Advances and challenges for ab initio calculations of medium-mass to heavy nuclei and nuclear matter

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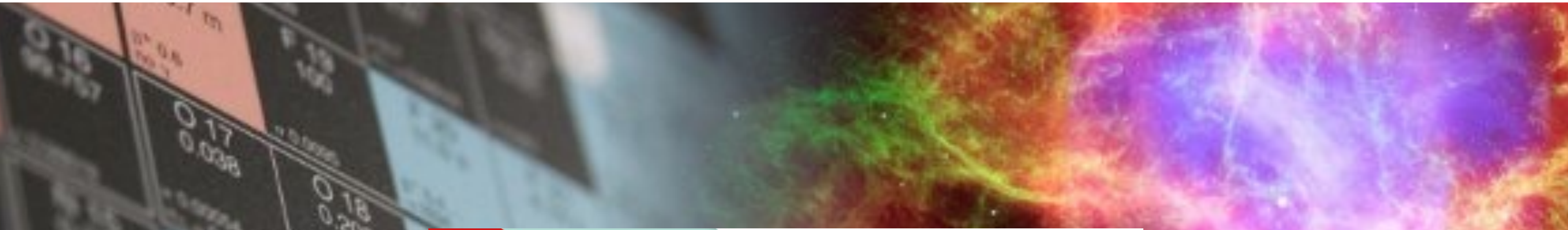

MITP Workshop

MITP
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WORKSHOP

Uncertainty Quantification in Nuclear Physics
June 24 – 28, 2024
https://indico.mitp.uni-mainz.de/event/357

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June 25, 2024

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Exzellente Forschung für Hessens Zukunft

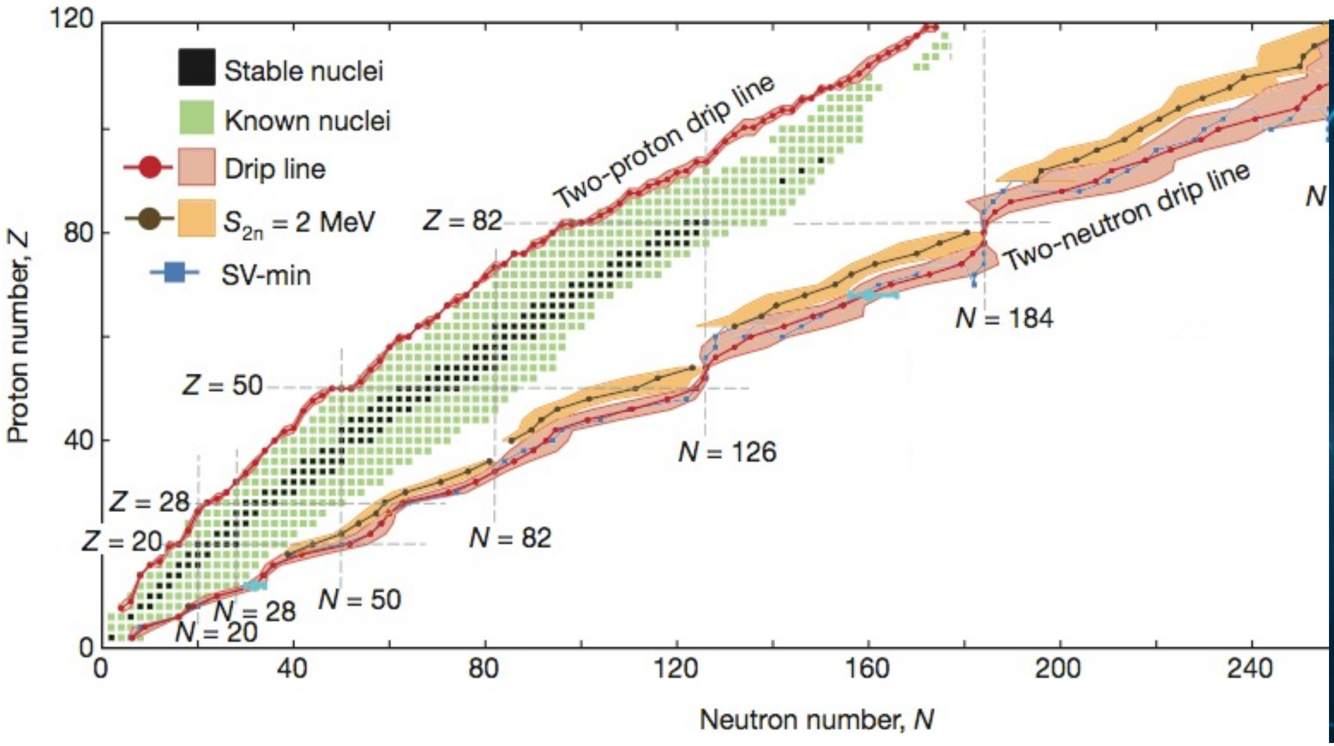
Structure of nuclei and dense matter in neutron stars

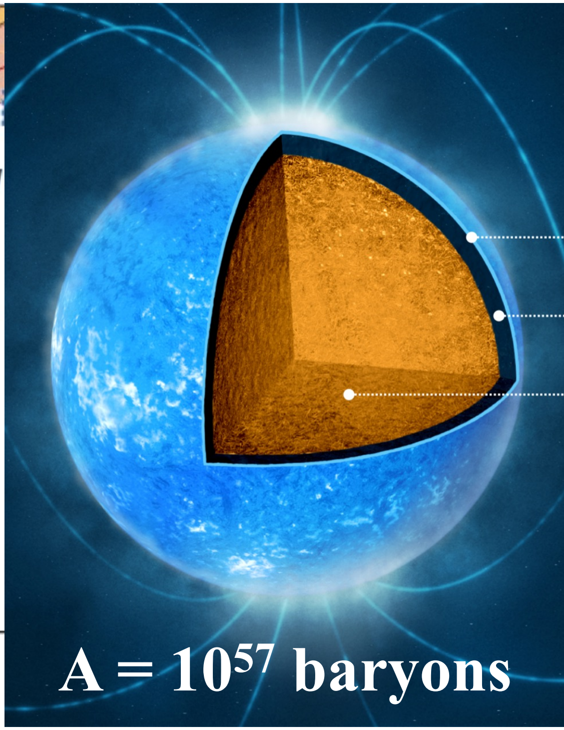
doi:10.1038/nature11188

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



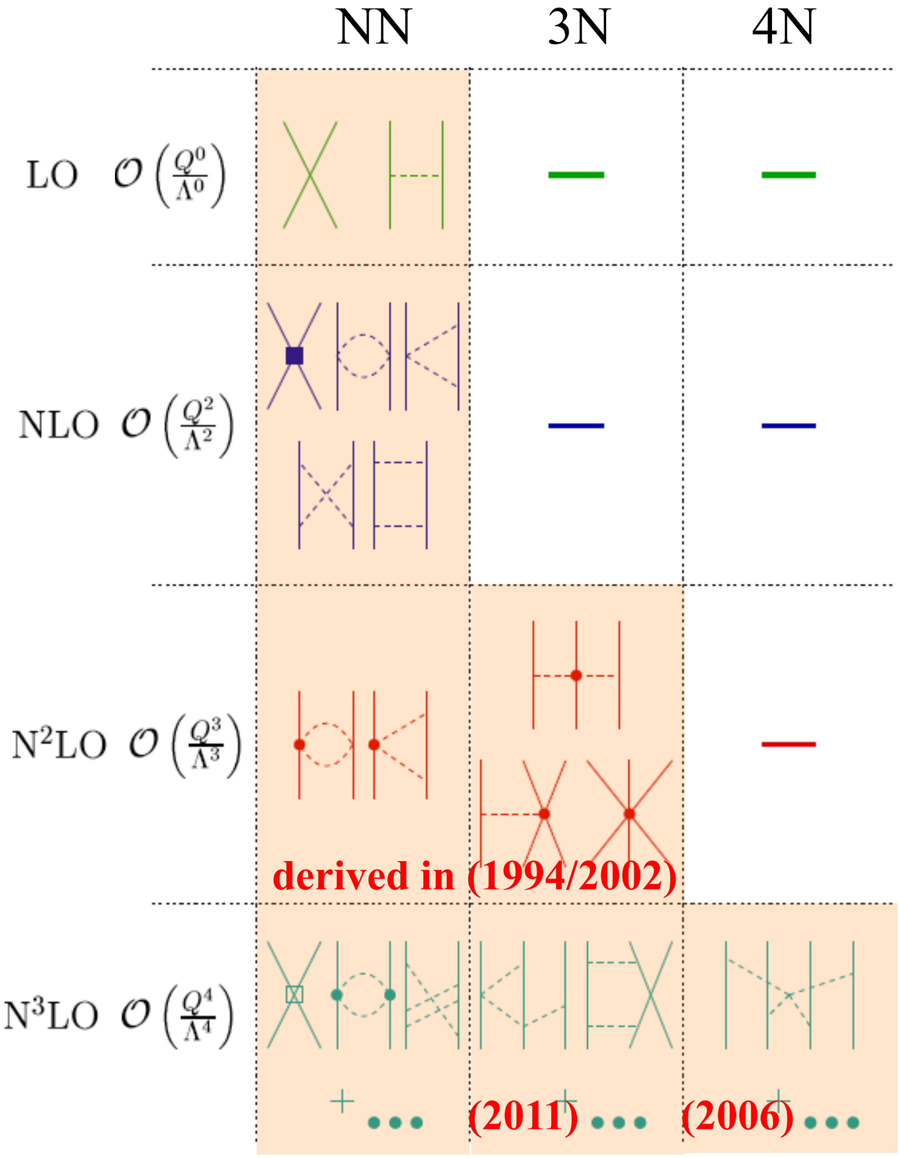


A = 10^{57} baryons

Extreme neutron-rich matter in neutron stars

Chiral effective field theory for nuclear forces

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



based on symmetries of strong interaction (QCD)

long-range interactions governed by pion exchanges

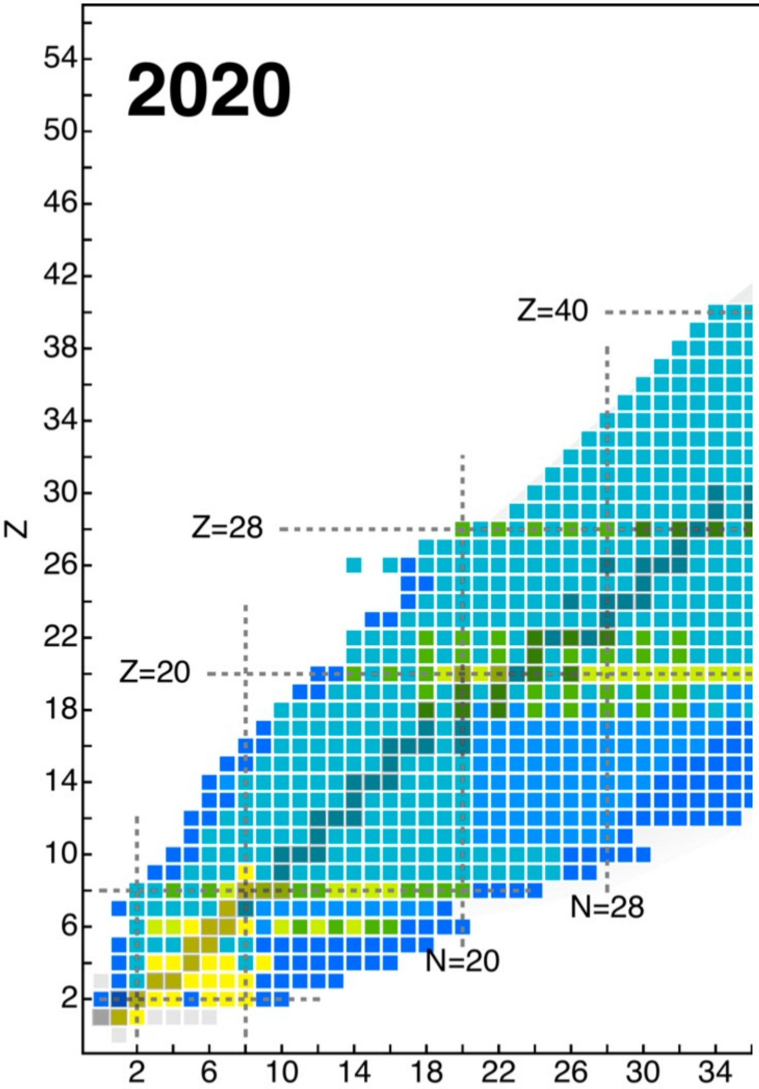
powerful approach for many-body interactions

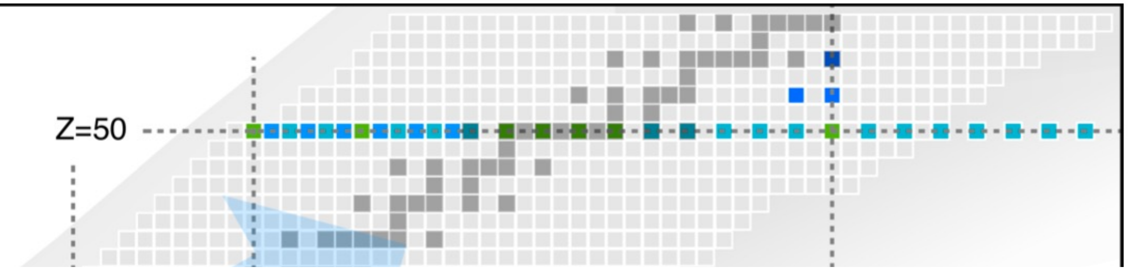
all 3- and 4-neutron forces predicted to N^{3}LO

Tews et al., PRL (2013)

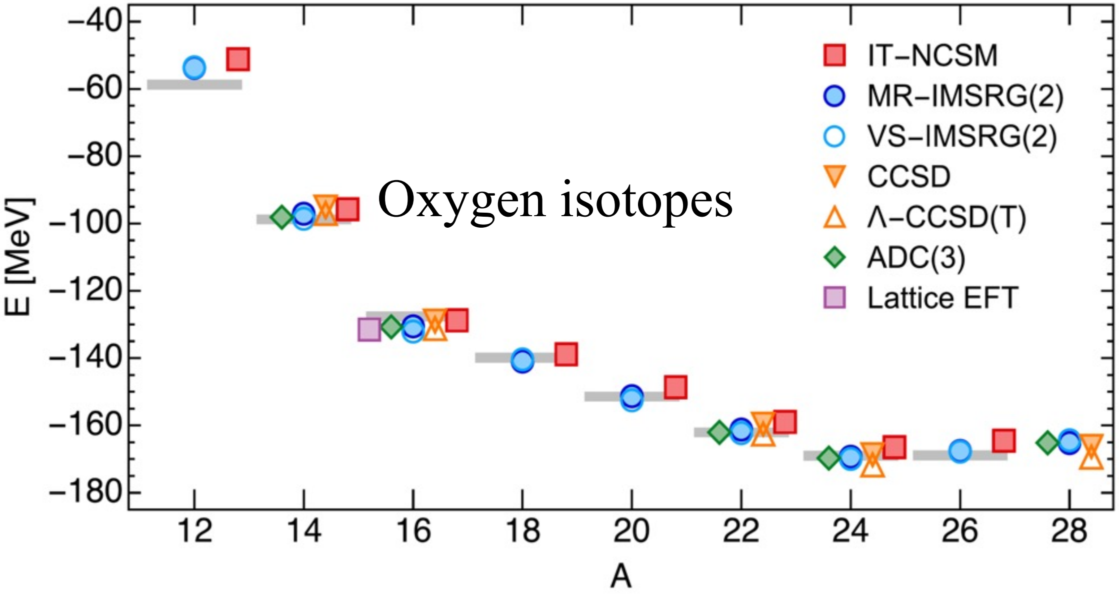
Weinberg (1990,91), van Kolck, Kaplan, Savage, Wise, Bernard, Epelbaum, Kaiser, Meißner,…

Great progress in ab initio calculations of nuclei





Chiral EFT interactions enable controlled solution of many-body Schrödinger eqn.



