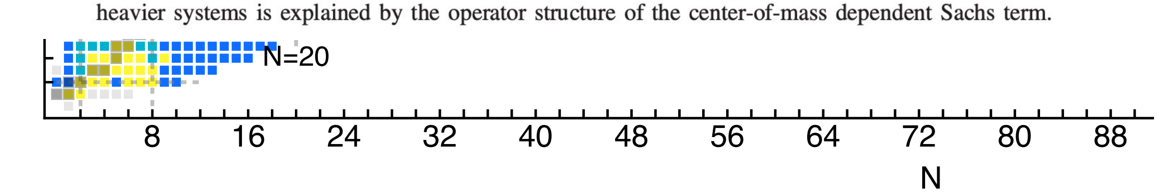
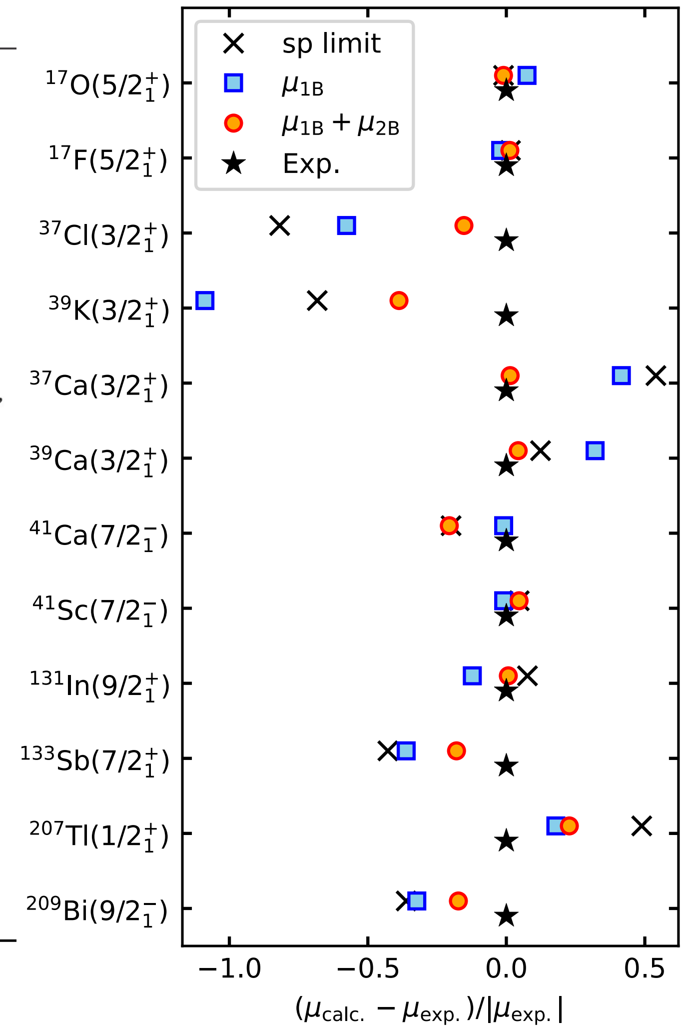
We investigate the effects of two-body currents on magnetic dipole moments of medium-mass and heavy nuclei using the valence-space in-medium similarity renormalization group with chiral effective field theory interactions and currents. Focusing on near doubly magic nuclei from oxygen to bismuth, we have 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

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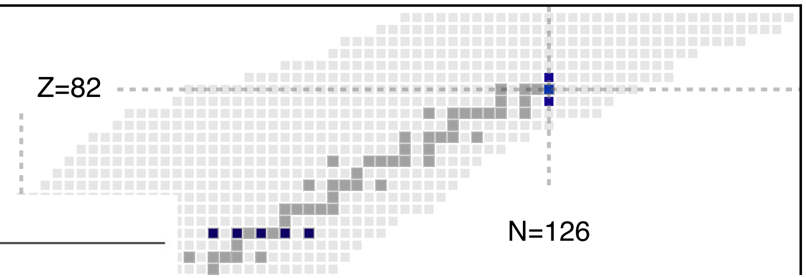
2025



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*
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[8]*Institute of Theoretical Physics, Jagiellonian University, Kraków, 30-348, Poland*
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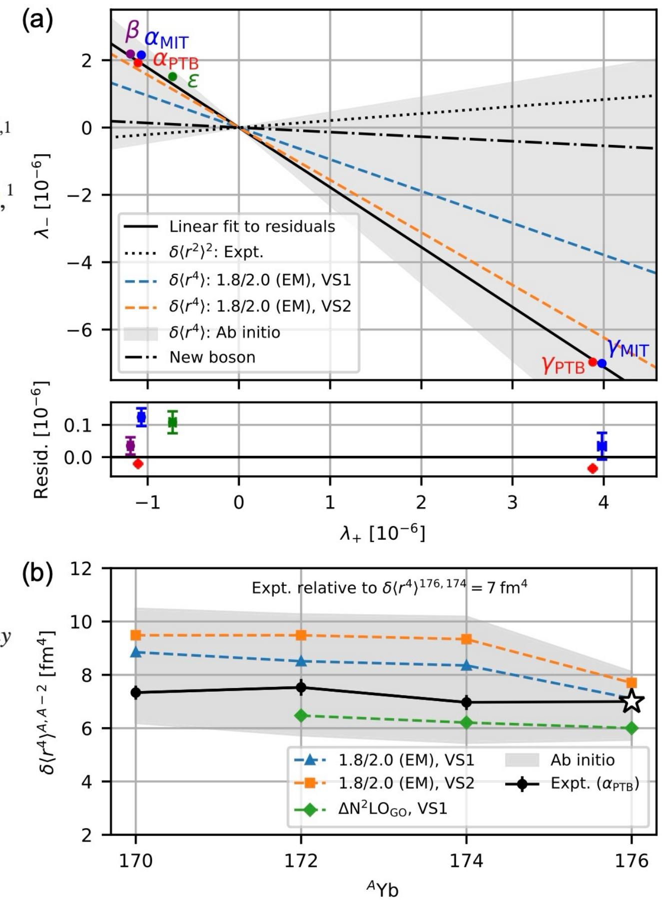
In this Letter, we present mass-ratio measurements on highly charged Yb^{42+} ions with a precision of 4×10^{-12} and isotope-shift measurements on Yb^{+} on the $^2S_{1/2} \rightarrow {}^2D_{5/2}$ and $^2S_{1/2} \rightarrow {}^2F_{7/2}$ transitions with a precision of 4×10^{-9} for the isotopes $^{168,170,172,174,176}Yb$. 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.



Challenges

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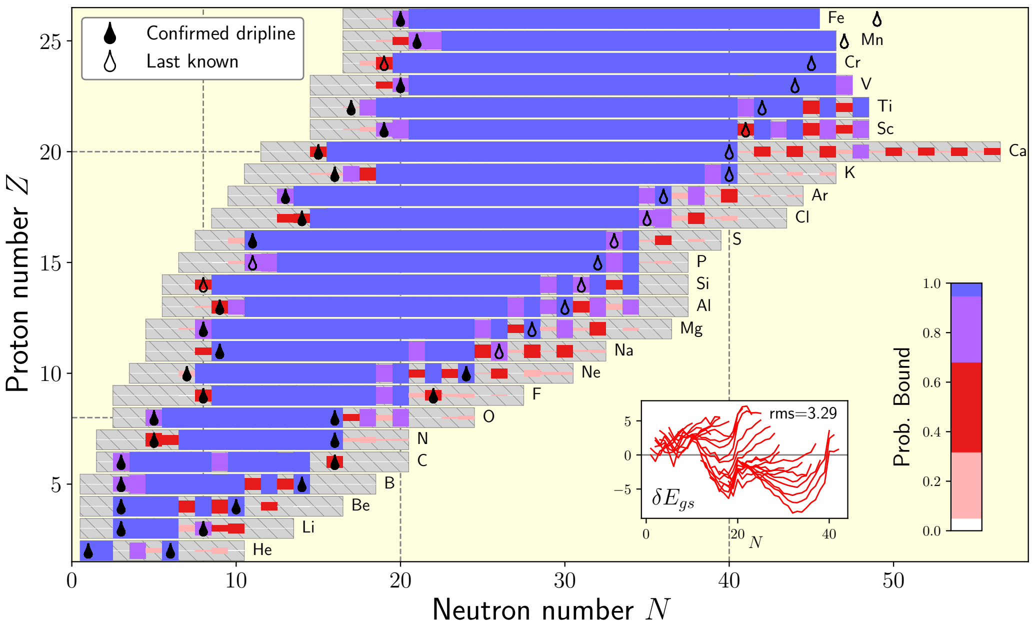
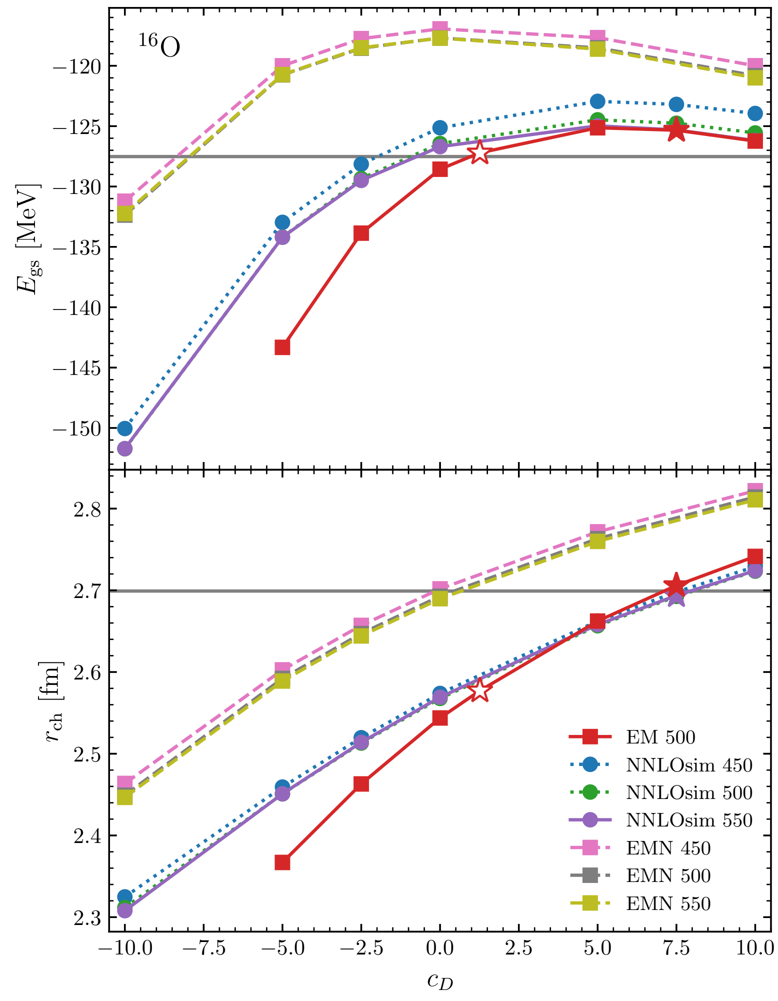
Chiral NN+3N interactions up to ^{208}Pb

only limited families of NN+3N interactions for global ab initio calcs

- magic interaction 1.8/2.0 (EM) Hebeler et al., PRC (2011)
  NN N^{3}LO SRG evolved + 3N N^{2}LO
  fit to ^{3}H energy and ^{4}He radius