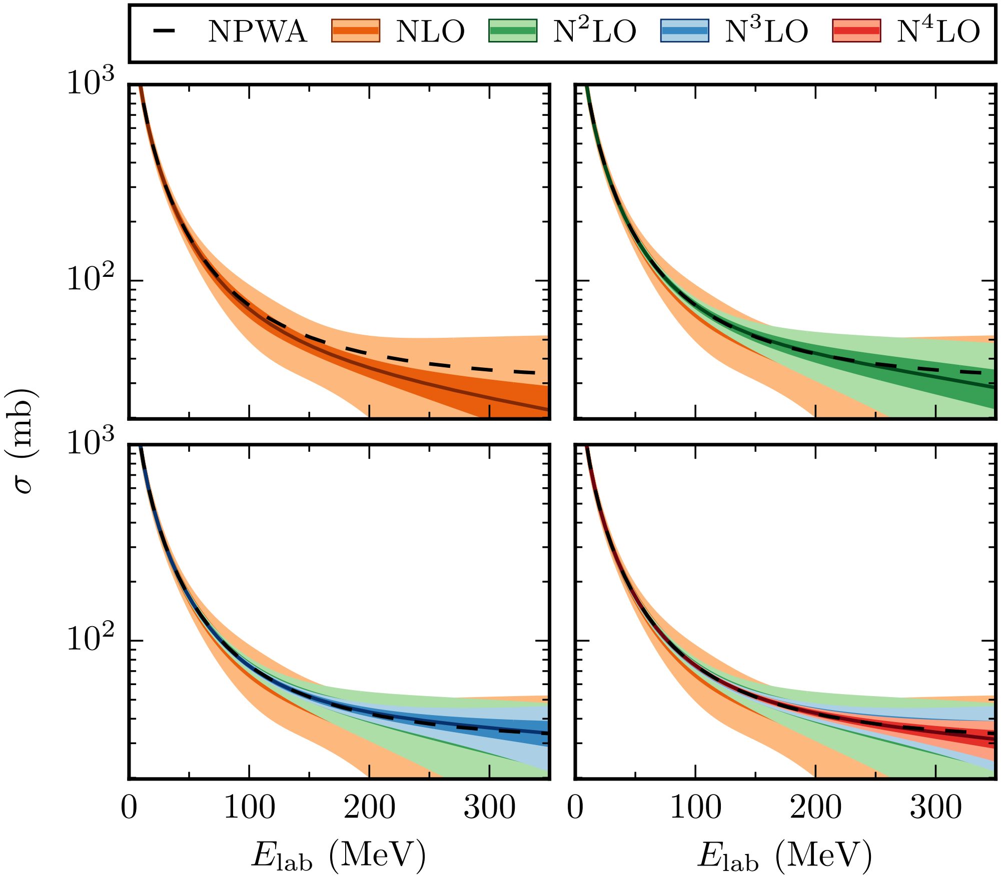
Interaction uncertainties dominate

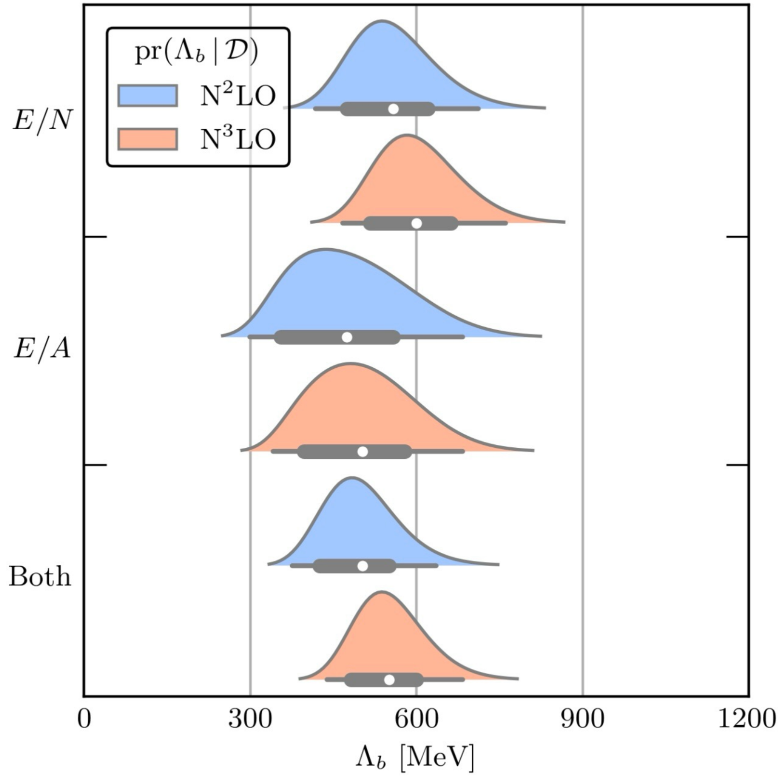
figures from Hergert (2020)

Chiral effective field theory for nuclear forces

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

Bayesian order-by-order uncertainty estimates based on power series in $(Q/\Lambda_b)^n$ with prior distribution for expansion coefficients



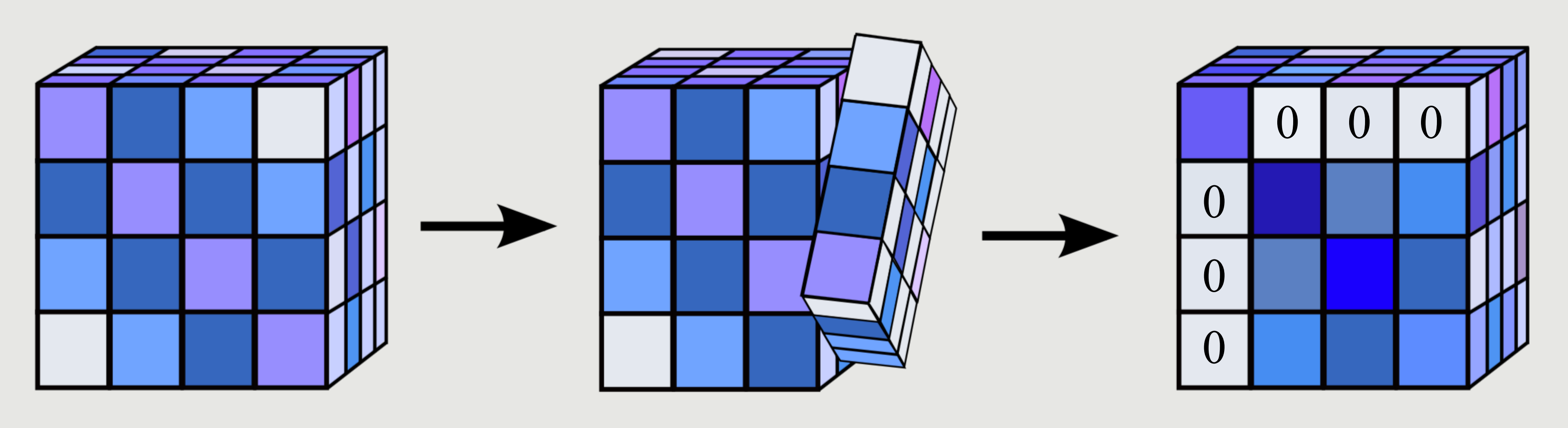


Furnstahl, Phillips, Klos, Wesolowski, Melendez, Drischler,… (2015-)

In-medium similarity renormalization group (IMSRG)

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

continuous transformation to block-diagonal form (→ decoupling)



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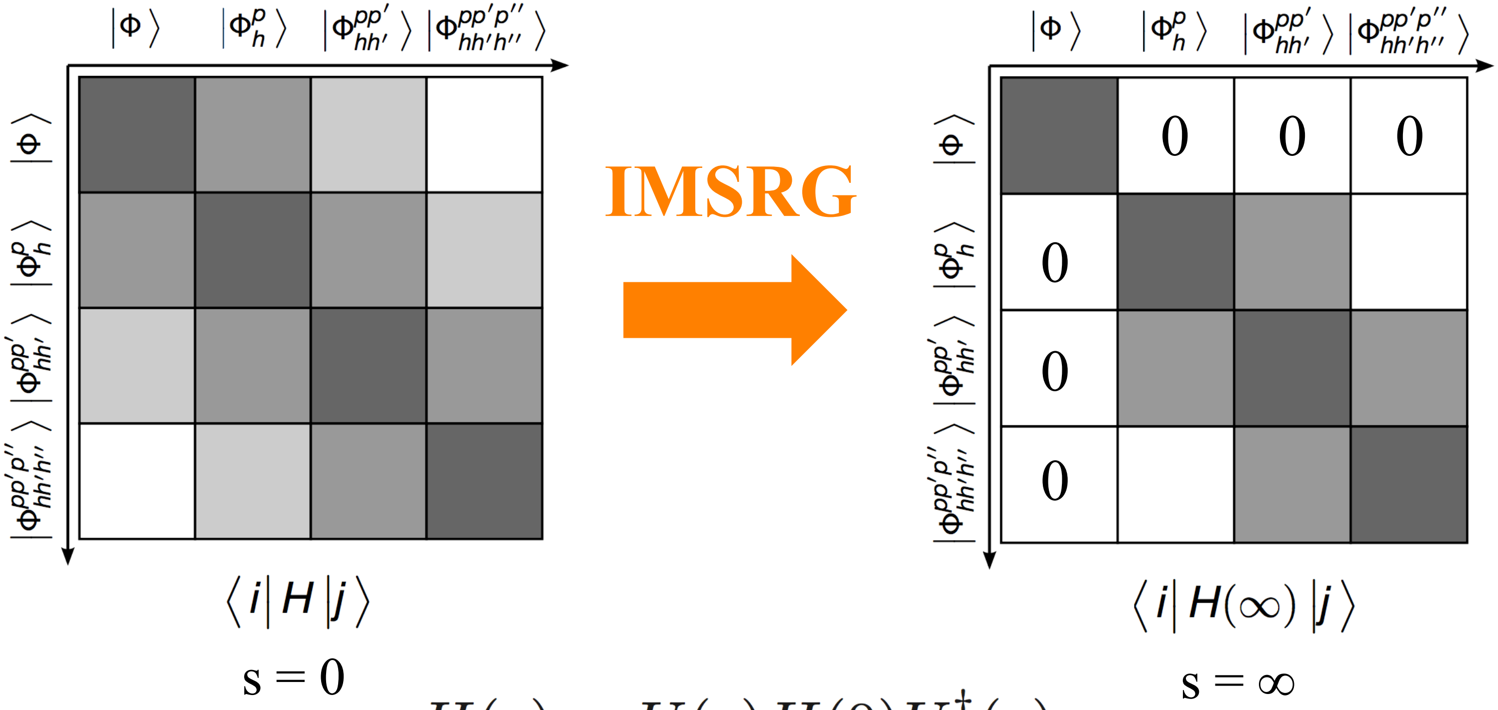
Tsukiyama, Bogner, AS, PRL (2011), Hergert et al., Phys. Rep. (2016)

RG flow equations to decouple higher-lying particle-hole states



$$H(s) = U(s)H(0)U^\dagger(s)$$

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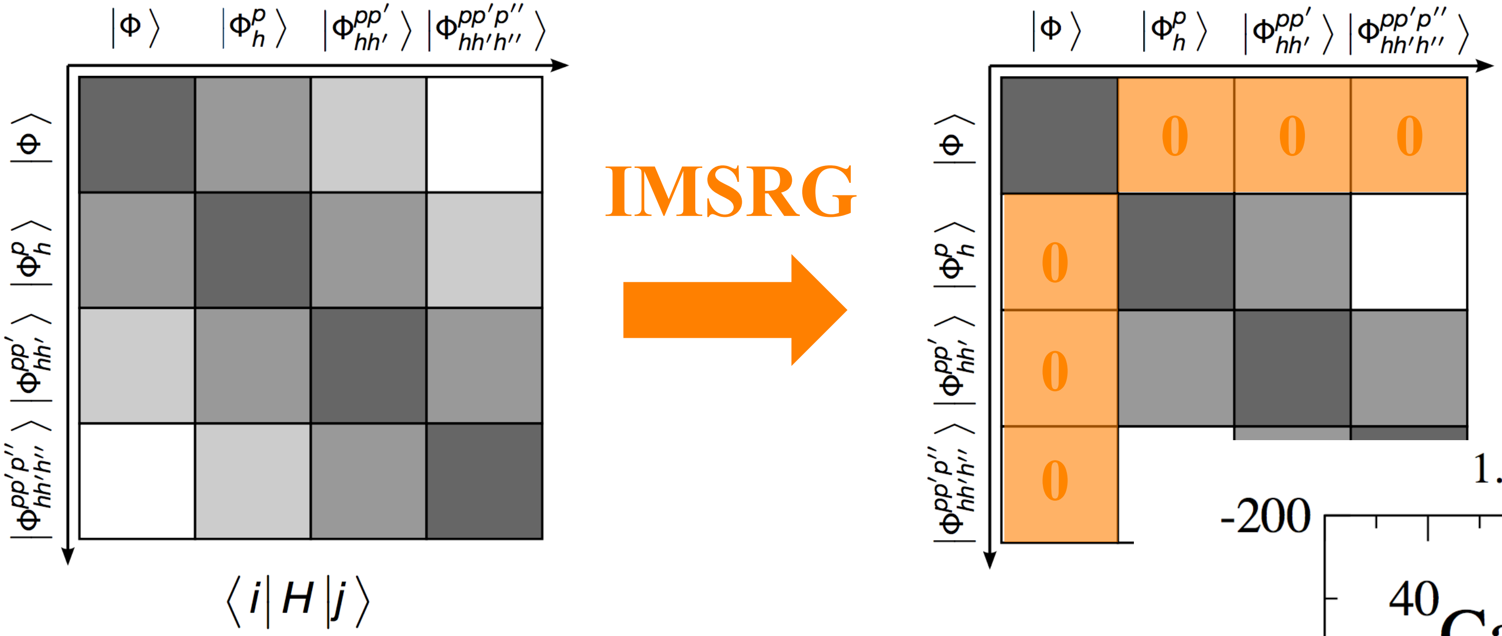
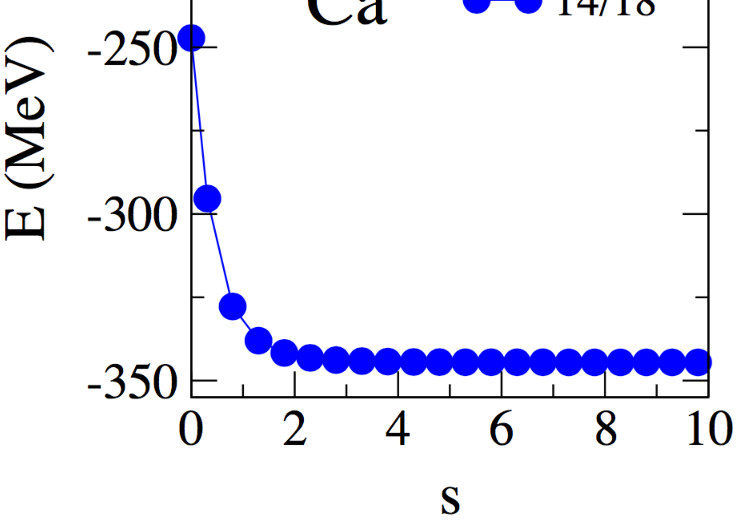