- fit to ^{3}H energy and ^{16}O energy/radius
  Arthuis et al., 2401.06675, see Pierre Arthuis' talk

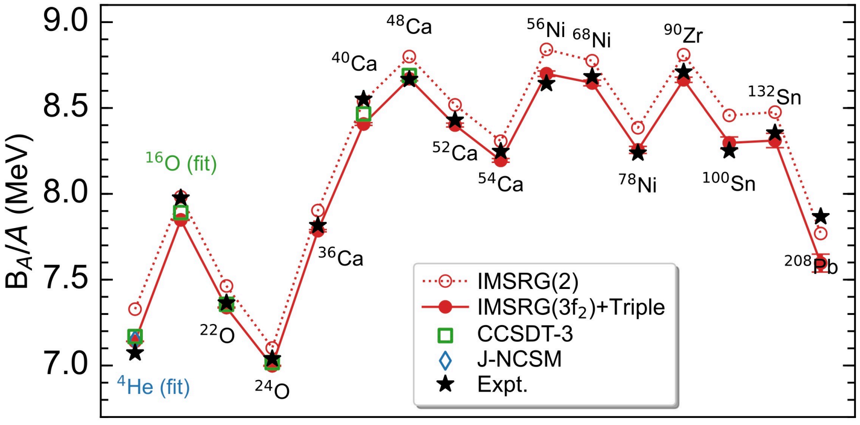
Chiral NN+3N interactions up to ^{208}Pb

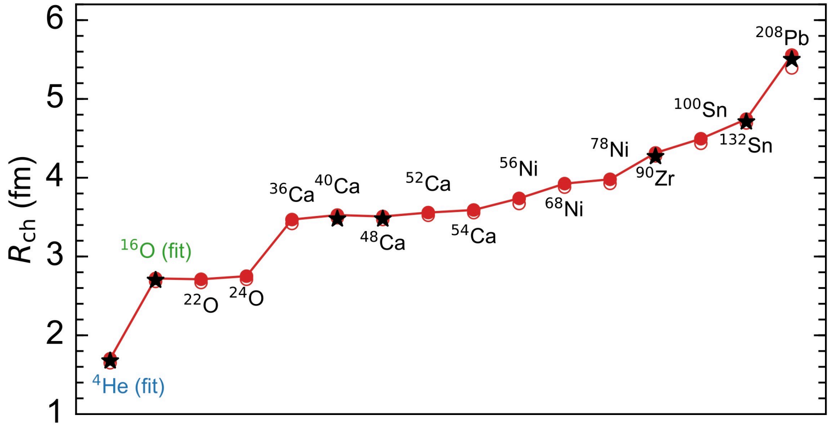
only limited families of NN+3N interactions for global ab initio calcs

- Δ-full interactions ΔN^2LO_{GO} (394 MeV) 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 via history matching
  Hu et al., Nat. Phys. (2024) great for uncertainty quantification

- N^3LO_{Texas} Hagen et al., see TRIUMF workshop
  similar fitting strategy, including also higher energy NN scattering

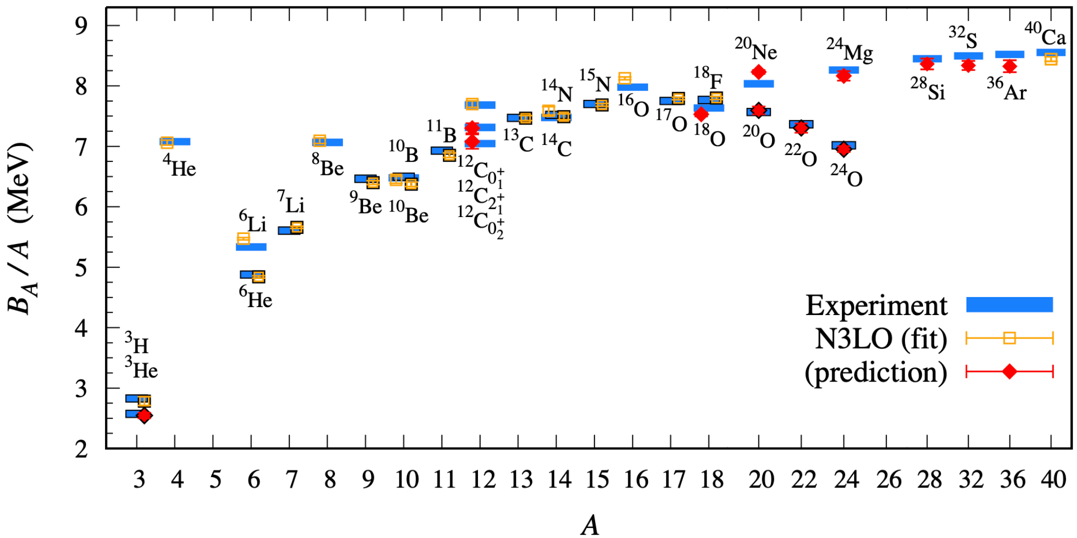


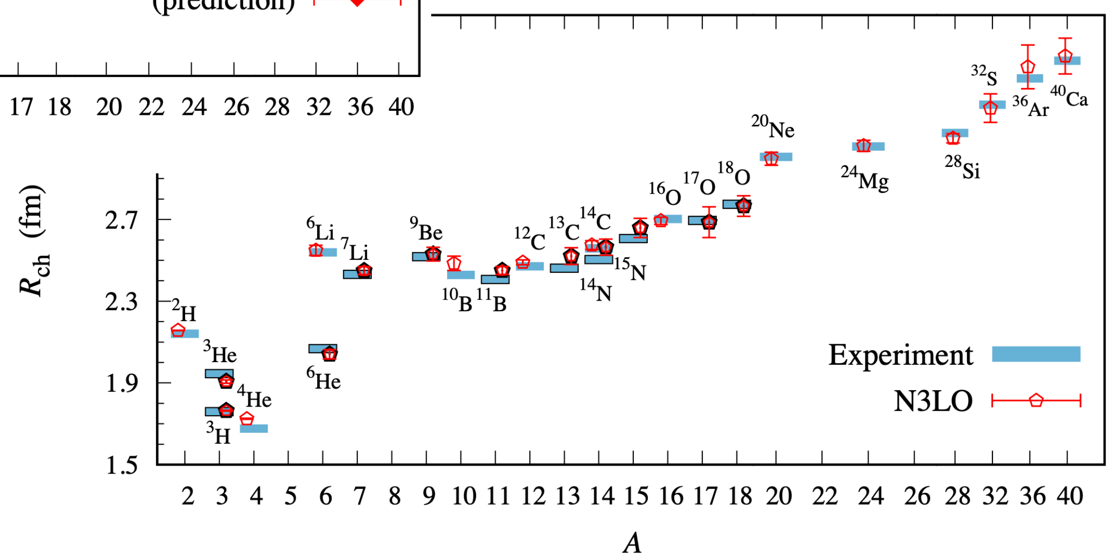


Chiral NN+3N interactions up to ^{208}Pb

only limited families of NN+3N interactions for global ab initio calcs

- Lattice EFT N^{3}LO Elhatisari et al., Nature (2024)
  NN N^{3}LO + 3N N^{2}LO at fixed lattice spacing
  +6 additional 3N parameters adjusted to selected nuclei





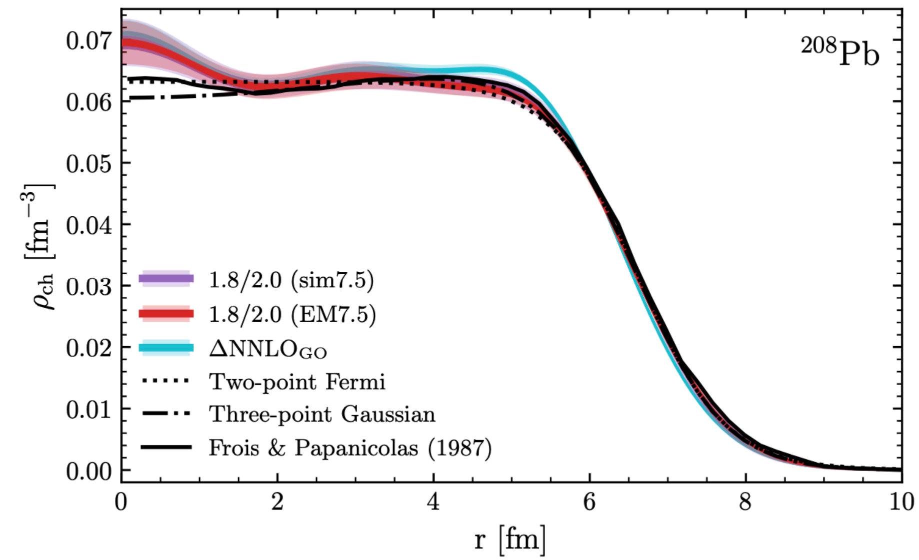
Next generation NN+3N interactions: wish list

- 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 Pierre Arthuis' talk

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



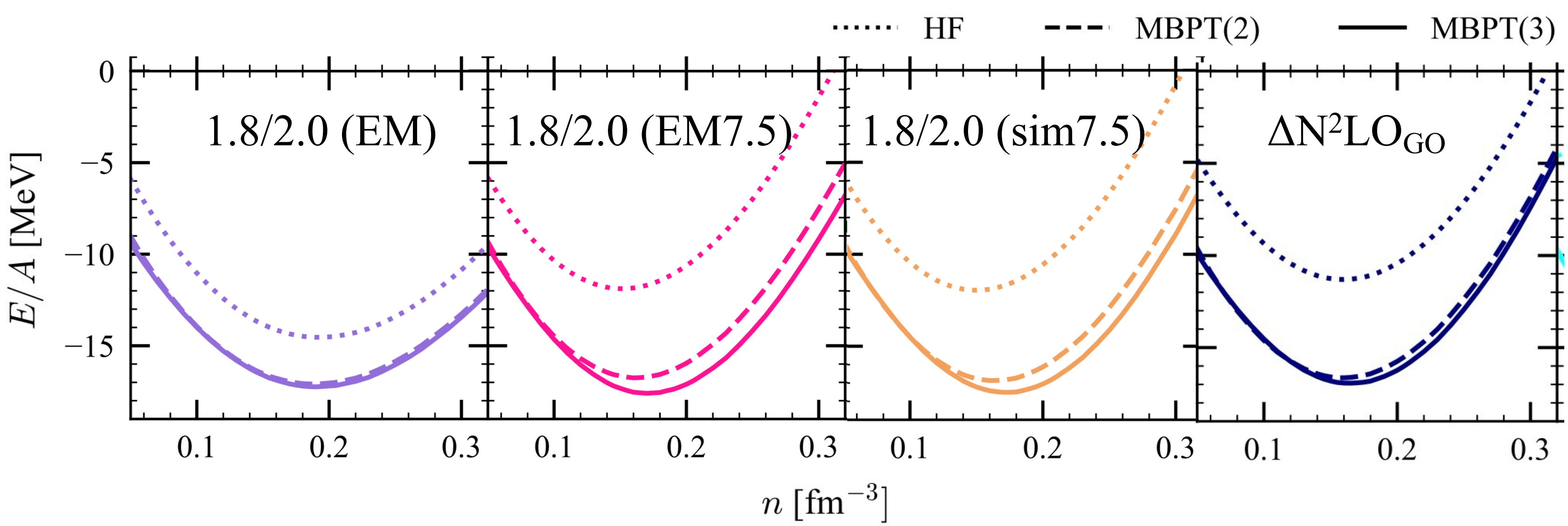
for these interactions

reasonable radii and densities

at Hartree-Fock level

compare with nuclear matter results

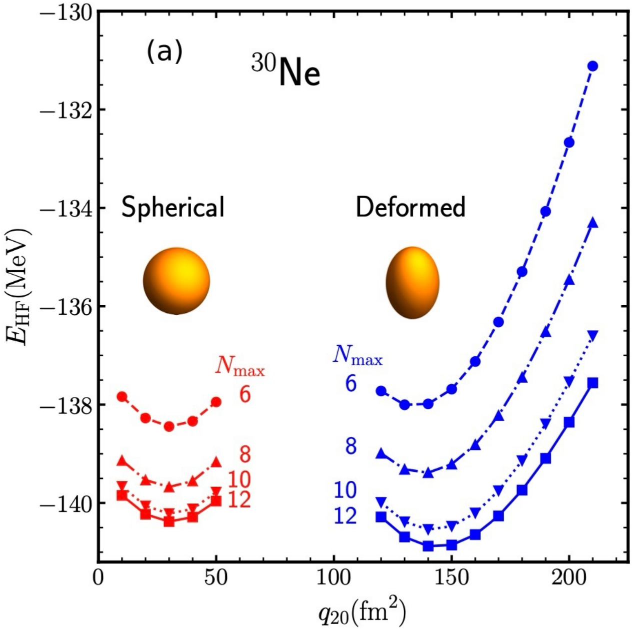
Alp, Dietz, Hebeler, AS, arXiv:2504.18259



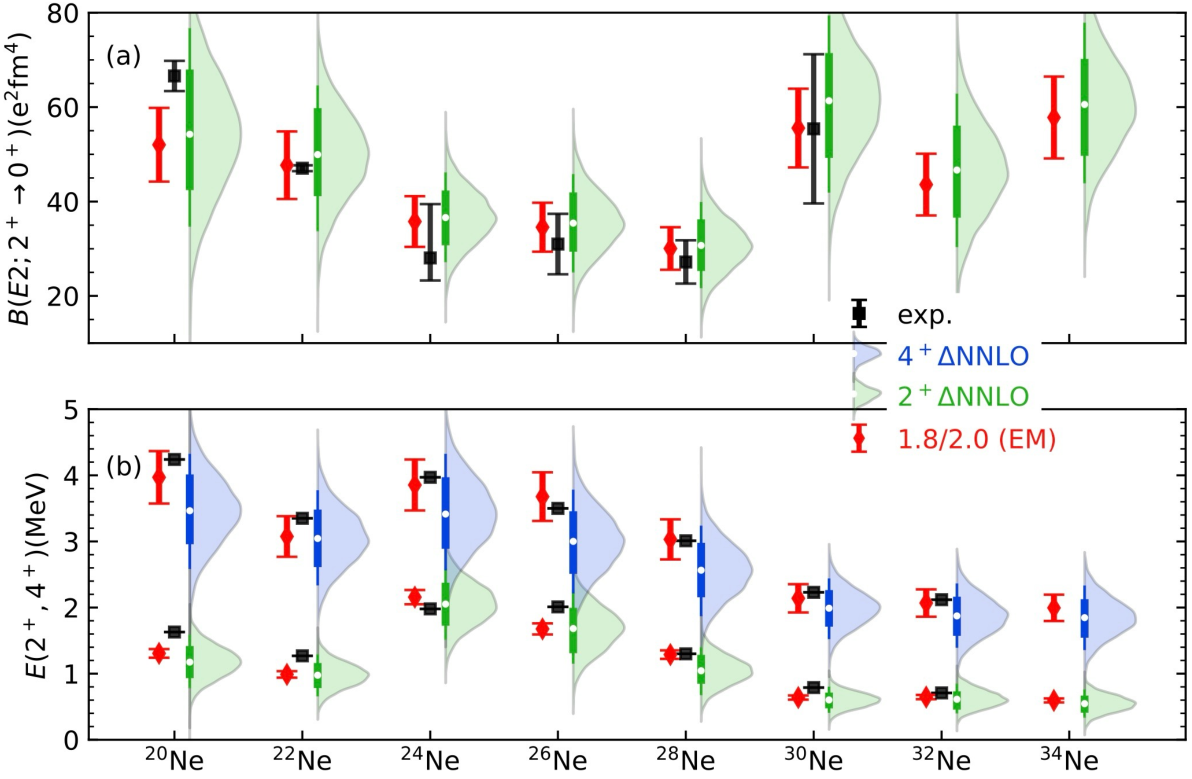
Ab initio calculations of deformed nuclei

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



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- 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,
  reasonable saturation density at HF level?

Challenges

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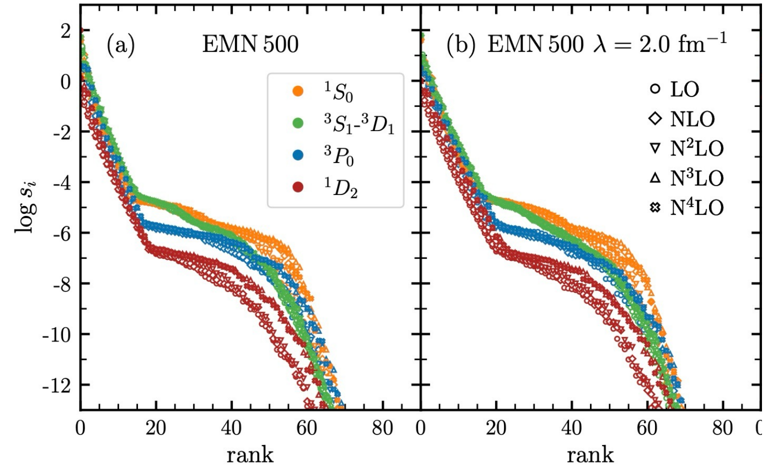
Uncertainty estimates for SRG-evolved interactions