s = 0

$$H(s) = U(s)H(0)U^\dagger(s)$$

$$\frac{d}{ds}H(s) = [\eta(s), H(s)]$$

with generator $\eta(s) = [H_{\text{od}}(s), H_{\text{d}}(s)]$



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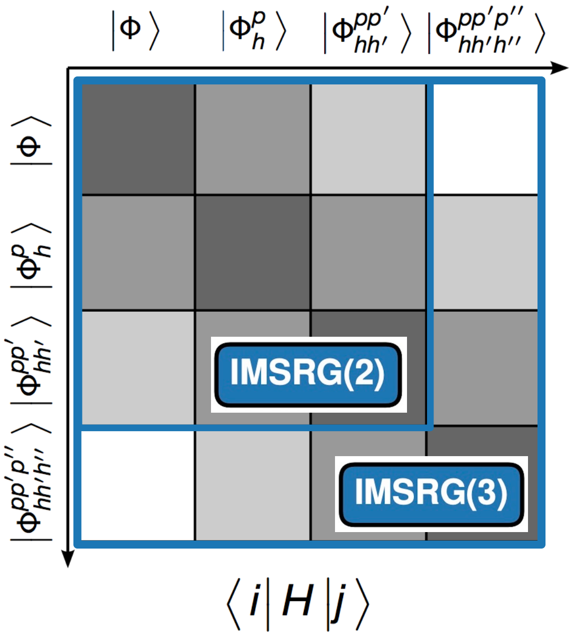
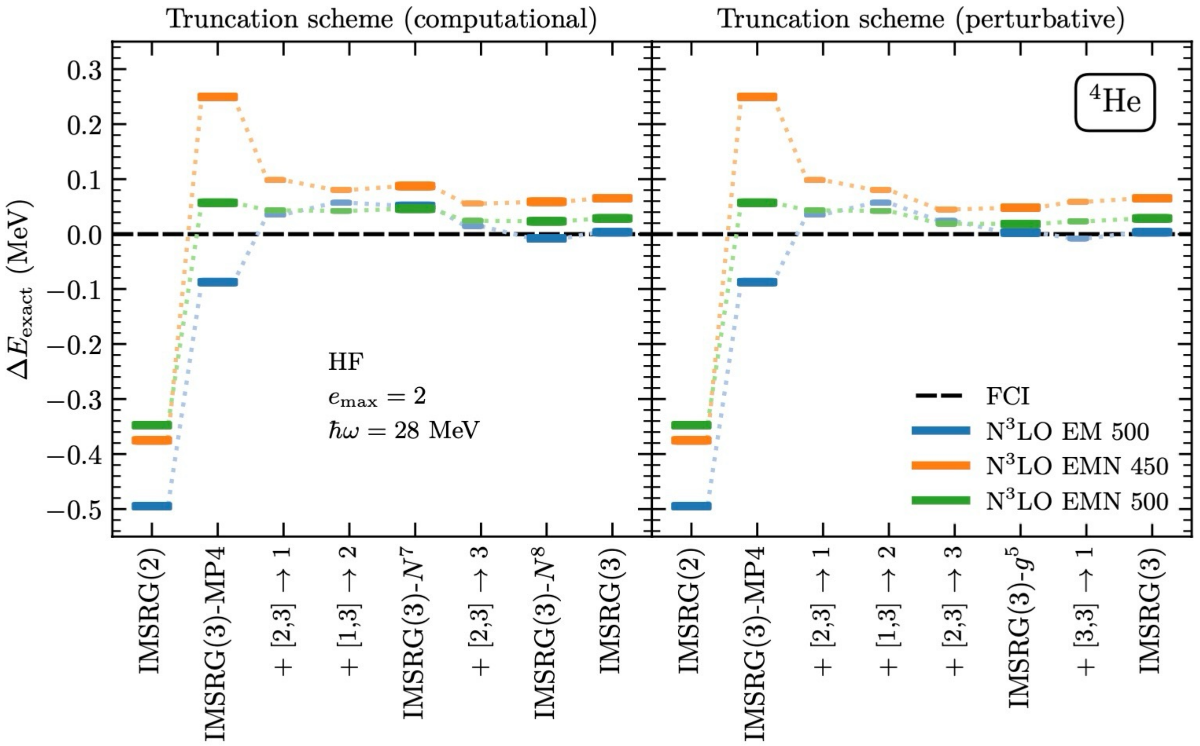
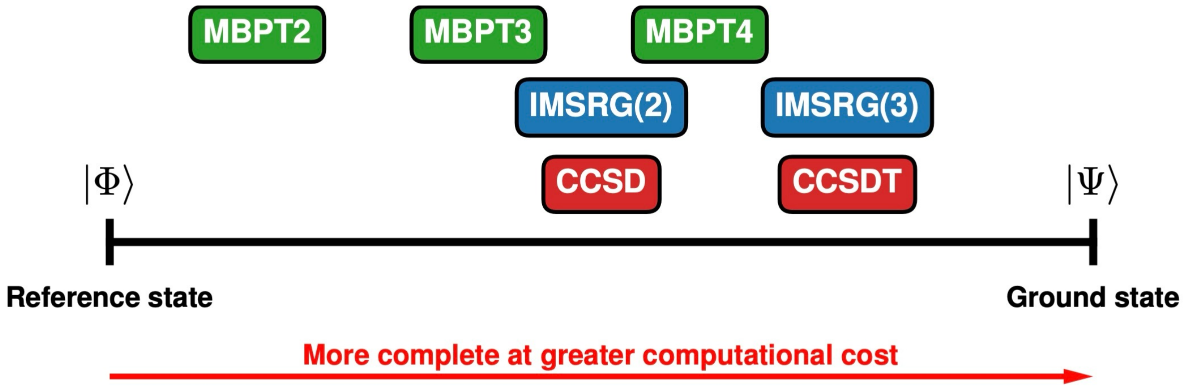




Standard truncation of IMSRG flow equations at normal-ordered 2-body level: IMSRG(2)



MBPT2

MBPT3

MBPT4

IMSRG(2)

IMSRG(3)

CCSD

CCSDT

$|\Phi\rangle$

$|\Psi\rangle$

Reference state

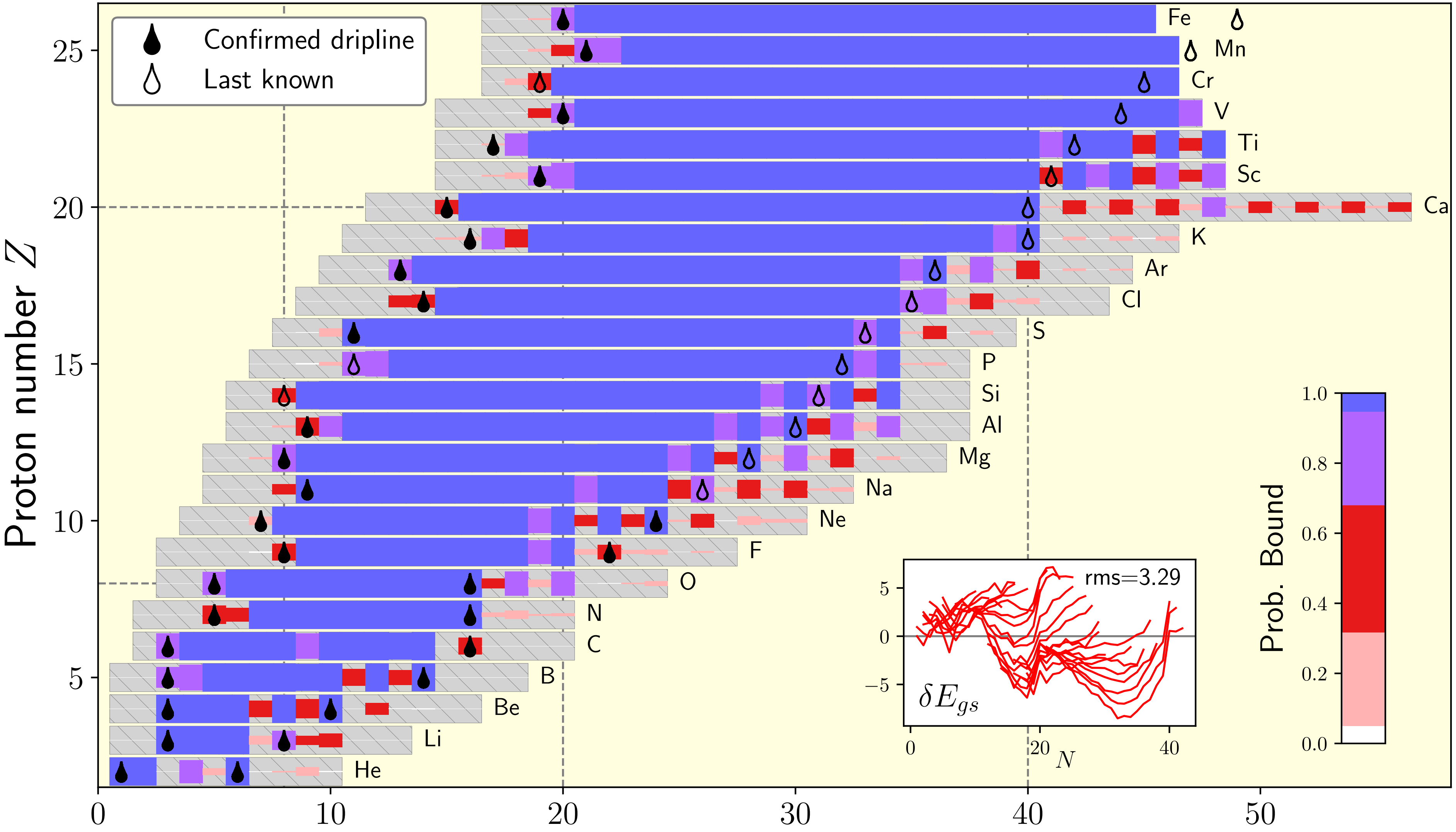
Ground state

More complete at greater computational cost

First IMSRG(3) results

Heinz et al., PRC (2021)

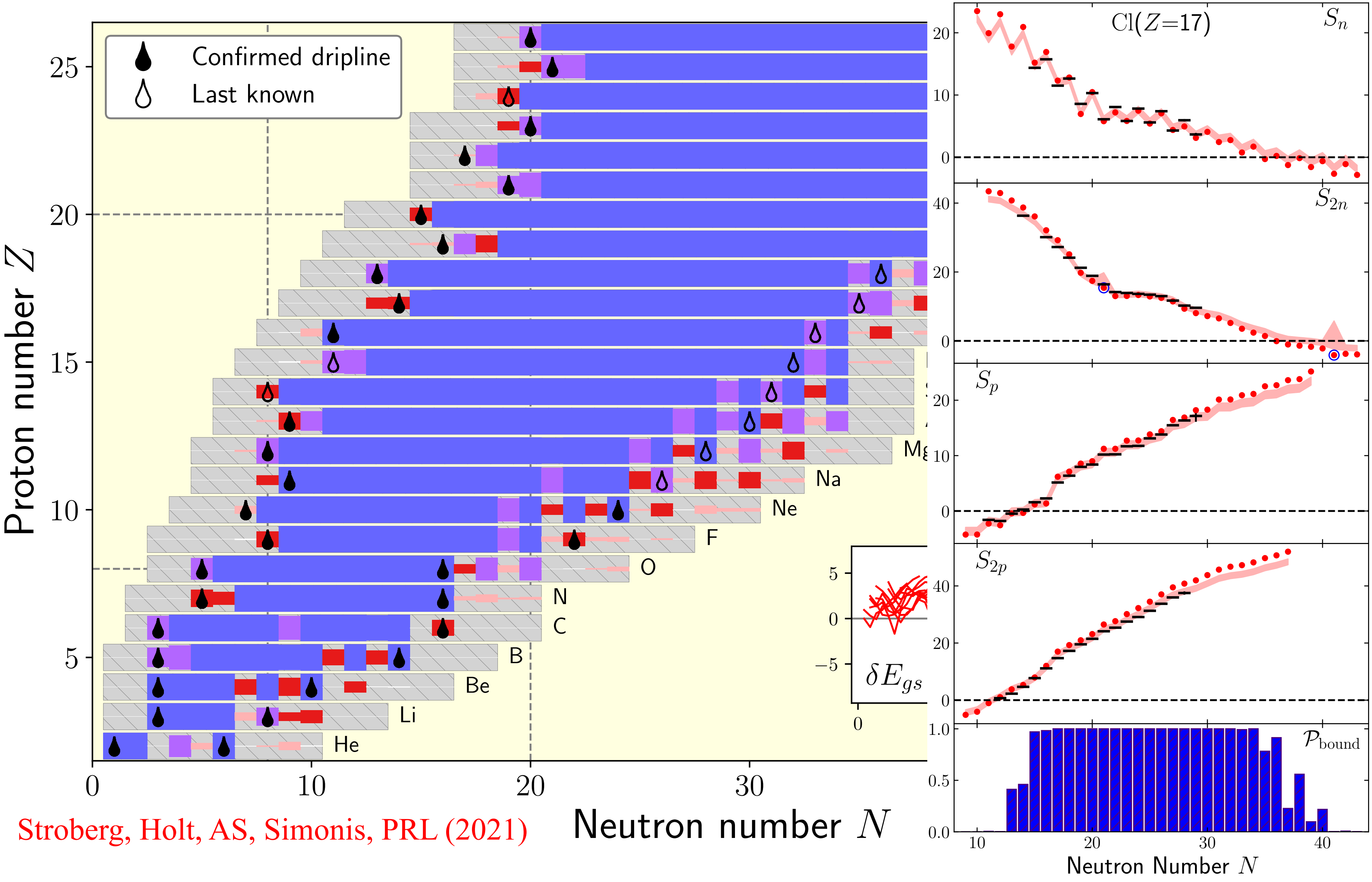
Nuclear landscape based on a chiral NN+3N interaction



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

ab initio is advancing to global theories, limitations due to input NN+3N

Nuclear landscape based on a chiral NN+3N interaction



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

ab initio is advancing to global theories, limitations due to input NN+3N

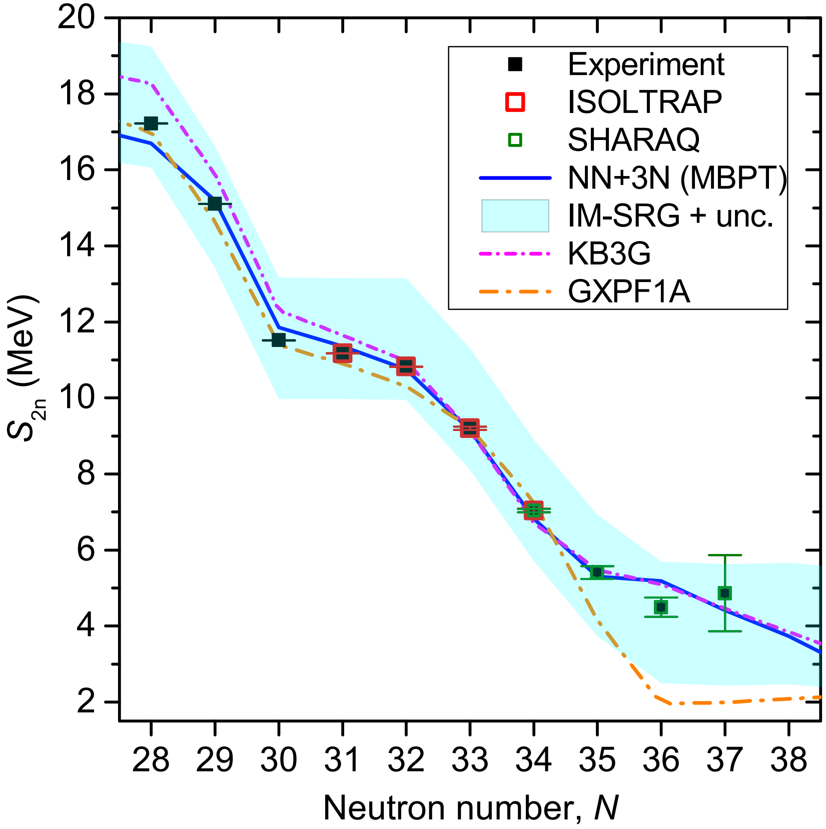
Highlights from ISOLDE/CERN and RIBF/RIKEN

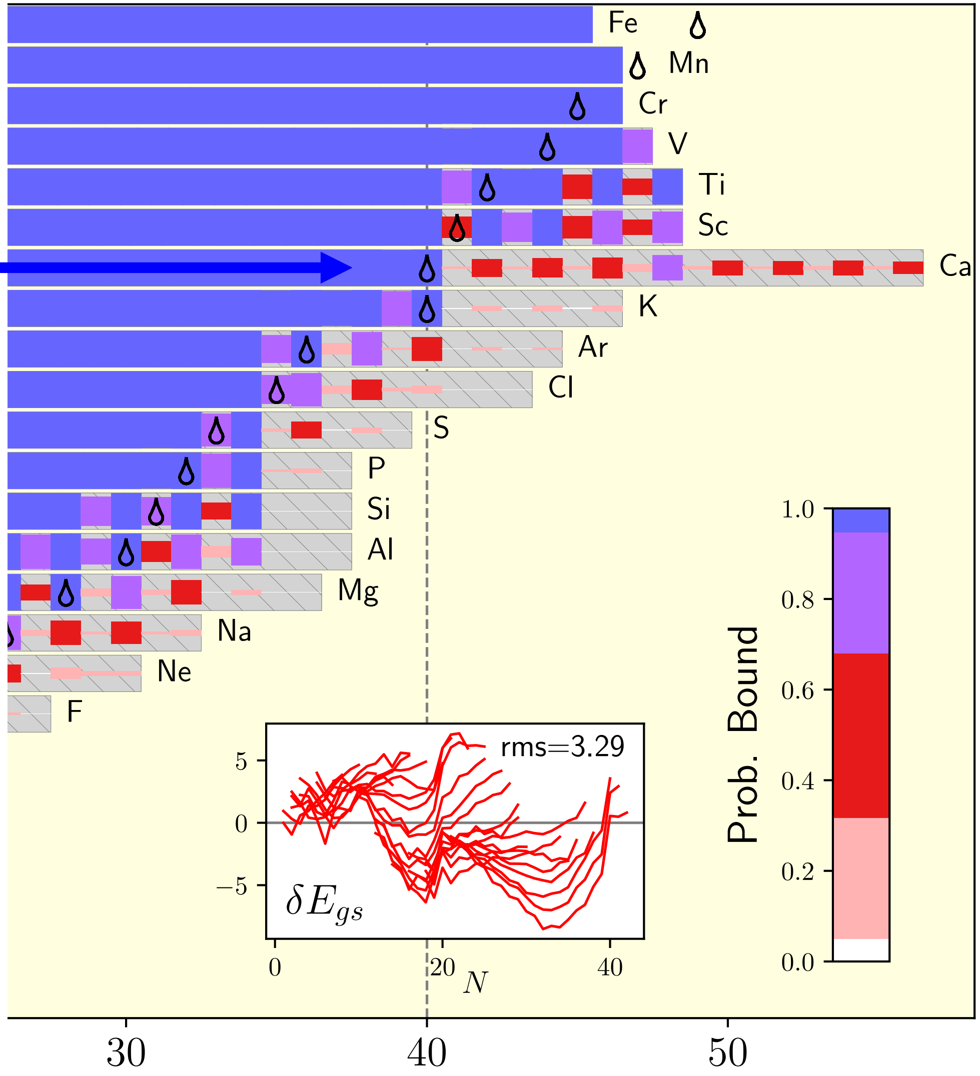
active exp-theory collaborations

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

Wienholtz et al., Nature (2013)

Michimasa et al., PRL (2019)





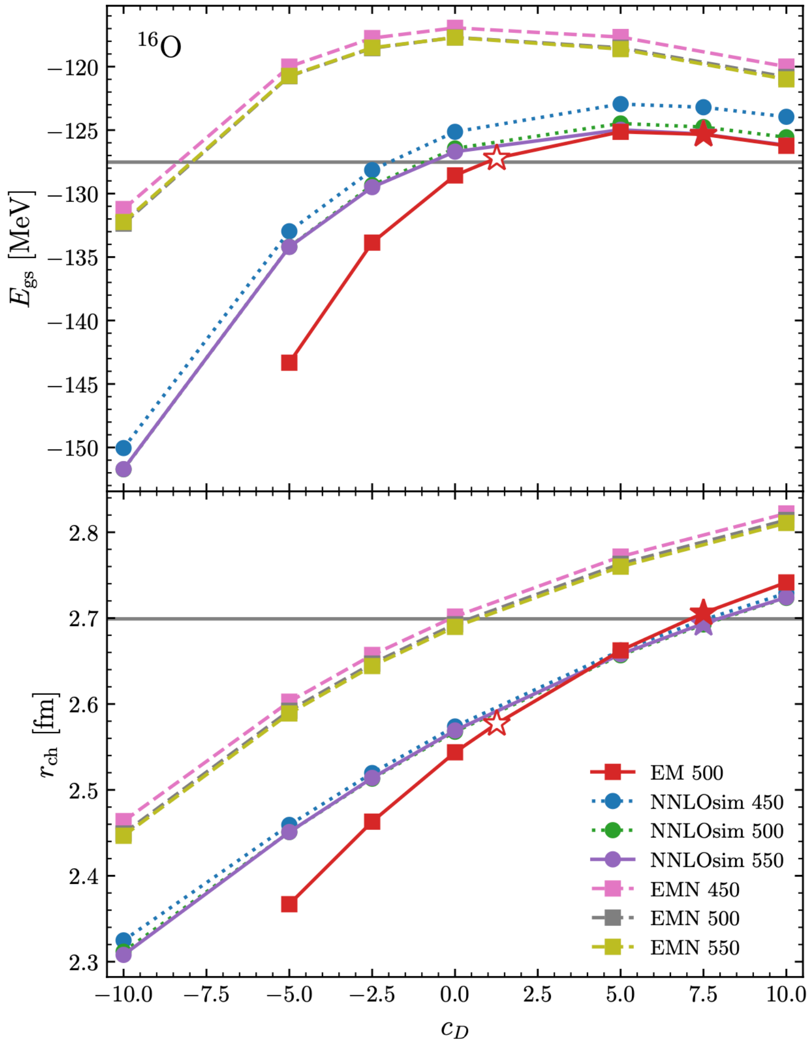
importance of 3N interactions
for neutron-rich shell structure

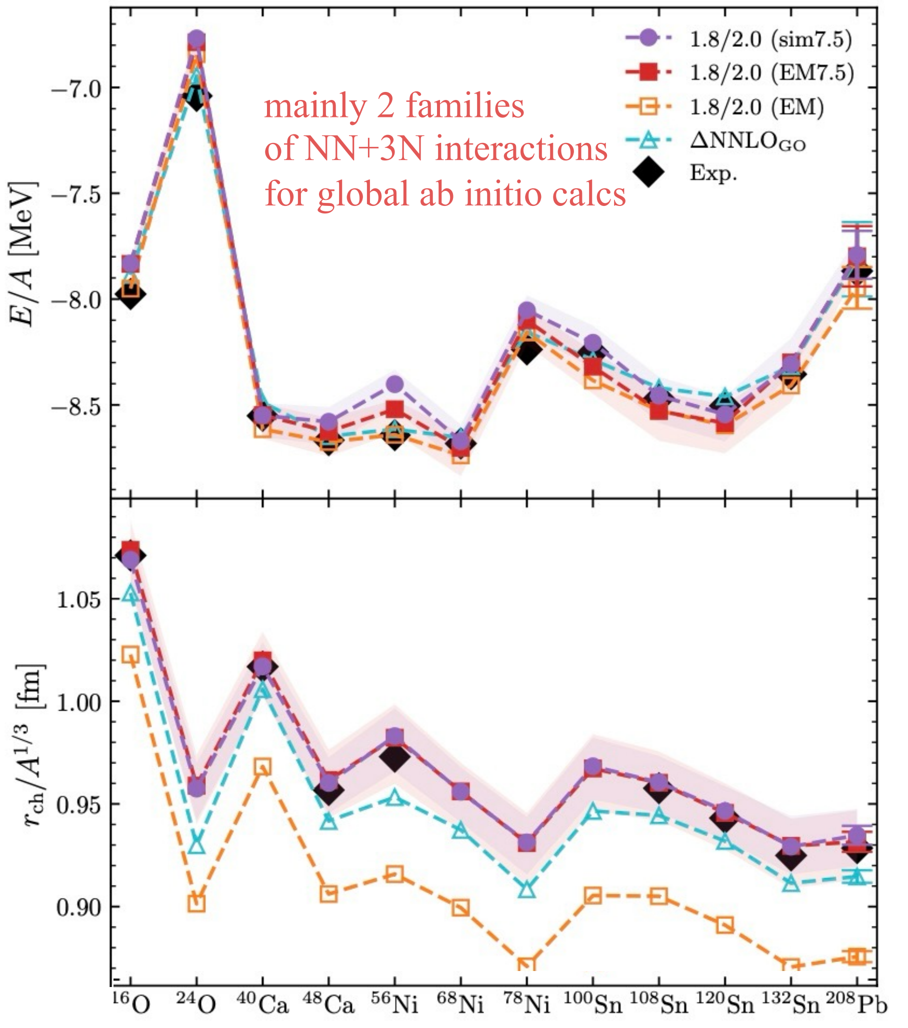
New chiral low-resolution interactions

Arthuis, Hebeler, AS, arXiv:2401.06675, see Kai Hebeler's talk

based on SRG-evolved NN interactions, 3N couplings fit to ^{3}H and ^{16}O

accurate for ground-state properties from ^{16}O to ^{208}Pb





mainly 2 families of NN+3N interactions for global ab initio calcs

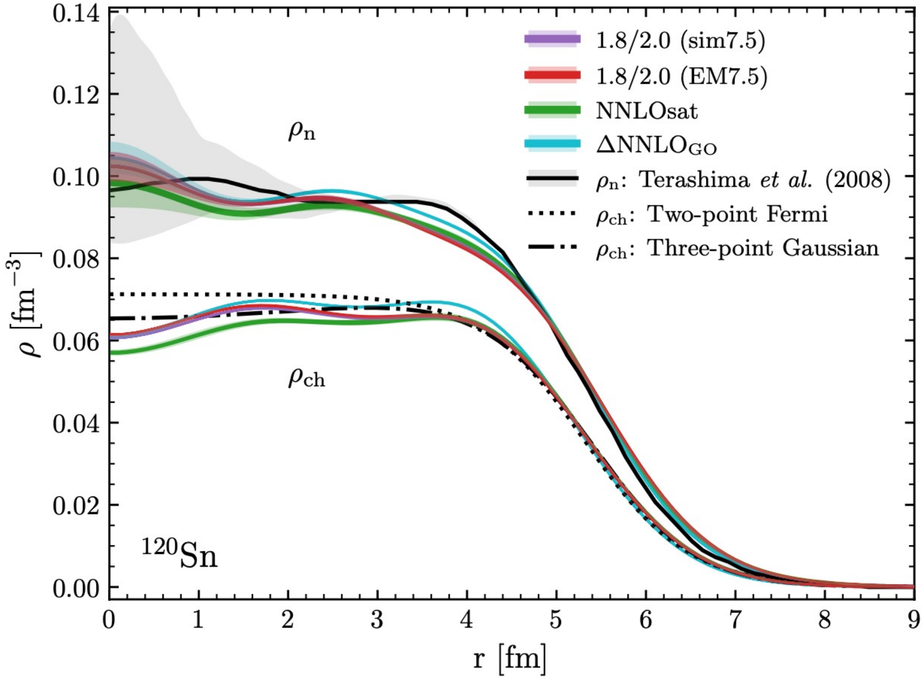
Neutron/proton density distributions in medium-heavy nuclei

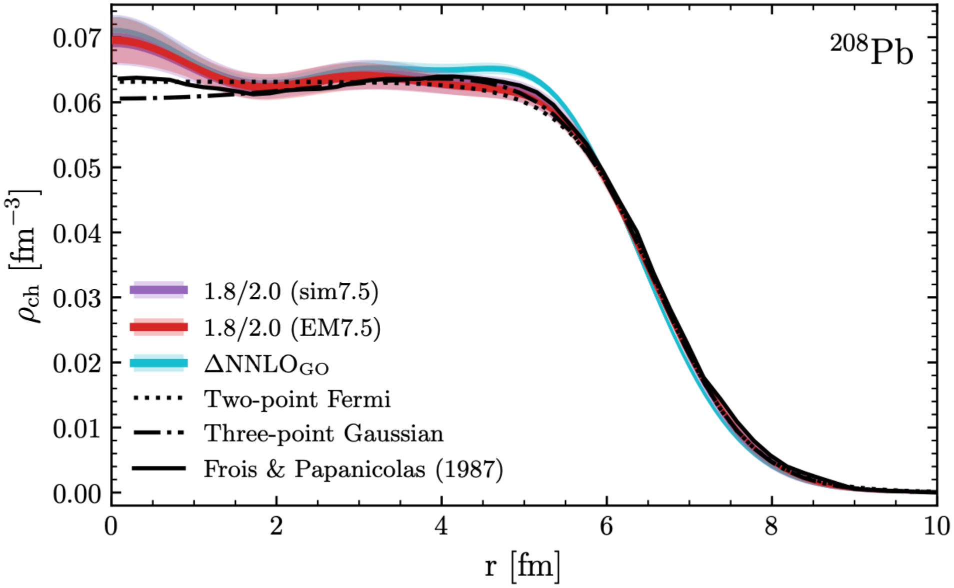
Arthuis, Hebeler, AS, arXiv:2401.06675

based on SRG-evolved NN interactions, 3N couplings fit to ^{3}H and ^{16}O

accurate for ground-state properties from ^{16}O to ^{208}Pb

very good agreement for density distributions in ^{120}Sn and ^{208}Pb



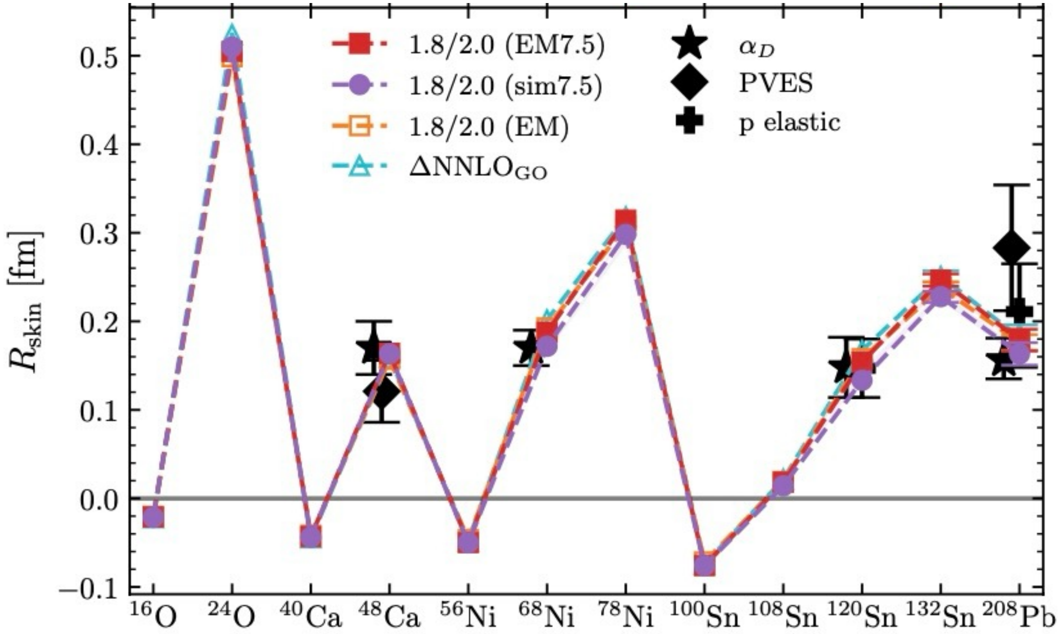


Neutron skins

Arthuis, Hebeler, AS, arXiv:2401.06675

very model independent

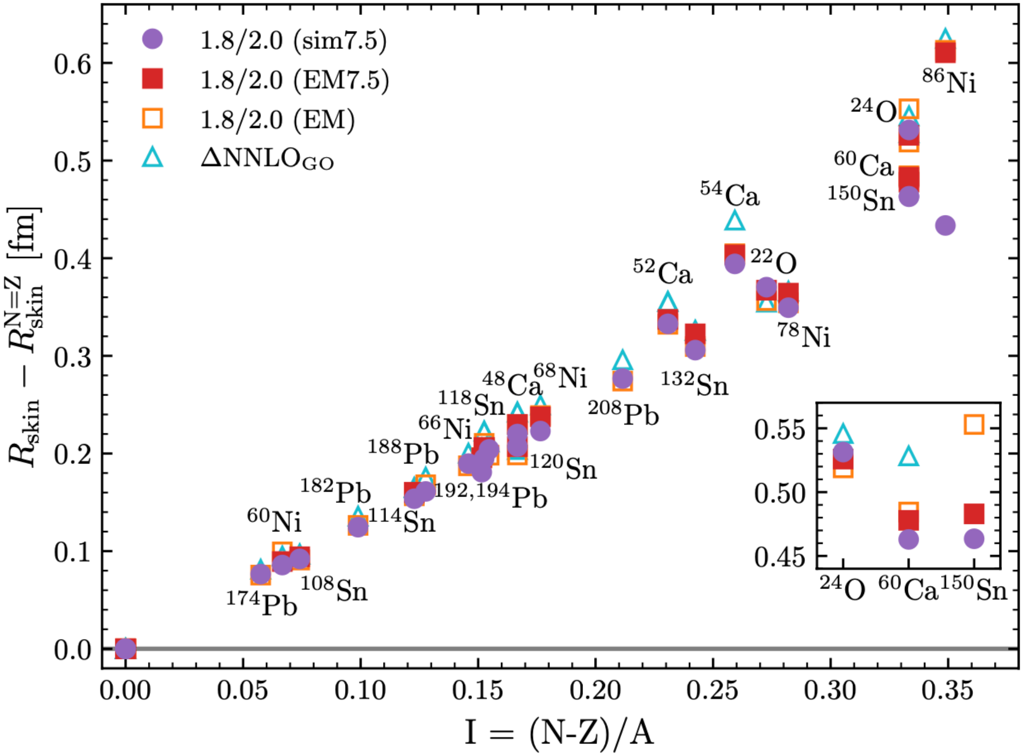
based on new (and previous) chiral NN+3N interactions