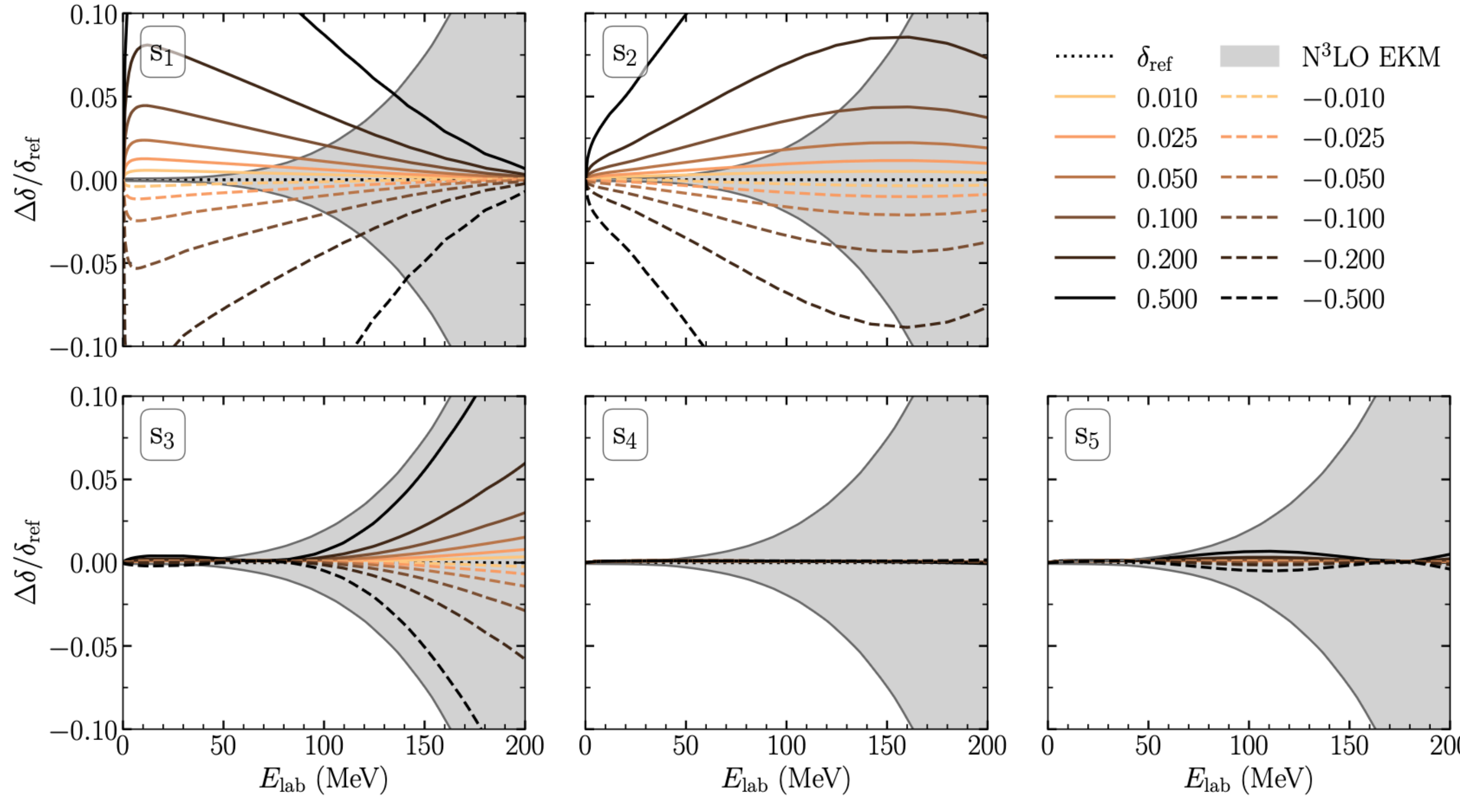
with Tom Plies and Matthias Heinz

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



consider largest 5 singular values/operators

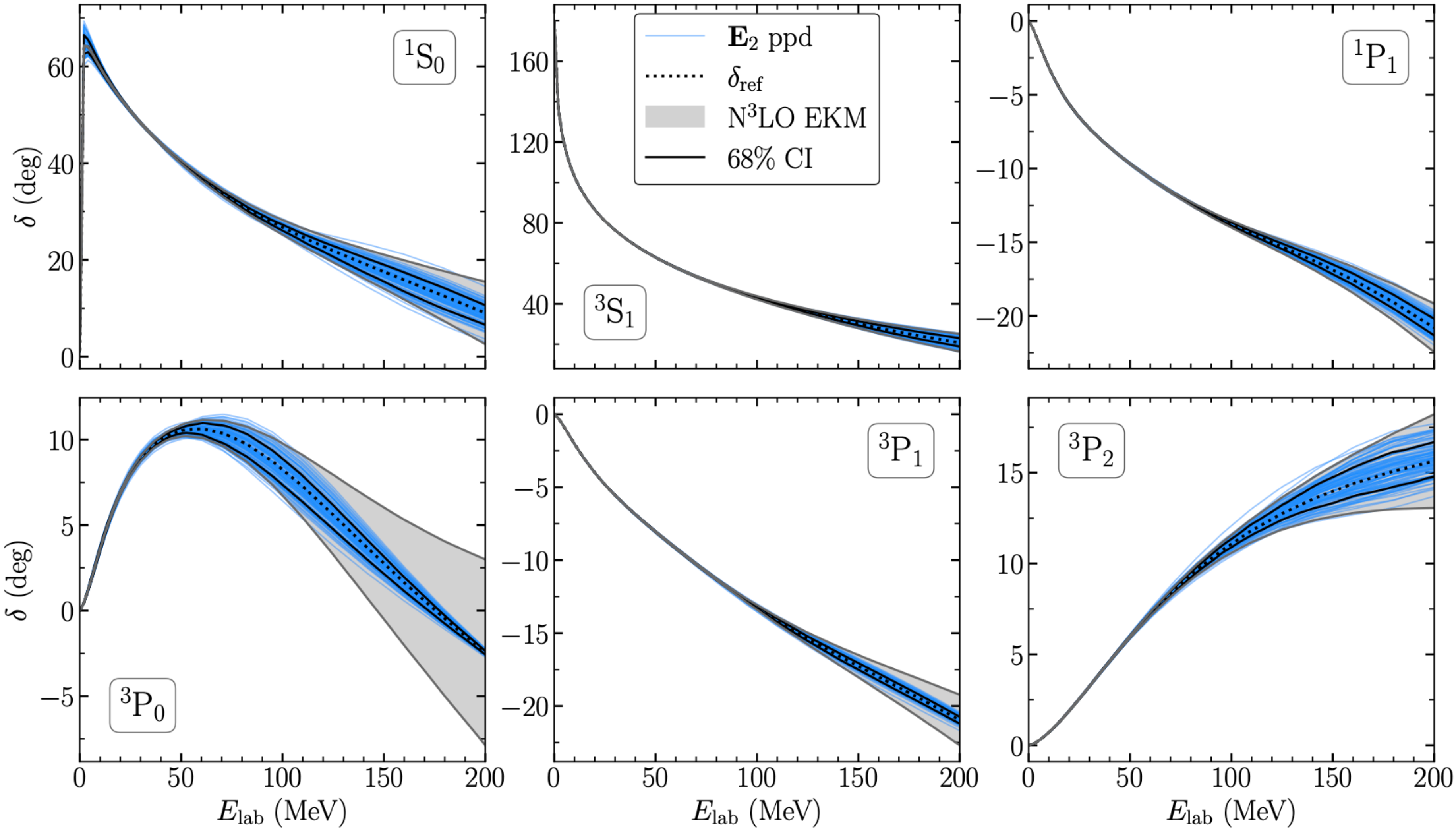
effectively 3 generate phase shift variation



Uncertainty estimates for SRG-evolved interactions

with Tom Plies and Matthias Heinz

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



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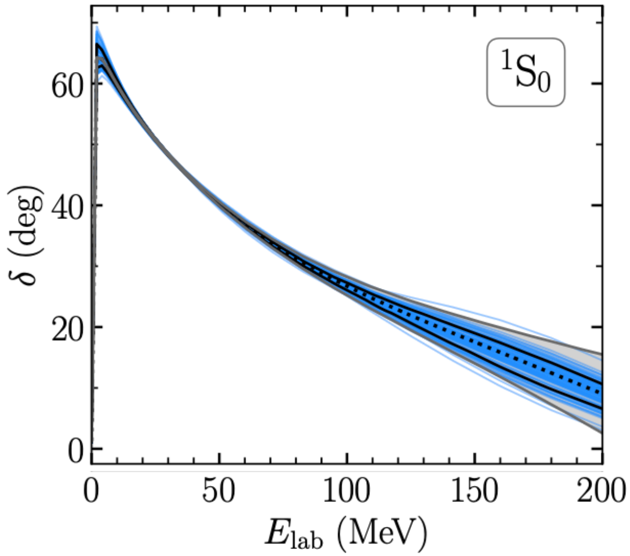
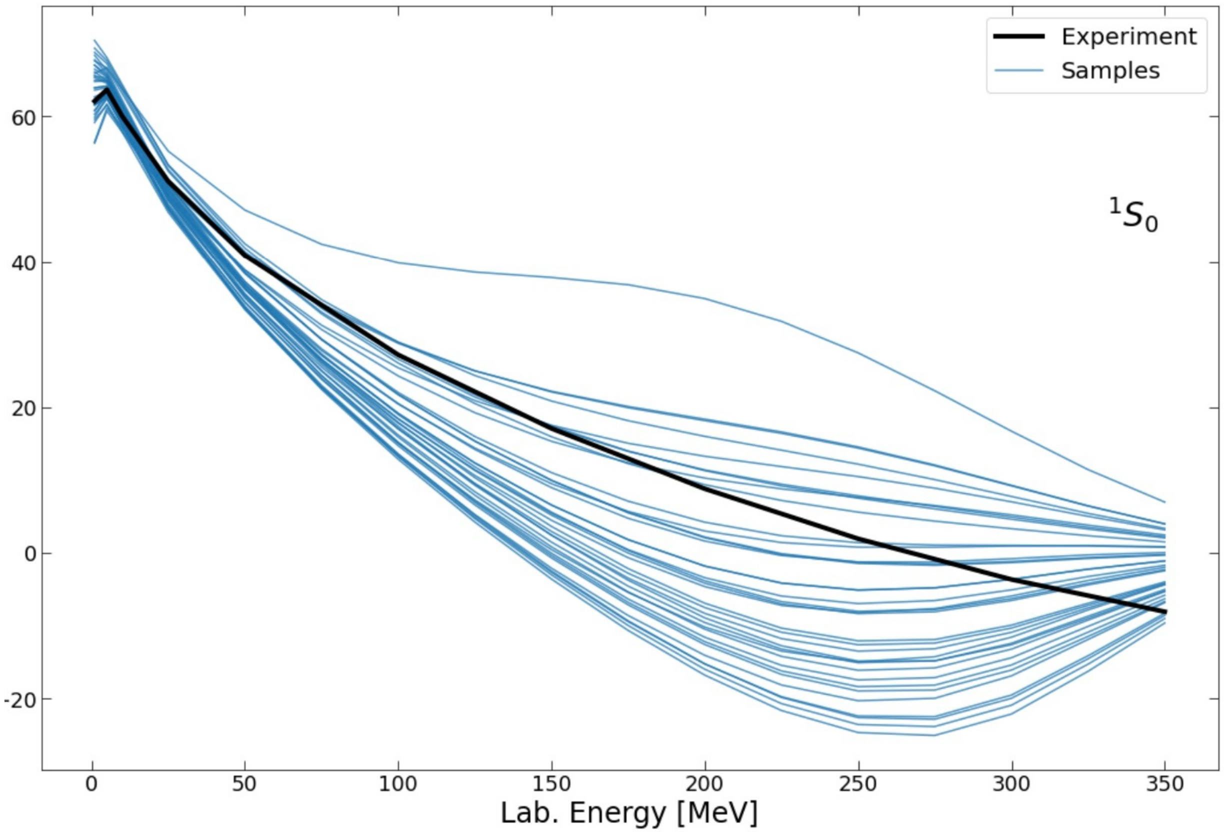




comparison to nonimplausible ΔN^2LO interactions Ekström, Forssen et al.