dependence of neutron skin corrected for Coulomb is linear in isospin

see also Novario et al., PRL (2023)

interesting predictions for extreme n-rich nuclei



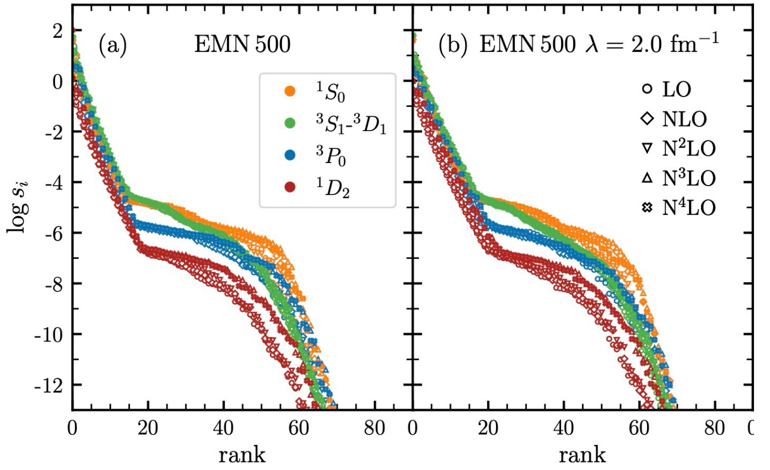
EFT uncertainties for SRG-evolved interactions

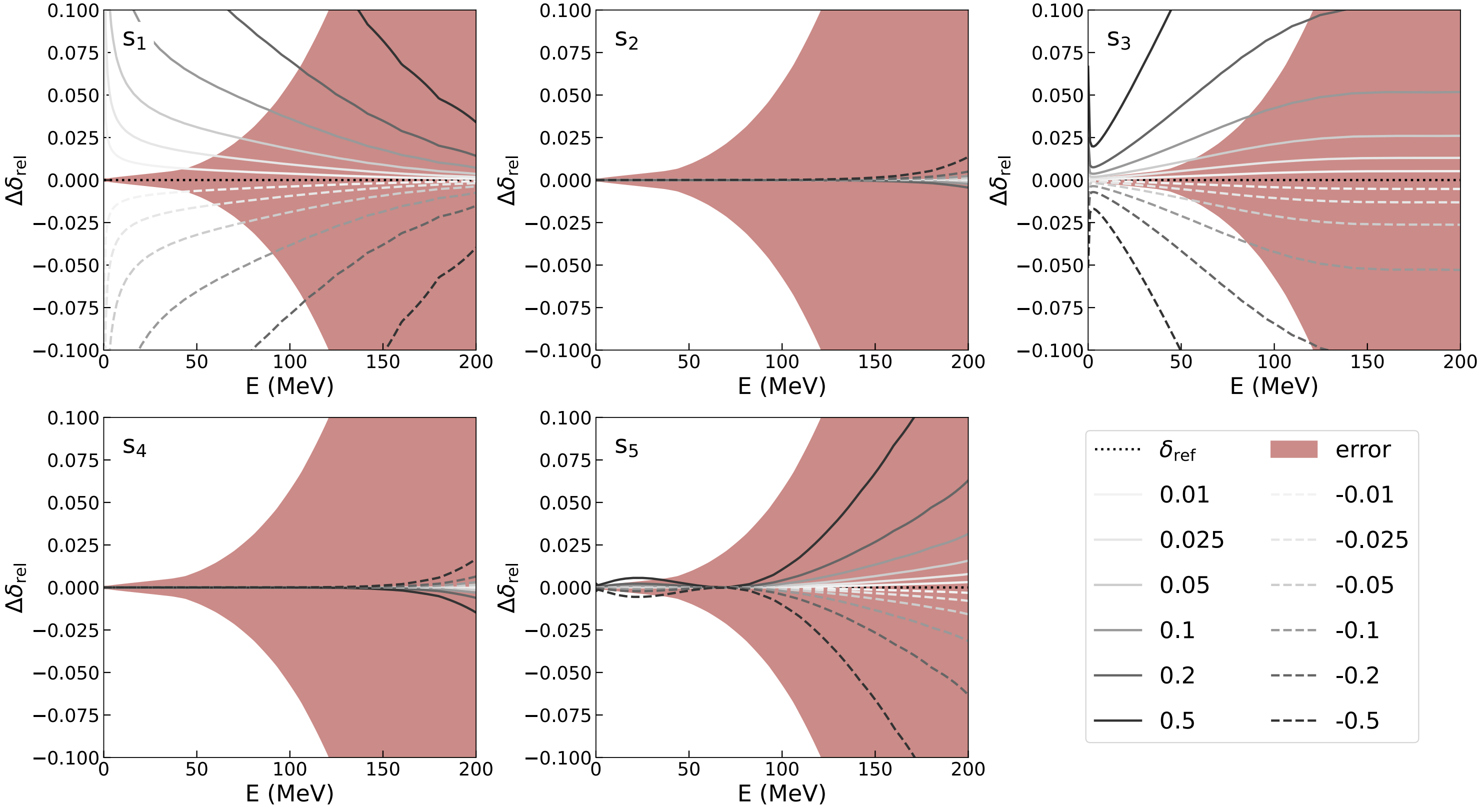
work of Tom Plies and Matthias Heinz, preliminary

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

consider lowest 5 singular values/operators

effectively 3 generate phase shift variation





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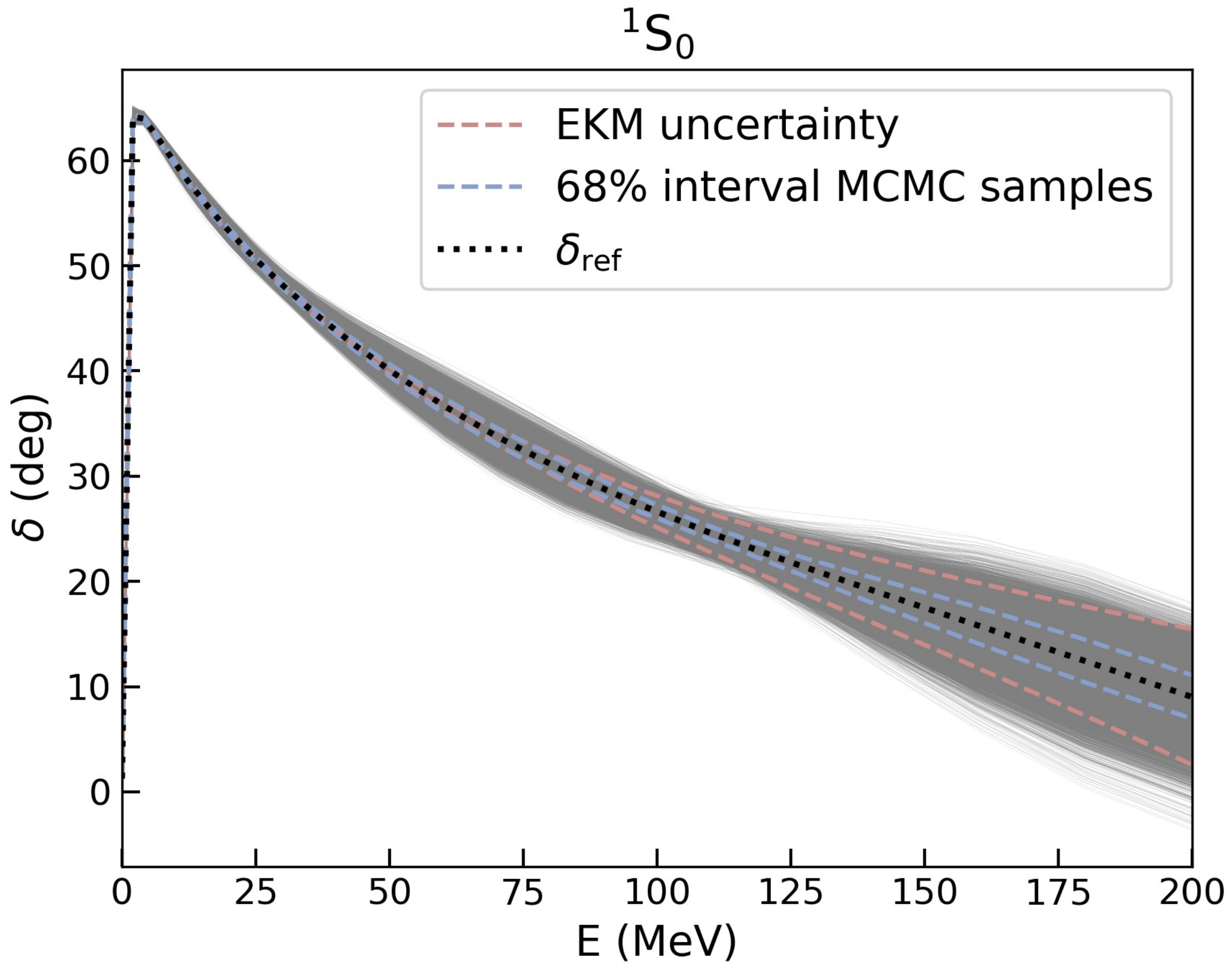
work of Tom Plies and Matthias Heinz, preliminary

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



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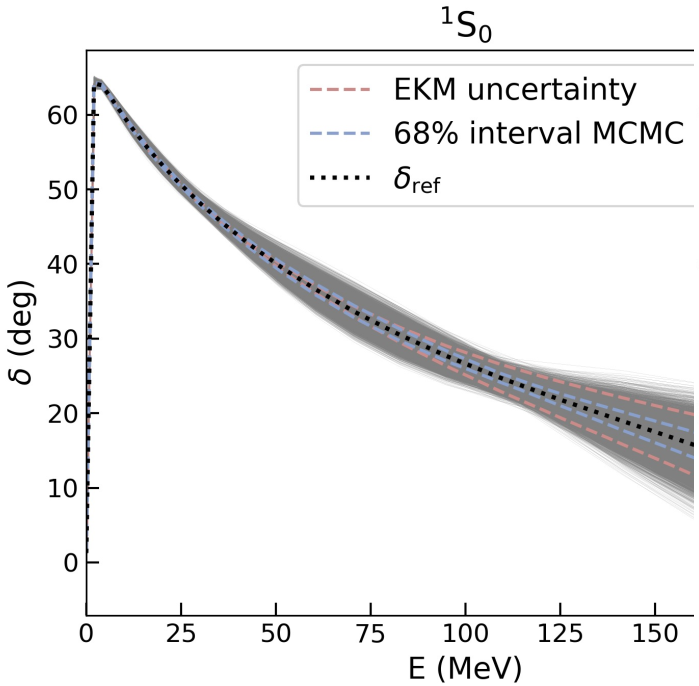
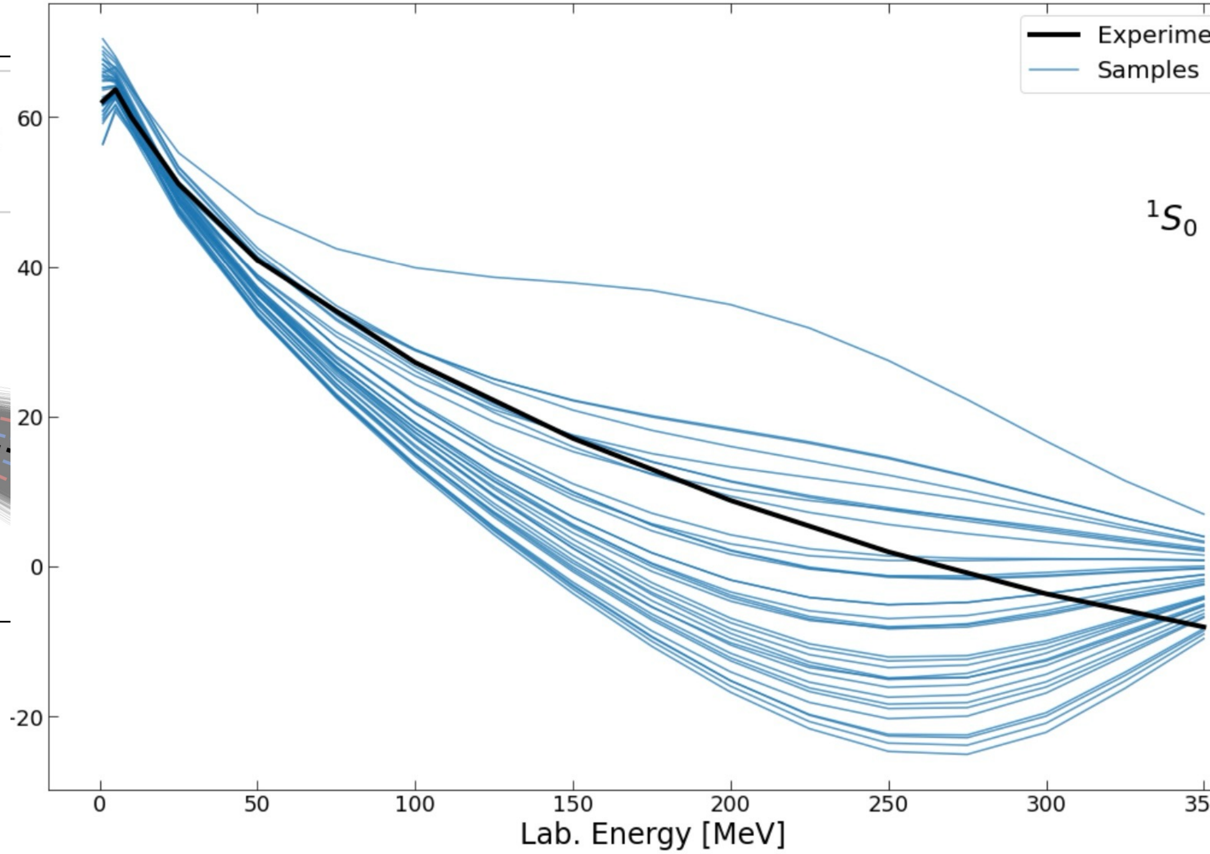