Uncertainty estimates for SRG-evolved interactions

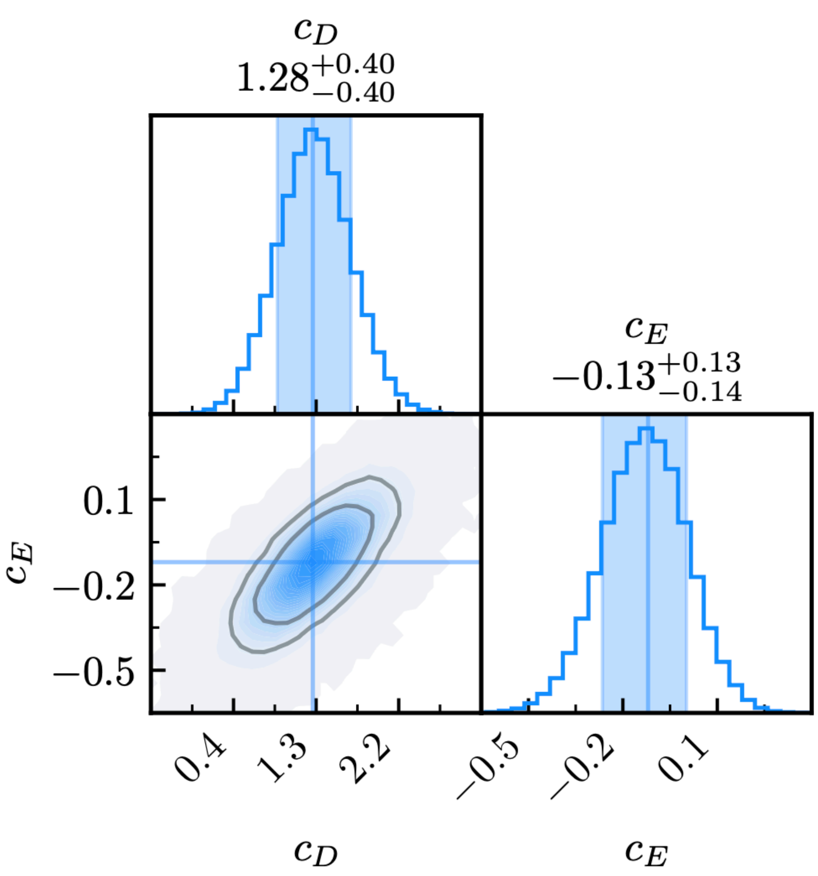
with Tom Plies and Matthias Heinz

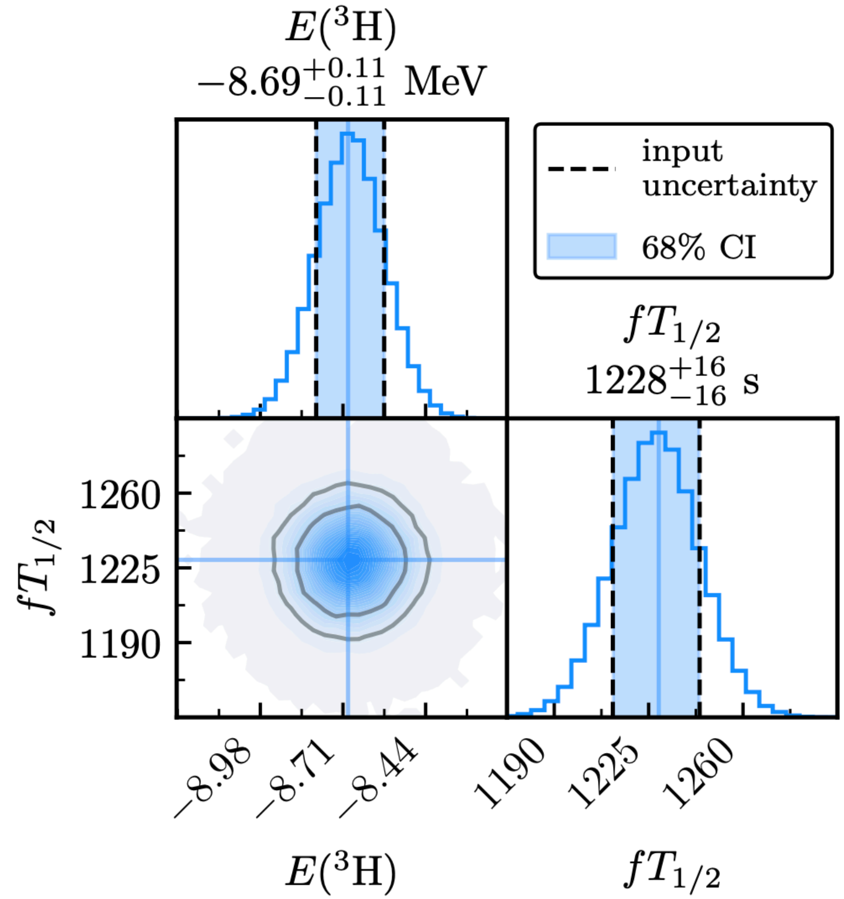
generate range of low-resolution NN+3N interactions

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)





Uncertainty estimates for SRG-evolved interactions

with Tom Plies and Matthias Heinz

generate range of low-resolution NN+3N interactions

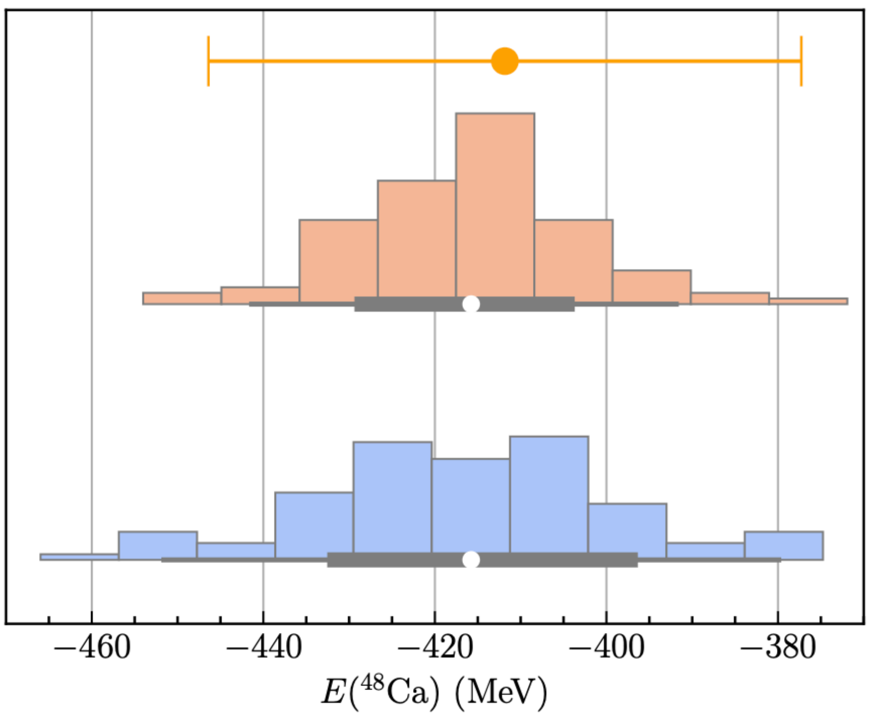
NN: S and P waves, higher partial waves unvaried

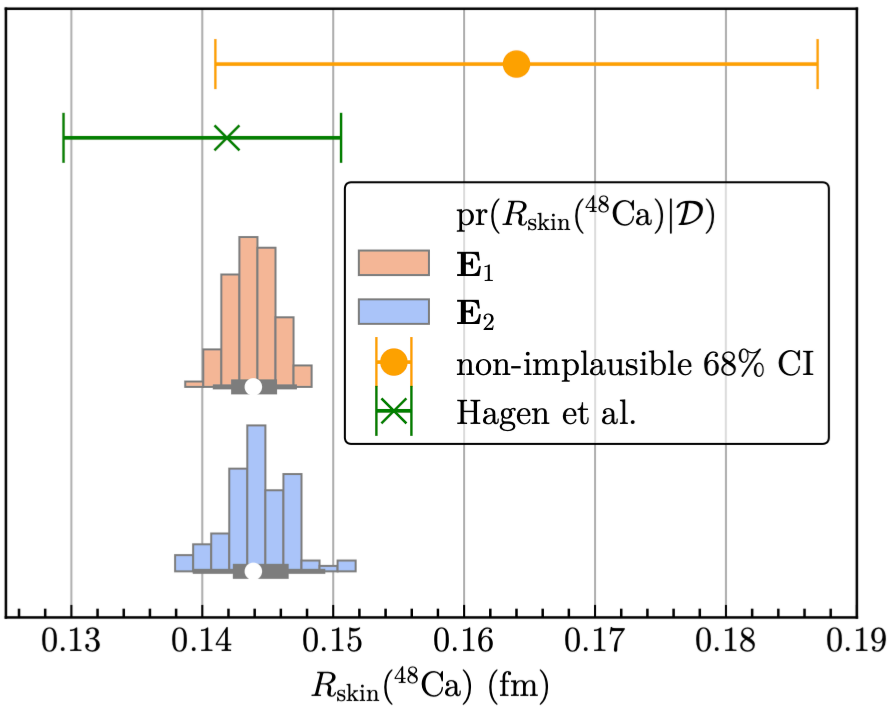
3N uncertainties from ^{3}H energy and half-life

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





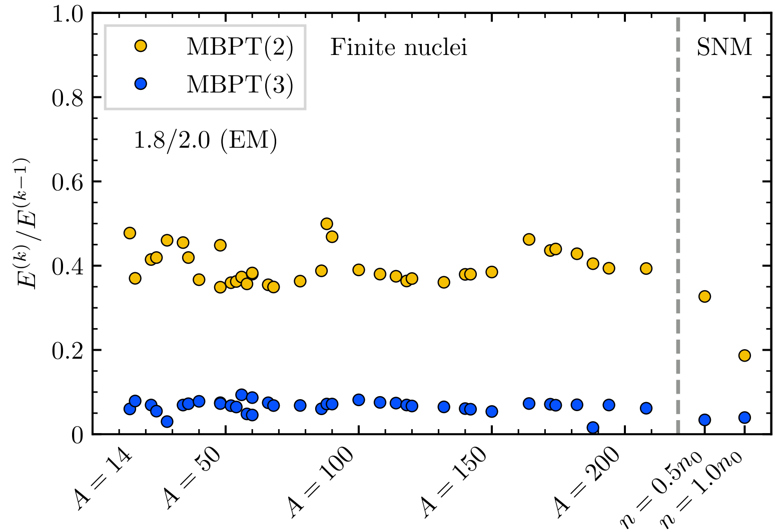
Many-body truncation uncertainties

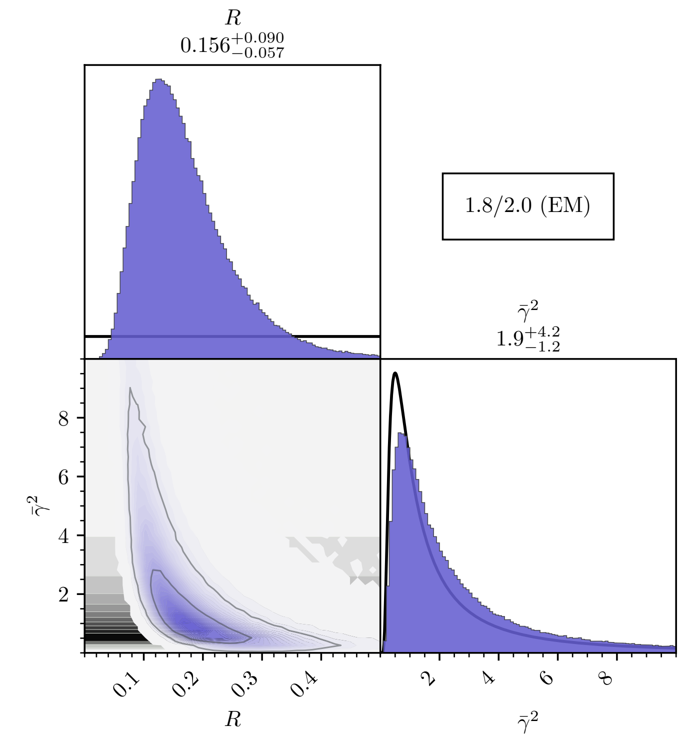
Svensson, Tichai, Hebeler, AS, arXiv:2507.09079