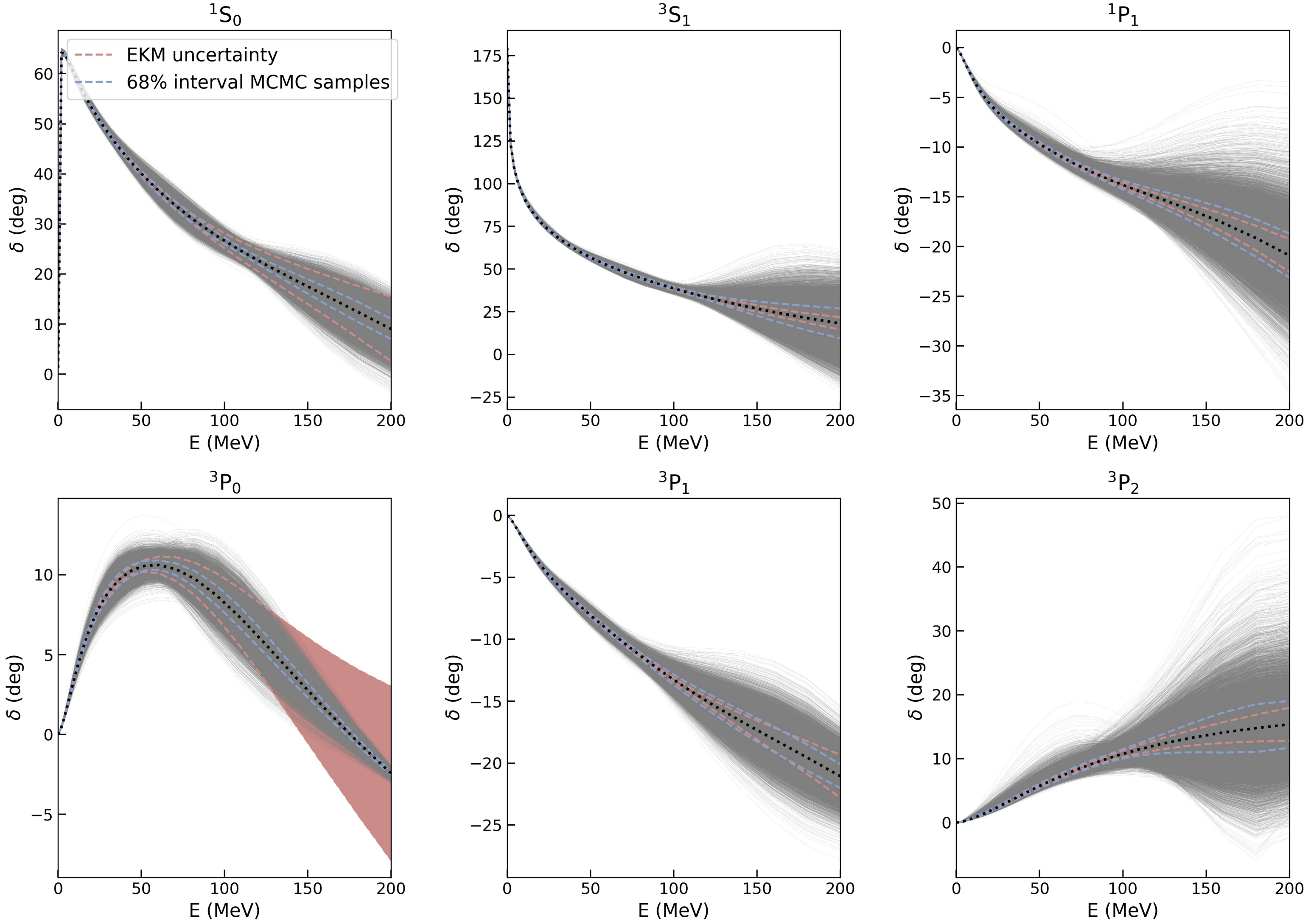
comparison to nonimplausible ΔN^2LO interactions Ekström, Forssen et al.

EFT uncertainties for SRG-evolved interactions

work of Tom Plies and Matthias Heinz, preliminary

generate range of low-resolution NN interactions

here: SRG-evolved EMN, S and P waves, higher partial waves unvaried



EFT uncertainties for SRG-evolved interactions

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generate range of low-resolution NN interactions

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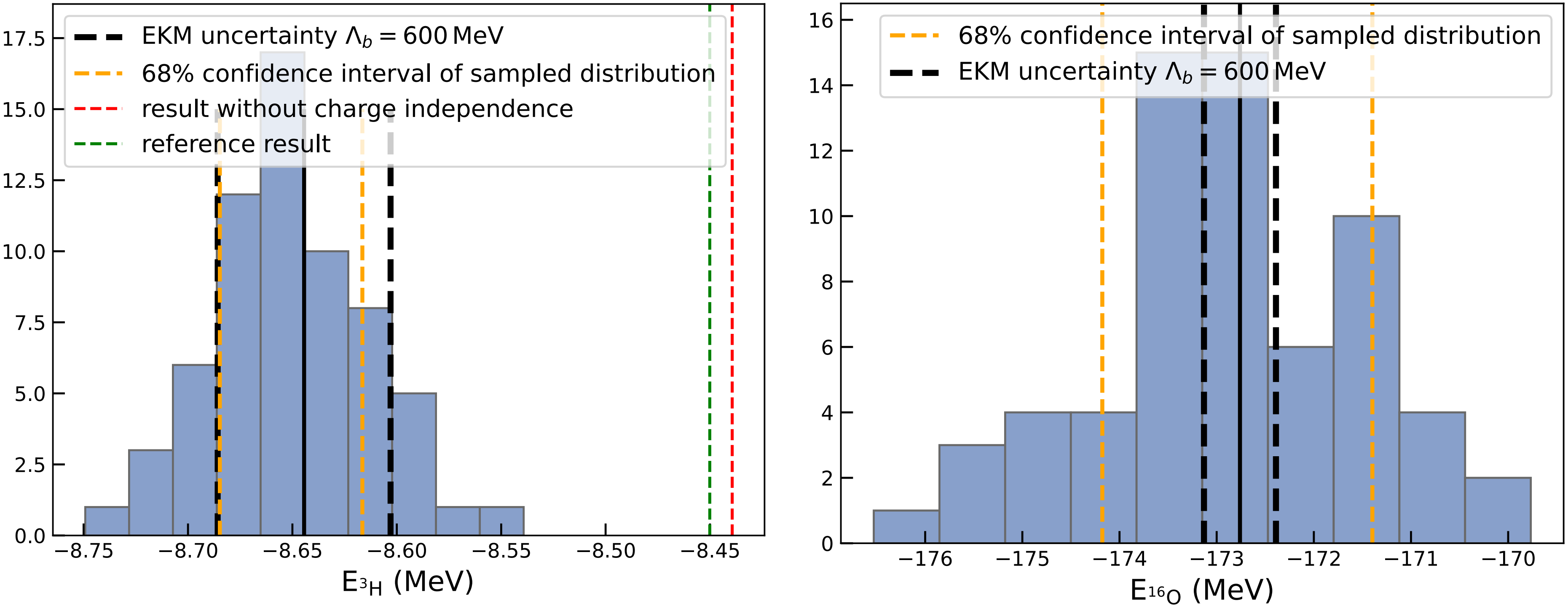
resulting posterior distributions for ^{3}H and ^{16}O ground-state energies



^{3}H uncertainties agree well with EKM, ^{16}O broader (good!)

next steps: improve sampling and include 3N interactions

Isotope shifts in ^{168,170,172,174,176}Yb

Door, Yeh, Heinz, Kirk, Lyu, Miyagi et al., arXiv:2403.07792

isotope shifts of atomic transitions

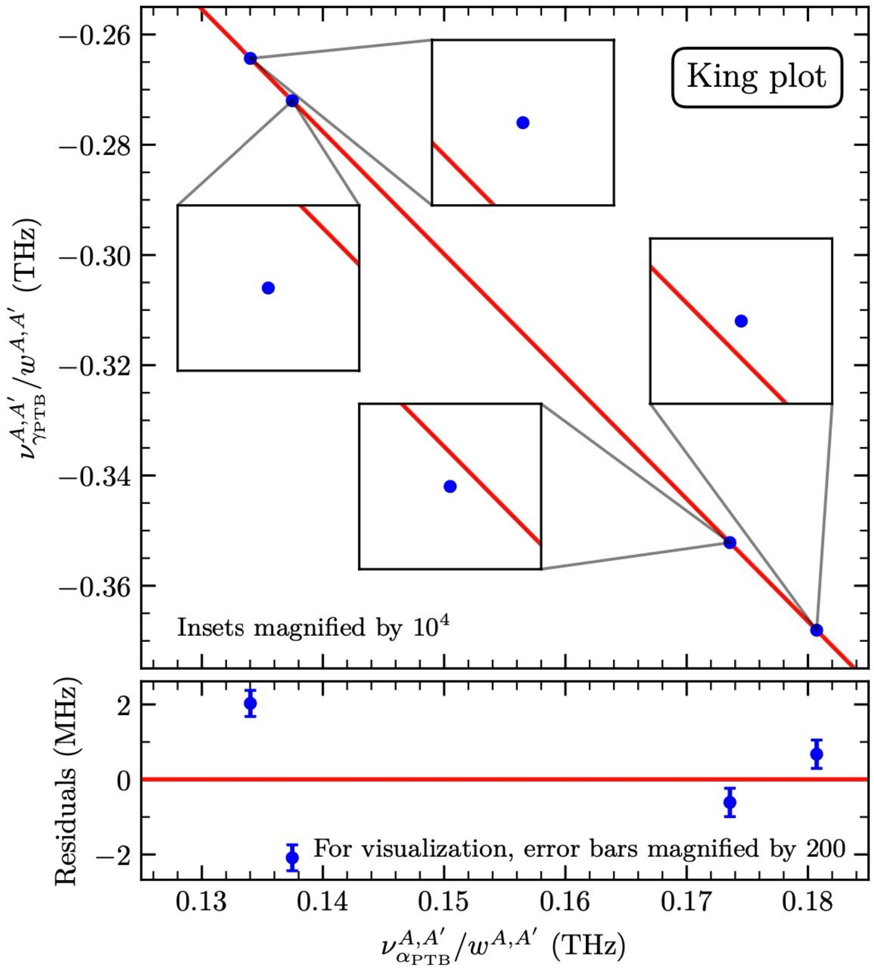
$$\nu_\tau^{A,A'} = \nu_\tau^{A} - \nu_\tau^{A'} \approx \underset{\textbf{mass shift}}{K_\tau w^{A,A'}} + \underset{\textbf{field shift}}{F_\tau \delta\langle r^2\rangle^{A,A'}}$$

leading terms give linear King plot

nonlinearities from higher-order **Standard Model** and **BSM**

$$\nu_{\tau,\text{nonlin.}}^{A,A'} = \underset{\textbf{higher-order nuclear structure}}{G_\tau^{(2)}(\delta\langle r^2\rangle^2)^{A,A'} + G_\tau^{(4)}\delta\langle r^4\rangle^{A,A'}}$$

$$\underset{\textbf{possible new boson}}{+\frac{\alpha_{\text{NP}}}{\alpha_{\text{EM}}} D_\tau h^{A,A'}} + \dots$$



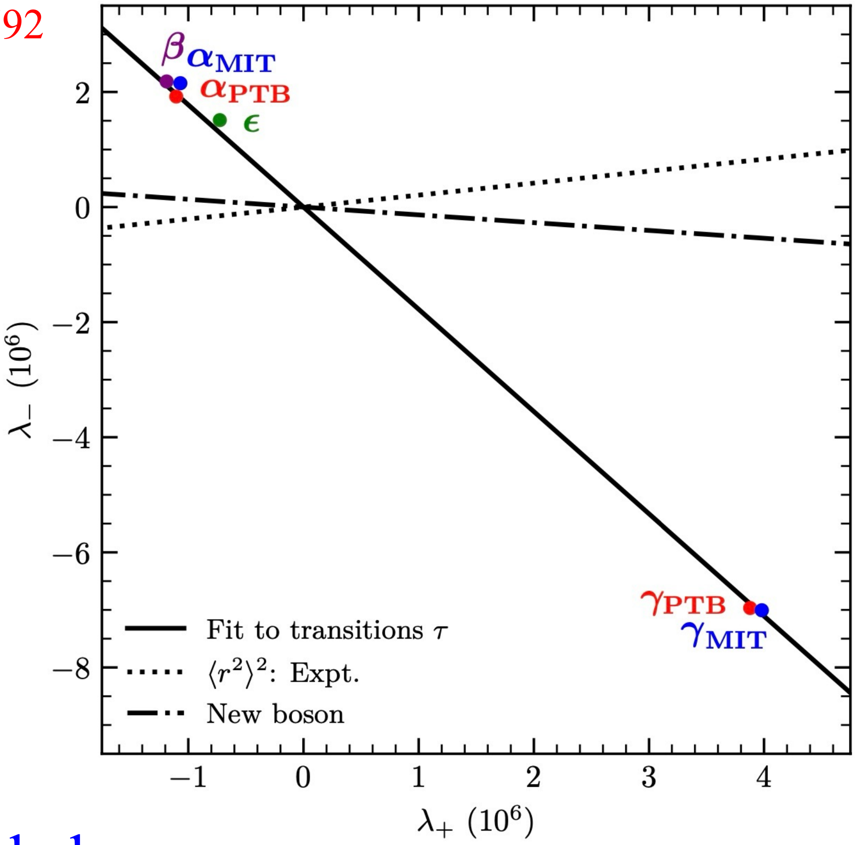
laser spectroscopy (PTB) + Penning trap mass measurements (MPIK) show clear nonlinearities

Isotope shifts in ^{168,170,172,174,176}Yb

Door, Yeh, Heinz, Kirk, Lyu, Miyagi et al., arXiv:2403.07792

nonlinearity decomposition suggests one dominant contribution

$$\nu^{A,A'}_{\tau,\mathrm{nonlin.}} = \underbrace{G^{(2)}_\tau(\delta\langle r^2\rangle^2)^{A,A'} + G^{(4)}_\tau\delta\langle r^4\rangle^{A,A'}}_{\text{higher-order nuclear structure}} \underbrace{+\frac{\alpha_{\mathrm{NP}}}{\alpha_{\mathrm{EM}}}D_\tau h^{A,A'}}_{\text{possible new boson}} + \ldots$$



→ not quadratic field shift

→ not new boson

theory predictions of quartic radius needed

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Door, Yeh, Heinz, Kirk, Lyu, Miyagi et al., arXiv:2403.07792

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→ not quadratic field shift

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theory predictions of quartic radius:

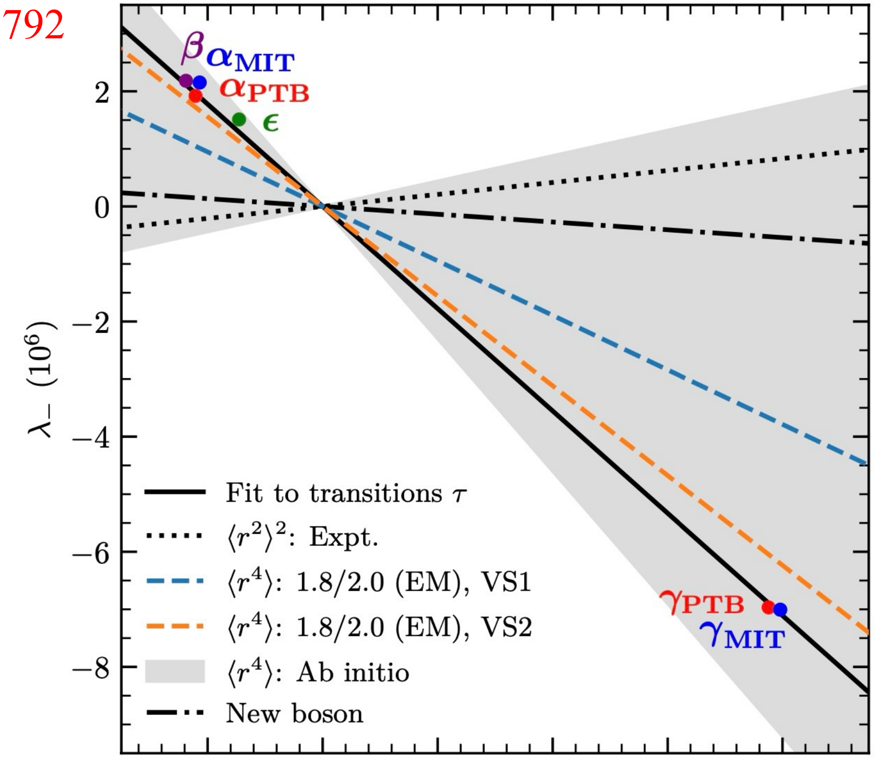
VS-IMSRG calculations,

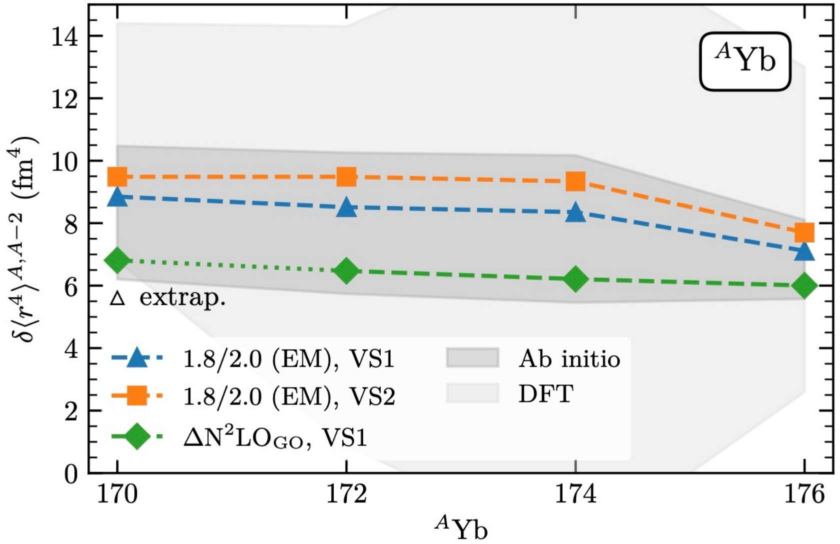
uncertainty estimates from:

1.8/2.0 (EM), $\Delta\mathrm{N}^2\mathrm{LO}_{\mathrm{GO}}$ interactions,

two valence spaces,

many-body estimated from IMSRG(3)





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$$\underbrace{+\frac{\alpha_{\text{NP}}}{\alpha_{\text{EM}}}D_{\tau}h^{A,A'}}_{\text{possible new boson}} + \ldots$$

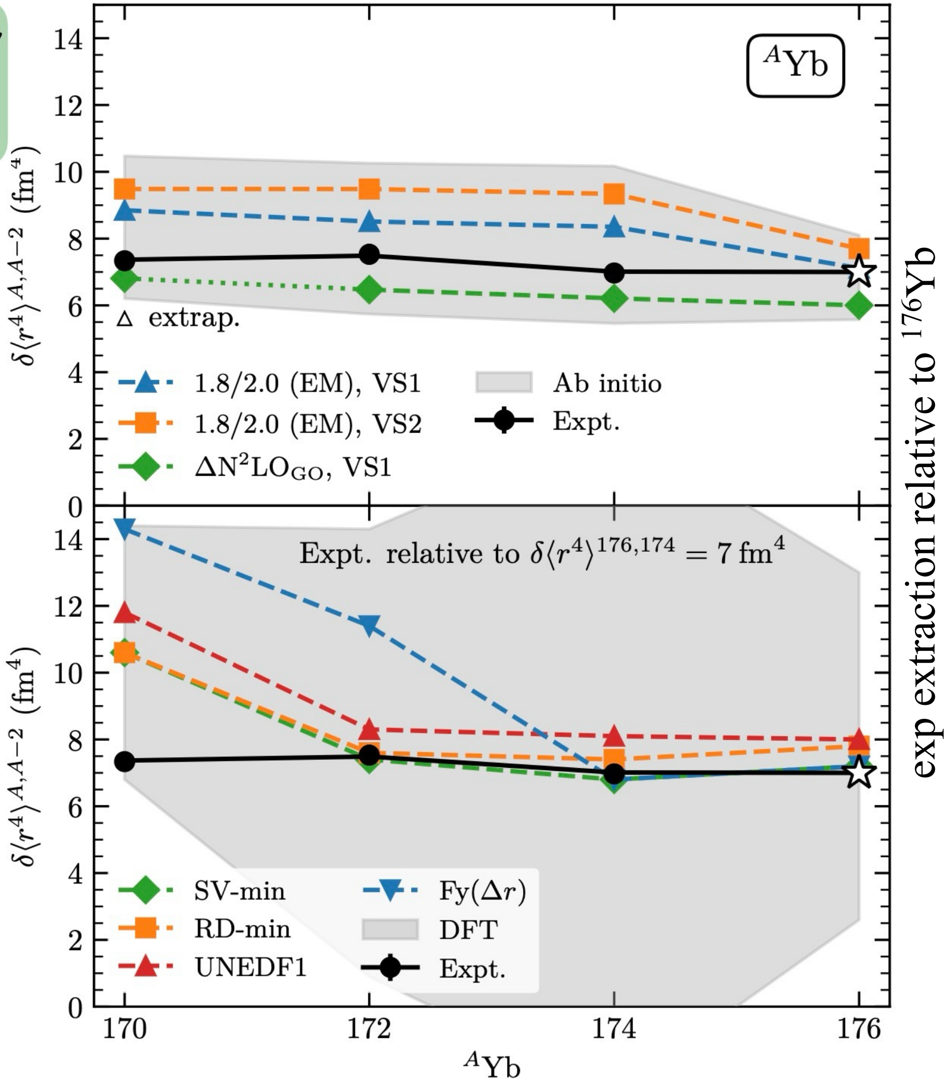
→ not quadratic field shift

→ not new boson

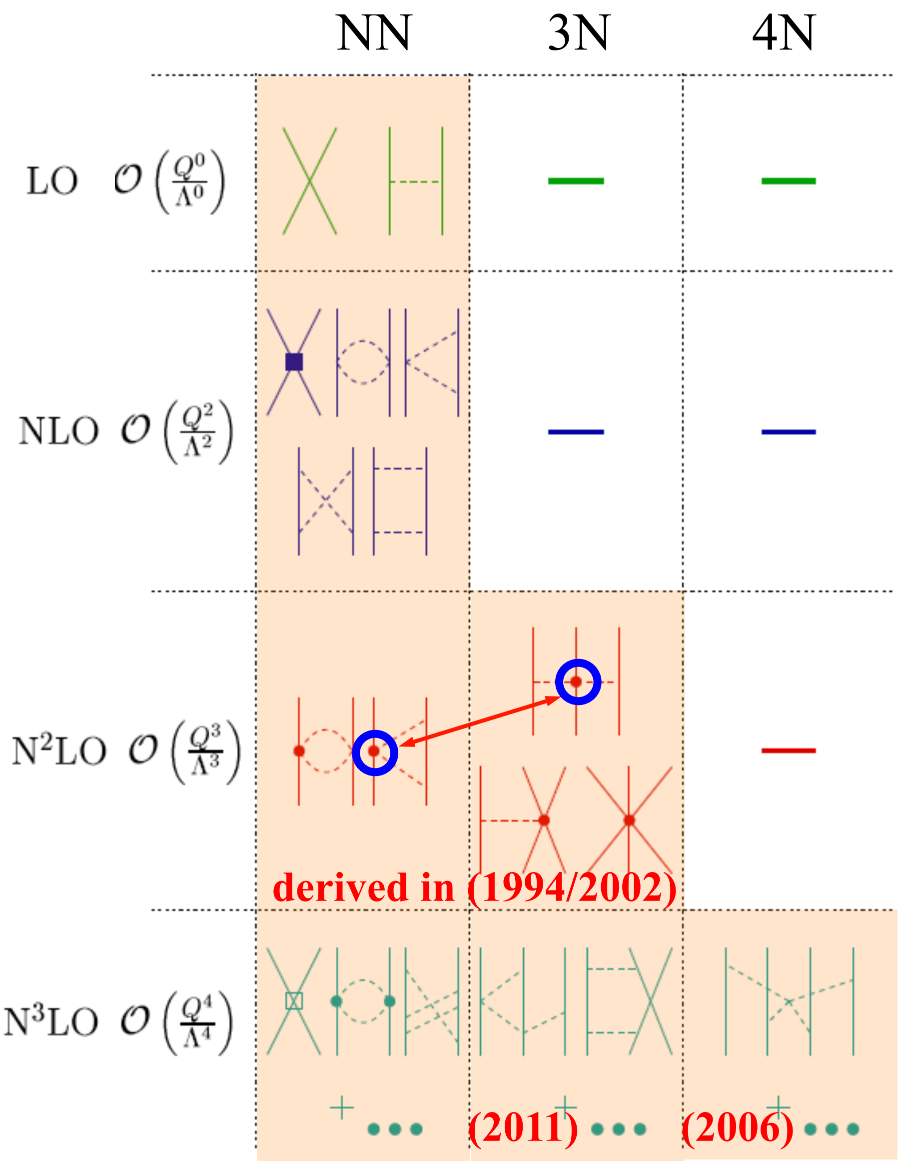
→ dominant nonlinearity from quartic radius term

NEW: extract quartic radius from experimental data:

observable related to deformation, trends consistent with ab initio

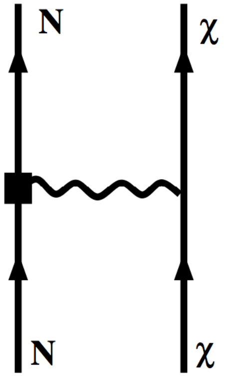


Chiral EFT for coupling to electroweak interactions

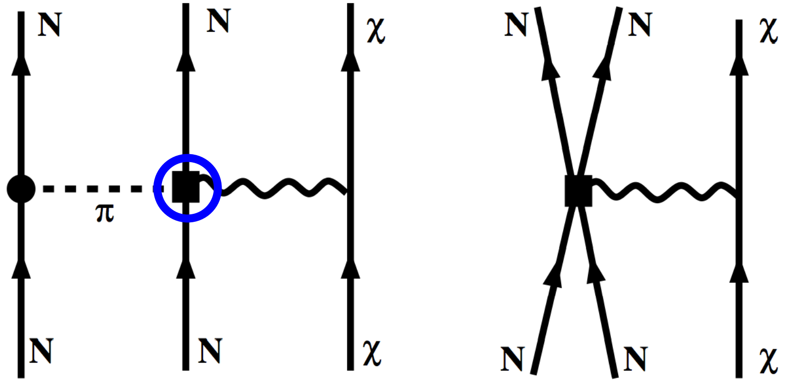


axial-vector currents (beta decays)

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



+ two-body currents at Q^3



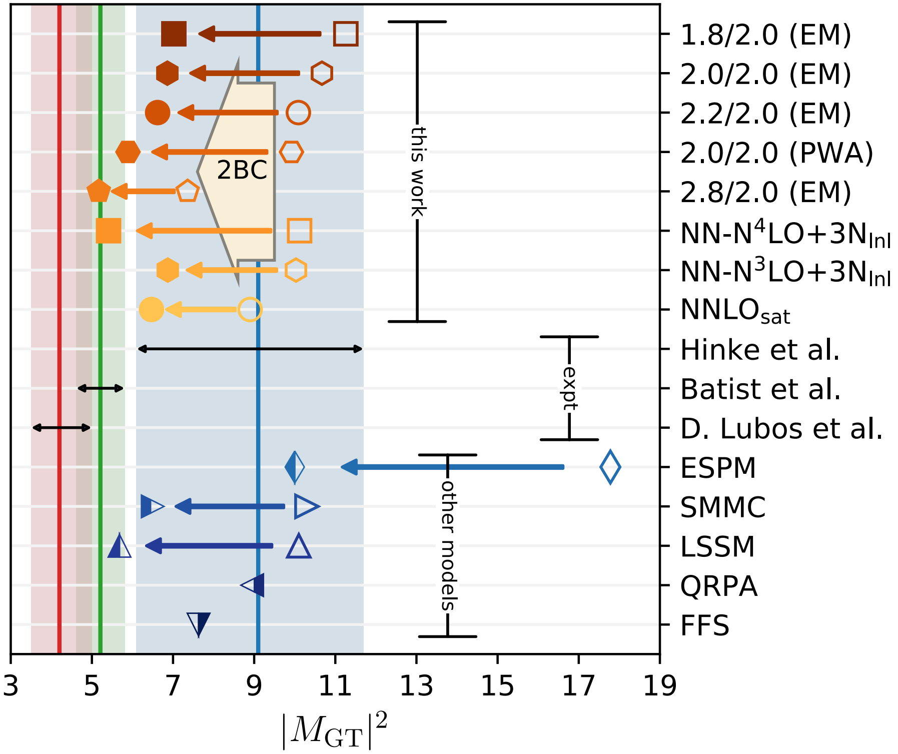
same couplings in forces and currents

Chiral EFT for coupling to electroweak interactions

consistent electroweak one- and two-body currents

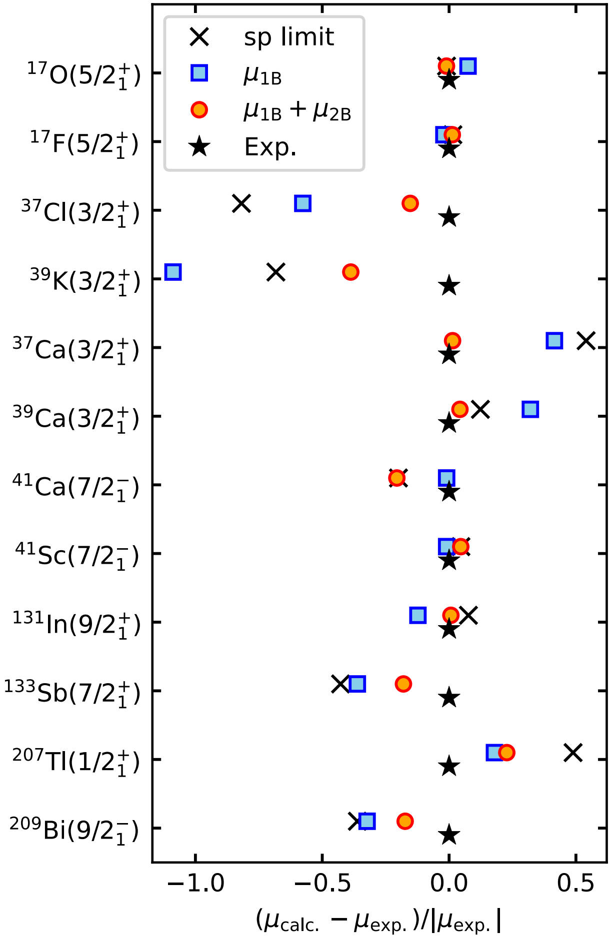
Gamow-Teller beta decay of ^{100}Sn

Gysbers et al., Nature Phys. (2019)



Magnetic moments of nuclei

Pastore et al. (2012-)



Miyagi et al., PRL (2024)