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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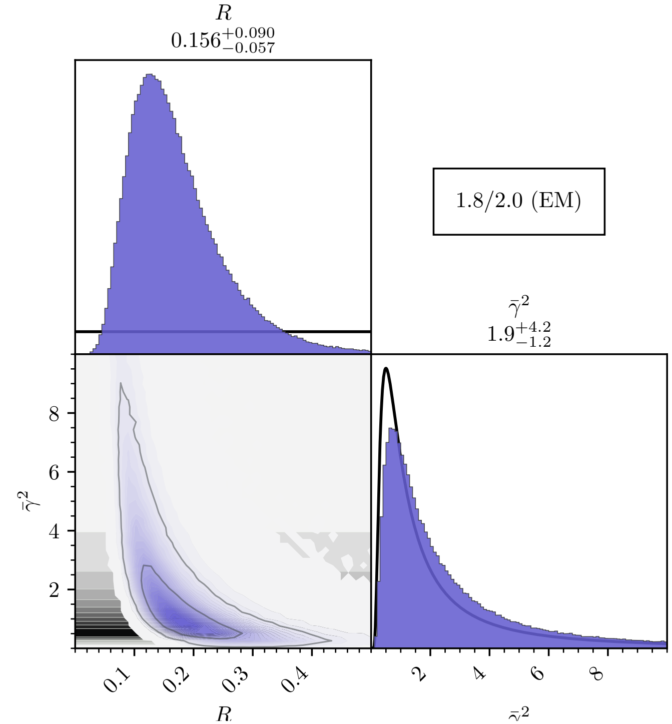
Svensson, Tichai, Hebeler, AS, arXiv:2507.09079

idea: use BUQEYE error model for MBPT expansion

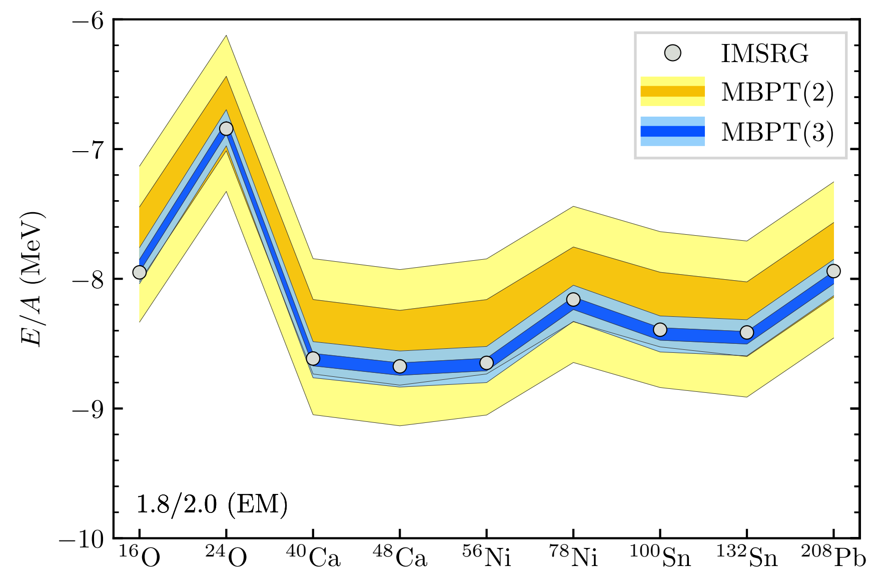
$$E_0 = \underbrace{E_{\text{ref}}\gamma_0}_{E_{\text{HF}}} + \underbrace{E_{\text{ref}}\gamma_1 R^1}_{\text{MBPT(2)}} + \underbrace{E_{\text{ref}}\gamma_2 R^2}_{\text{MBPT(3)}} + \ldots$$

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



posterior distributions at different orders

good agreement with IMSRG(2)



enables many-body uncertainty estimates beyond expert assessment

Challenges

Next generation NN+3N interactions up to heavy nuclei: status and wish list P. Arthuis, K. Hebeler, T. Plies, I. Svensson, U. Vernik

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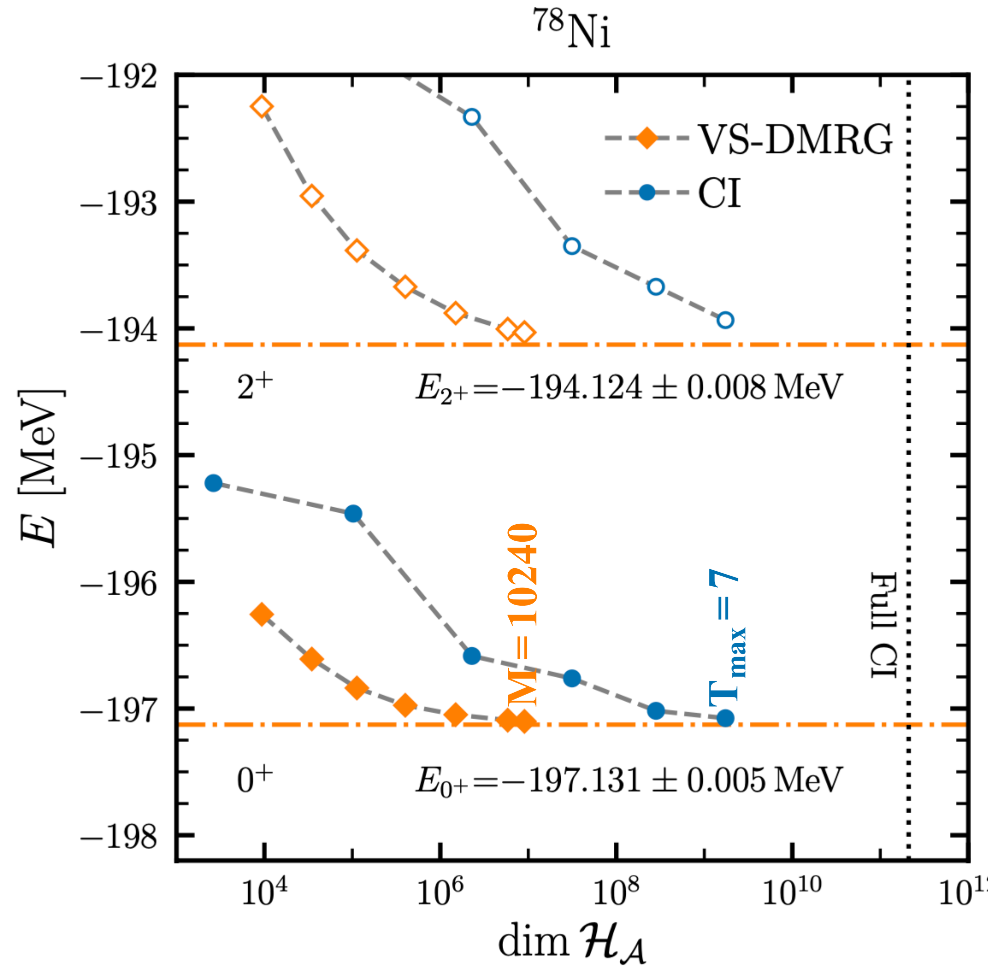
Valence-space density matrix renormalization group

Tichai et al., PLB (2023)

use valence-space IMSRG to decouple valence-space Hamiltonian

slow/poor convergence with typical particle-hole truncations in shell model (CI)

DMRG optimization of matrix product states efficiently samples correlations, good convergence in ~100 smaller dimensions



Can we use ideas from quantum information to more efficiently represent nuclear states?

Valence-space density matrix renormalization group

Tichai et al., PLB (2024)

dependence on orbital ordering

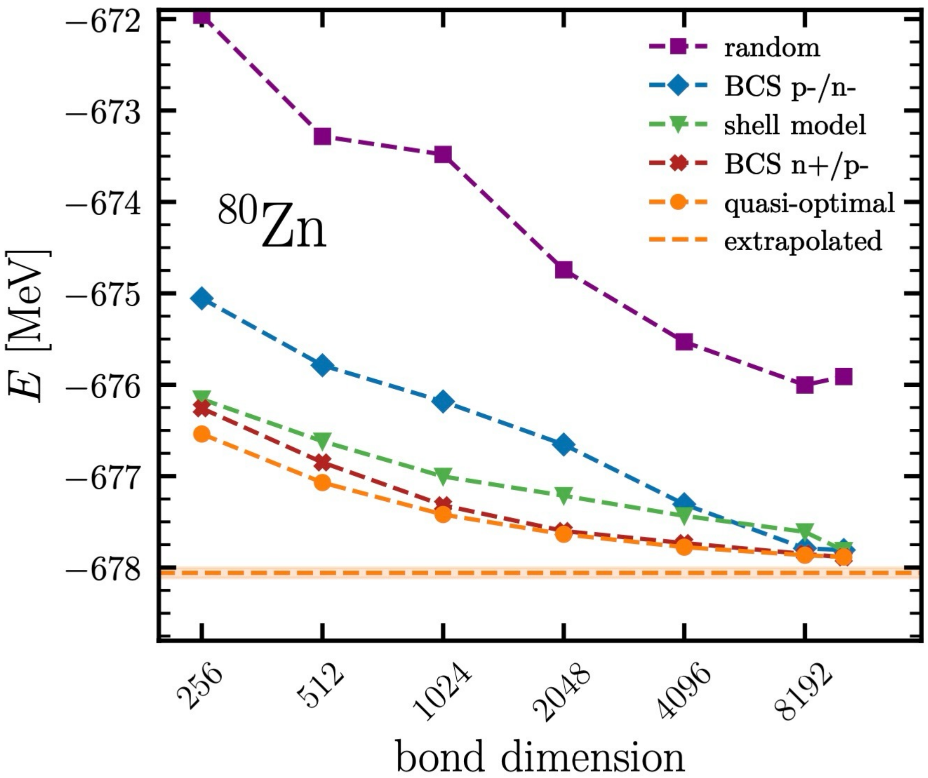
all orderings with physics insights better than random ordering

energetic/shell model ordering not optimal

improved convergence when including pairing correlations, BCS n+/p- has orbitals with high j (larger entropy) in center of chain

$$\{\nu : s_{1/2}\, d_{3/2}\, d_{5/2}\, g_{7/2}\, g_{9/2};\, \pi : f_{7/2}\, f_{5/2}\, p_{3/2}\, p_{1/2}\}$$

quasi-optimal ordering places orbitals with high entropy around chain center



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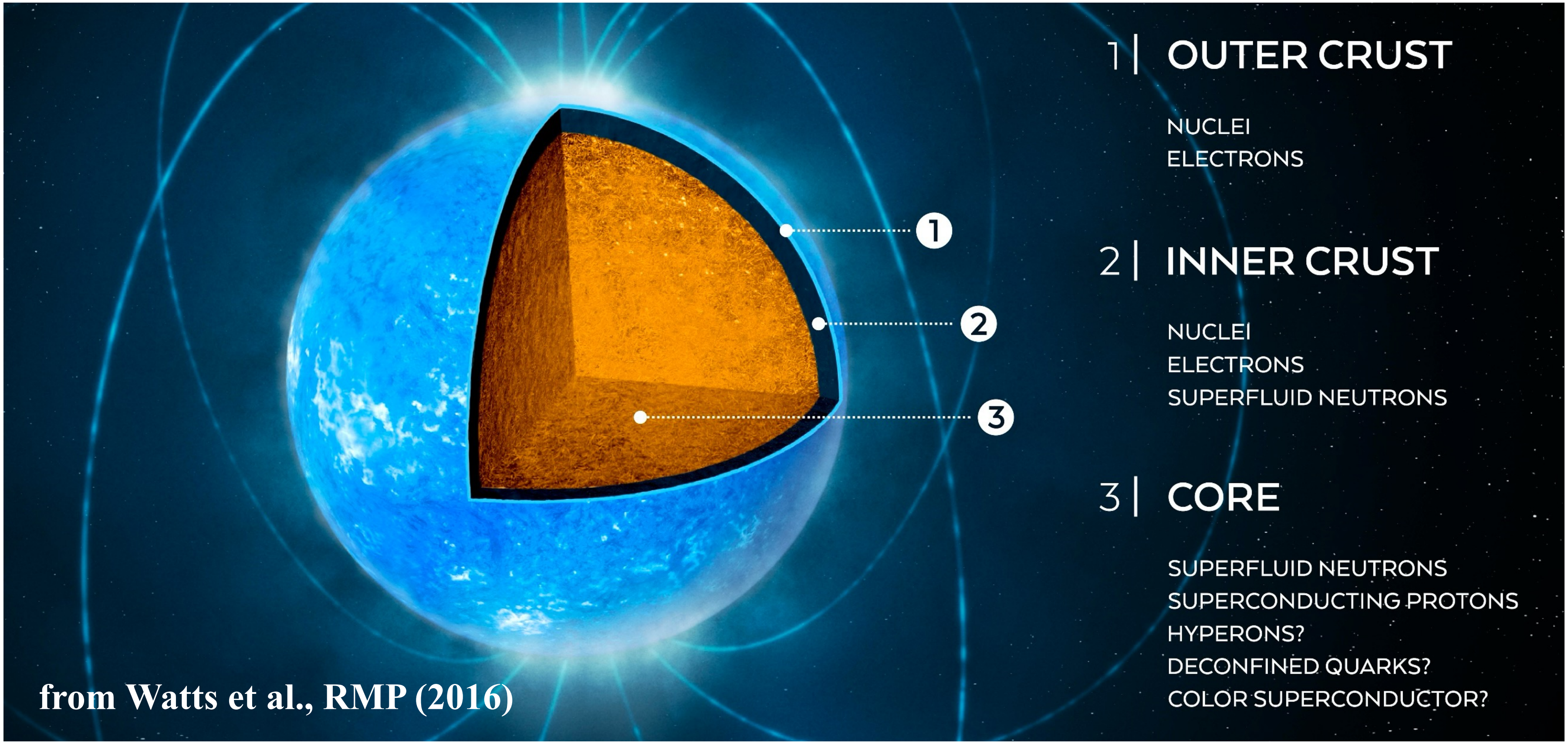
Extreme matter in neutron stars

Cold dense matter up to ~ 5-8 n_0 (in heaviest neutron stars)

governed by strong interactions, up to few n_0: n,p,e,μ

When/do degrees of freedom change?

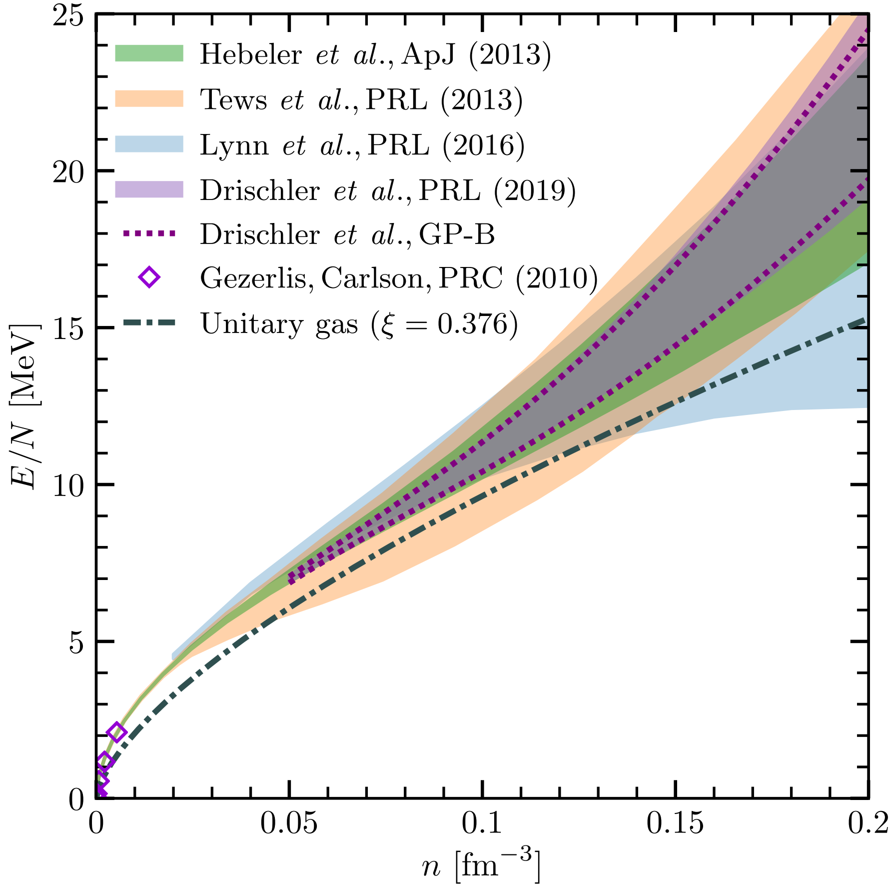
Chiral EFT sets pressure of first few km Hebeler et al., PRL (2010), ApJ (2013)



from Watts et al., RMP (2016)

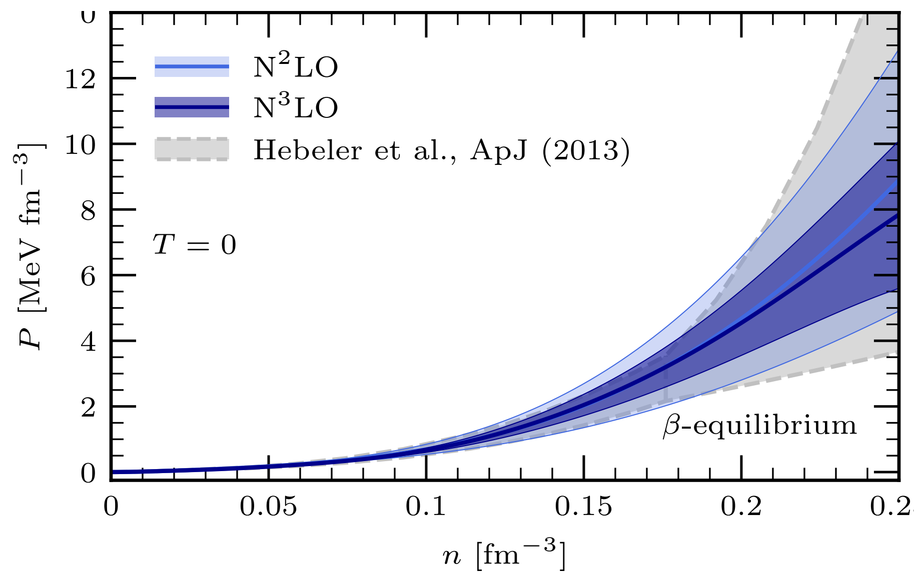
Chiral EFT calculations of neutron matter

good agreement up to saturation density
including NN, 3N, 4N interactions up to N^{3}LO



comparison from Huth et al., PRC (2021)

slope determines pressure of neutron matter



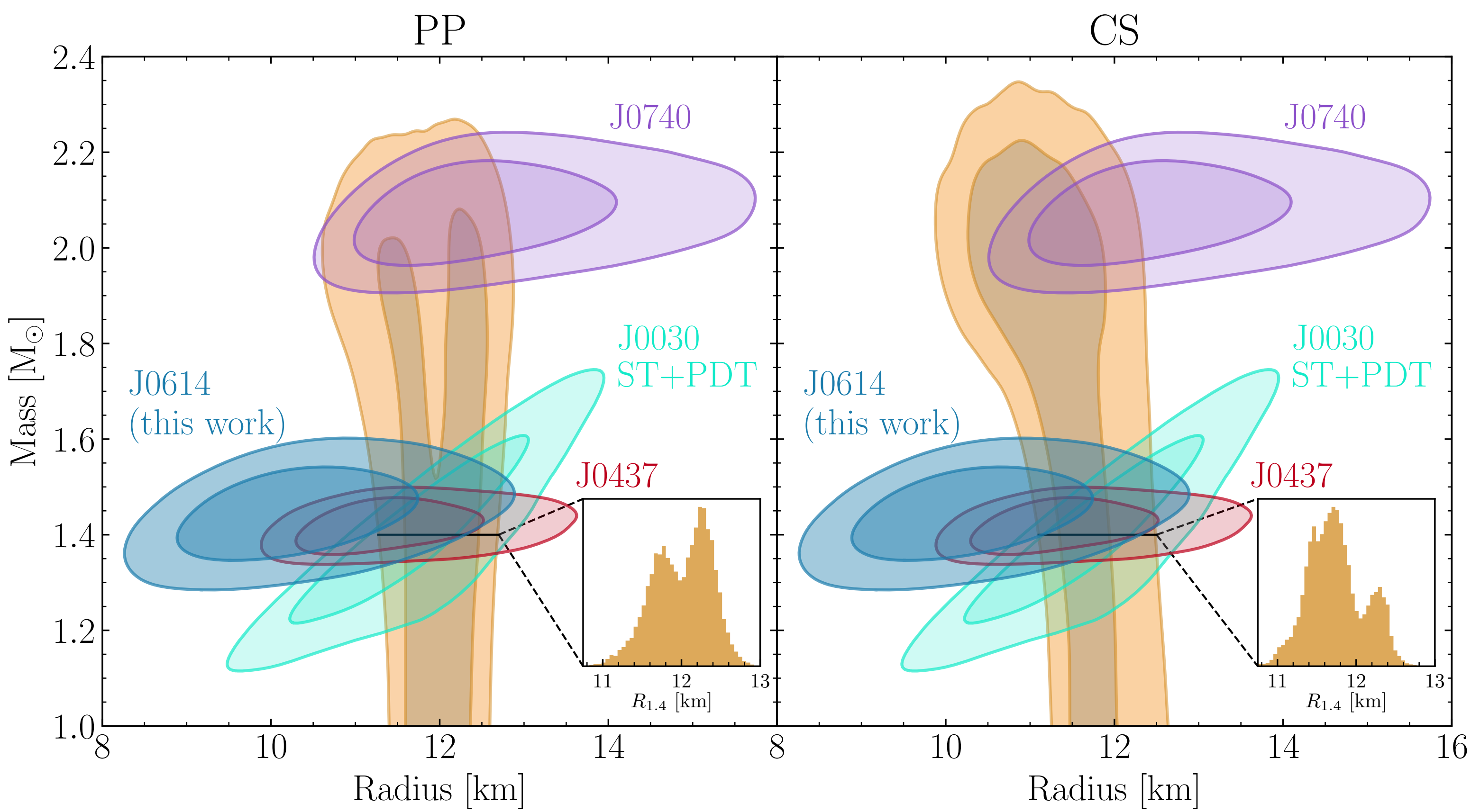
EOS for arbitrary proton fraction (and finite temperature) using Gaussian Process emulator

Keller, Hebeler, AS, PRL (2023)

LIGO/Virgo and NICER results

chiral EFT up to $1.5n_0$ + general EOS extrapolations + causality

including information from GW170817 and 4 stars studied by NICER



Raaijmakers et al., ApJL (2020), (2021), Rutherford, Mendes, Svensson et al., ApJL (2024)
Mauviard-Haag et al., arXiv:2506.14883

Constraints at intermediate densities

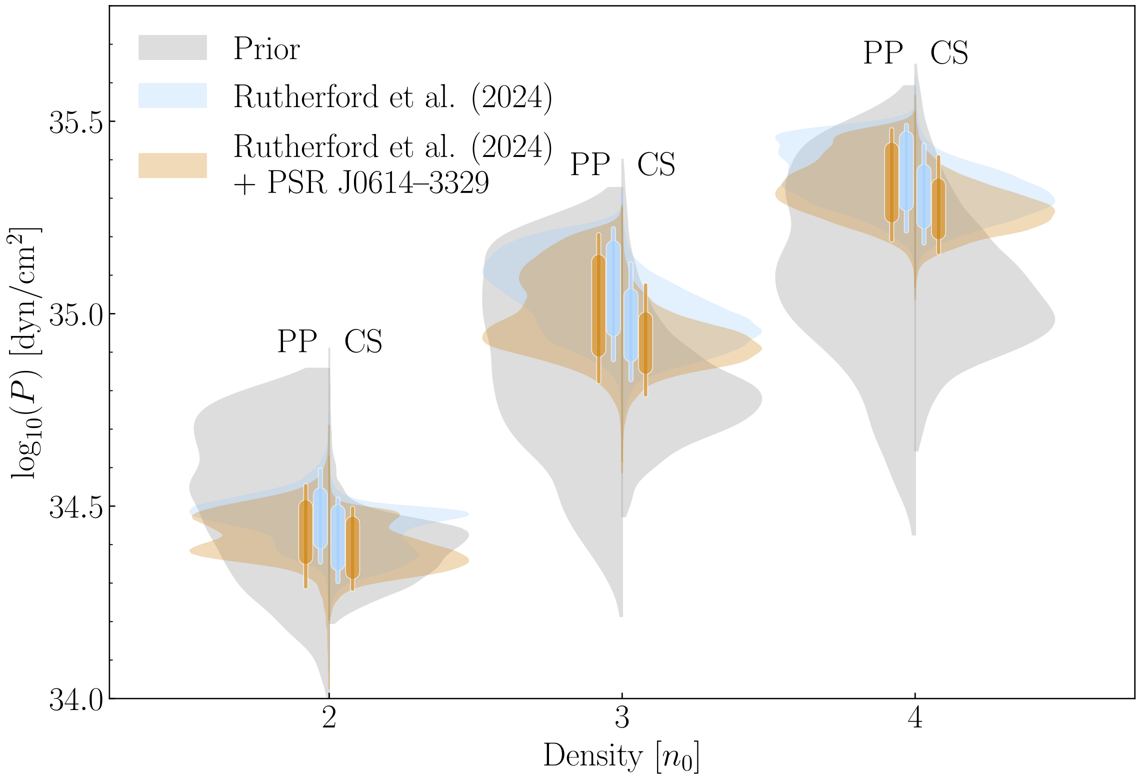
chiral EFT up to $1.5n_0$ + general EOS extrapolations + causality

including information from GW170817 and 4 stars studied by NICER

observations constrain pressure at intermediate densities

posteriors at 3-4n_0
→ astro prefers higher pressures

important to explore prior sensitivities



Rutherford, Mendes, Svensson et al., ApJL (2024)
Mauviard-Haag et al., arXiv:2506.14883

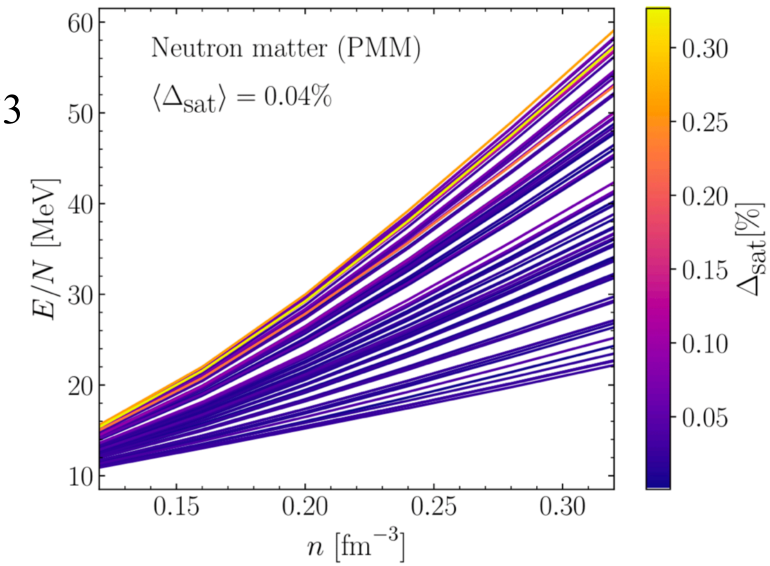
What can we expect from more observations?

Inferring 3N couplings from next generation observations

Somasundaram, Svensson et al., arXiv:2410.00247

prior: assume 100% uncertainty in c_1 and c_3

build PMM emulator for neutron matter

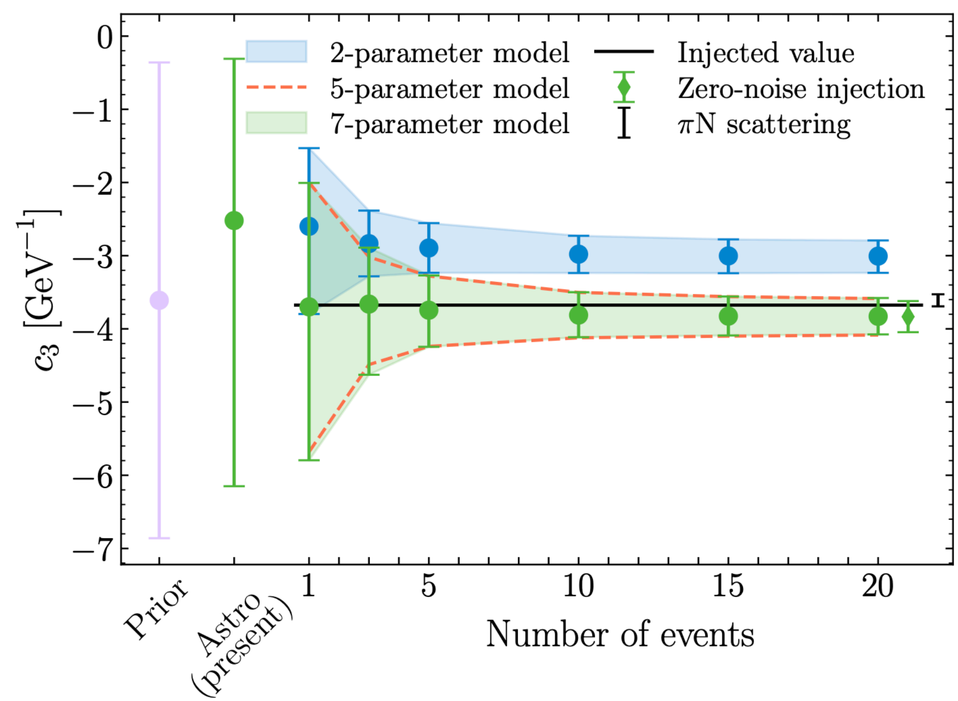


infer 3N couplings from astro data

present observations not very constraining

~20 future events will lead to interesting constraints for c_3

More work on connections between RIB measurements and astro impact is crucial



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