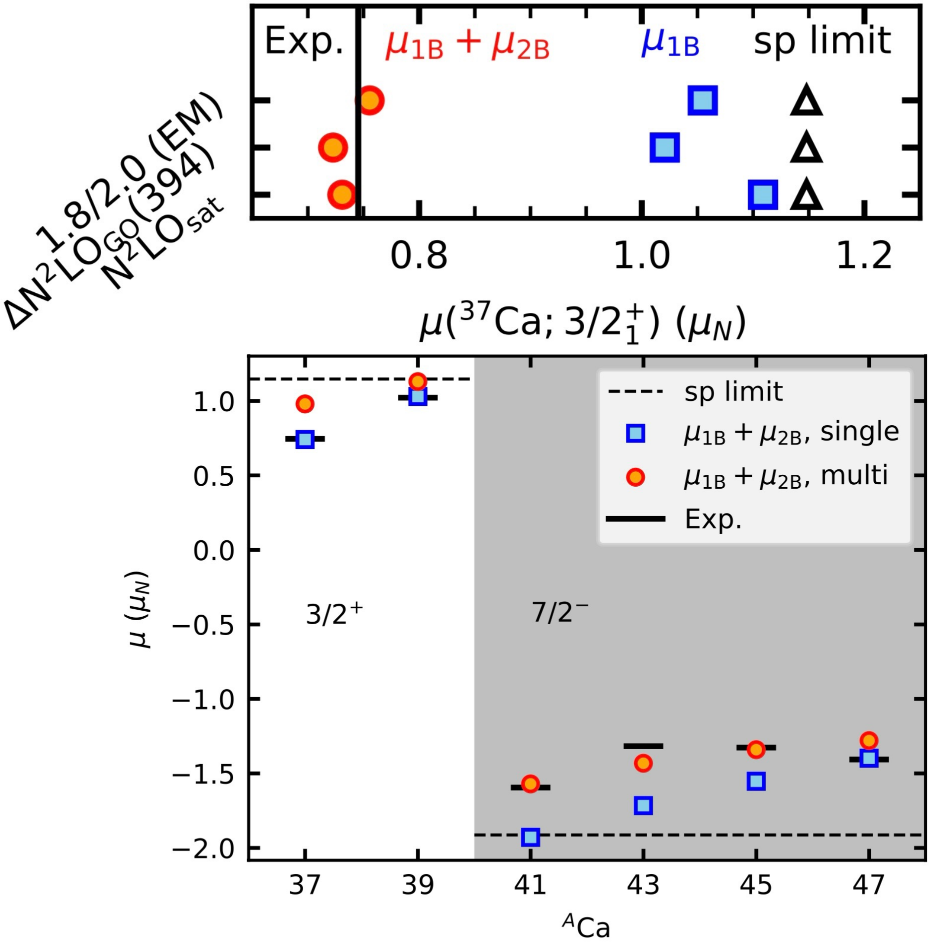
two-body currents (2BC) key for quenching puzzle of beta decays + always improve magnetic moments

Chiral EFT for coupling to electroweak interactions

consistent electroweak one- and two-body currents

Magnetic moments of nuclei

Pastore et al. (2012-)



Miyagi et al., PRL (2024)

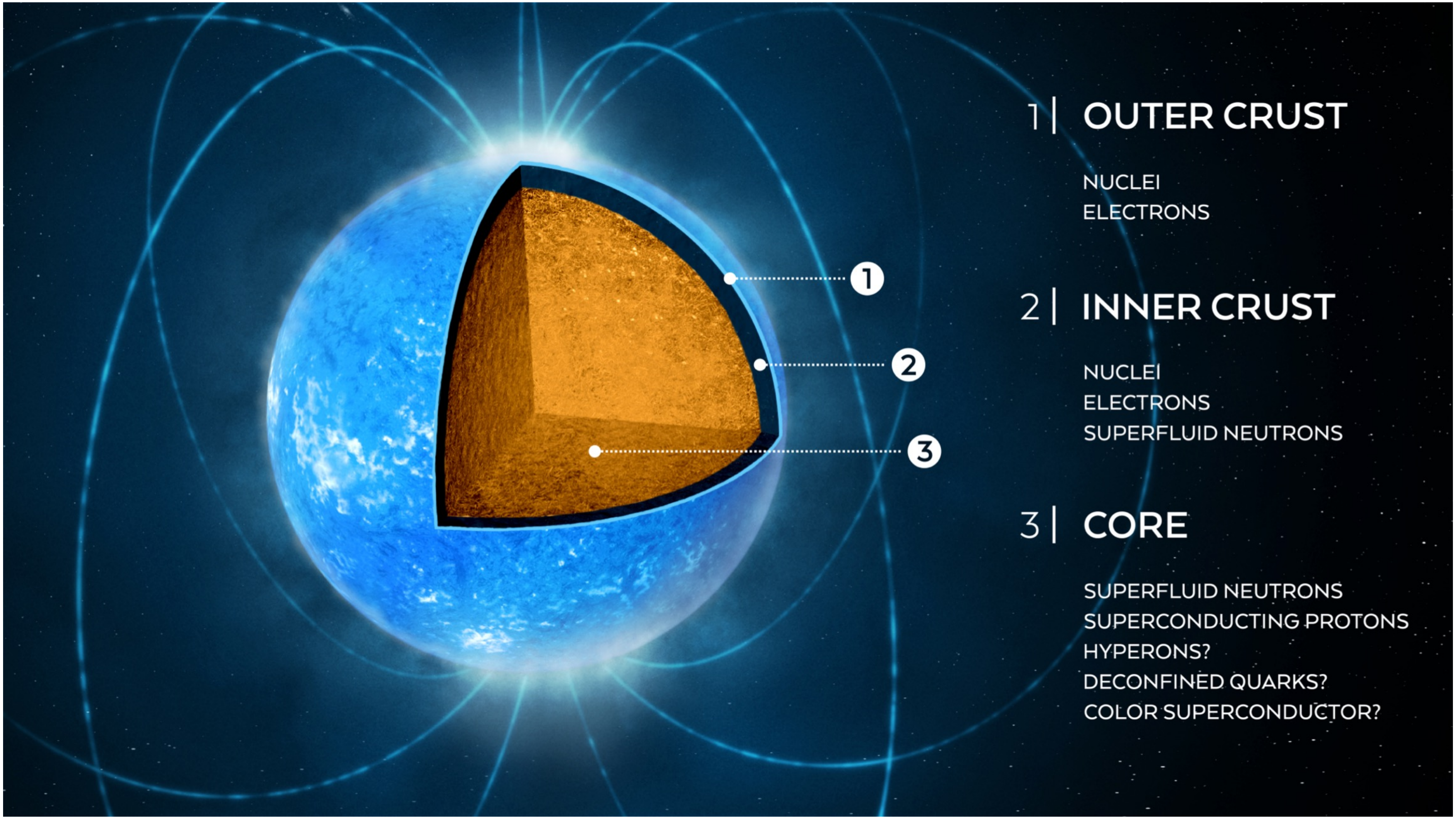
Interaction and many-body uncertainties explored, but need to work on order-by-order uncertainties

two-body currents (2BC) key for quenching puzzle of beta decays + always improve magnetic moments

Extreme matter in neutron stars

governed by the same strong interactions:

chiral EFT sets pressure of first few km to inside



1 | OUTER CRUST

NUCLEI
ELECTRONS

2 | INNER CRUST

NUCLEI
ELECTRONS
SUPERFLUID NEUTRONS

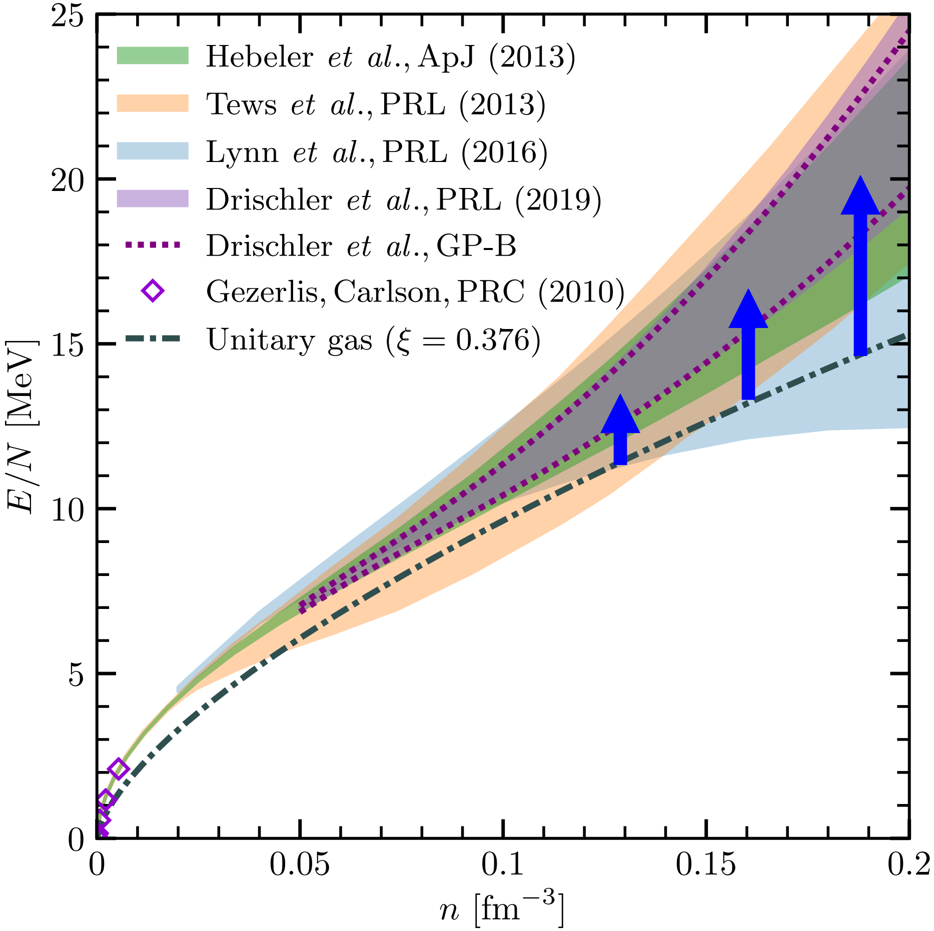
3 | CORE

SUPERFLUID NEUTRONS
SUPERCONDUCTING PROTONS
HYPERONS?
DECONFINED QUARKS?
COLOR SUPERCONDUCTOR?

Watts et al., RMP (2016)

Chiral EFT calculations of neutron matter

good agreement up to saturation density for neutron matter including NN, 3N, 4N interactions up to N^3LO



comparison from Huth et al., PRC (2021)

slope determines pressure of neutron matter

comparison to unitary Fermi gas measured with cold atoms

behavior very similar to 0.1 fm^{-3} because neutrons have large scattering length $a_s = -18.5$ fm

stronger increase towards higher densities (EOS becomes stiffer) due to repulsive 3N forces

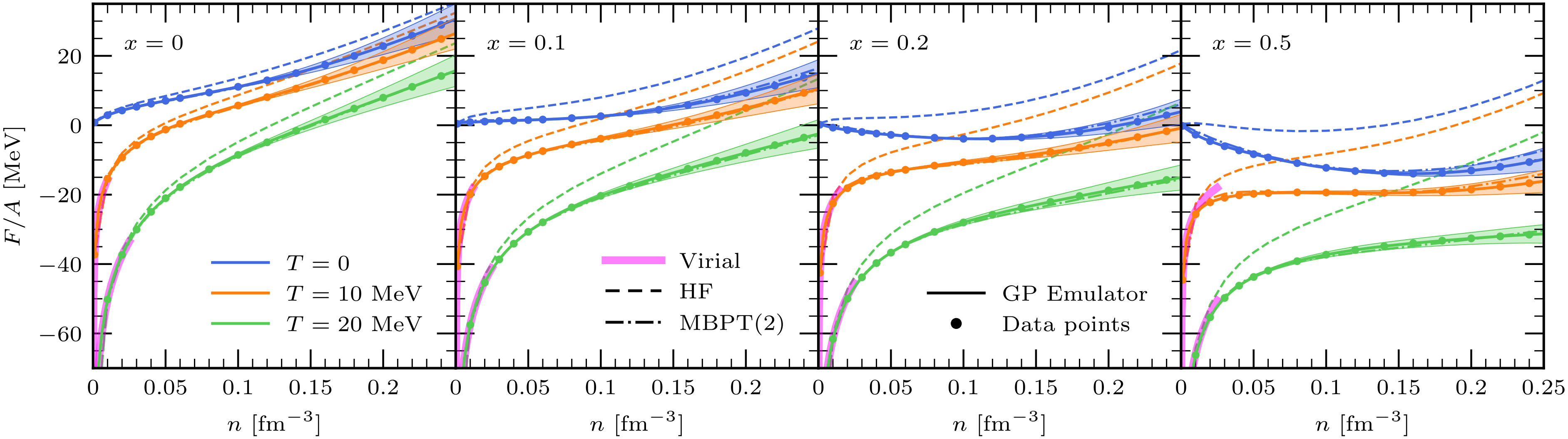
EOS for arbitrary proton fraction and temperature

Keller, Hebeler, AS, PRL (2023)

based on chiral EFT NN+3N interactions to N^{3}LO

order-by-order EFT uncertainties + (small) many-body uncertainties

see Hannah Göttling's talk for Bayesian EFT uncertainties



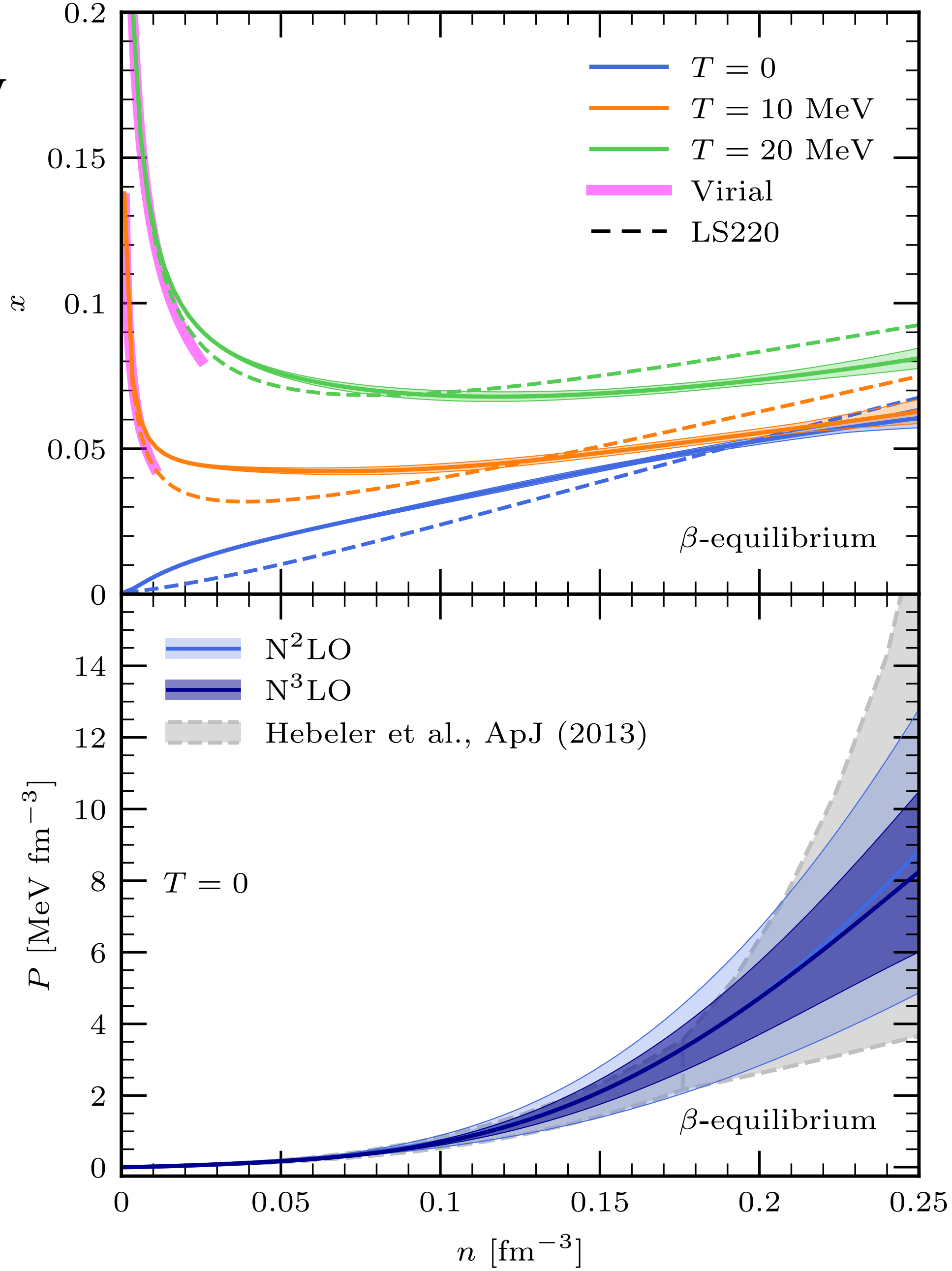
excellent reproduction of free energy data by Gaussian process (GP)

agrees with model-indep. virial EOS Horowitz, AS, NPA (2006) at low densities

EOS for neutron star matter in beta equilibrium

Keller, Hebeler, AS, PRL (2023)

use GP emulator to access arbitrary proton fraction,
solve for beta equilibrium



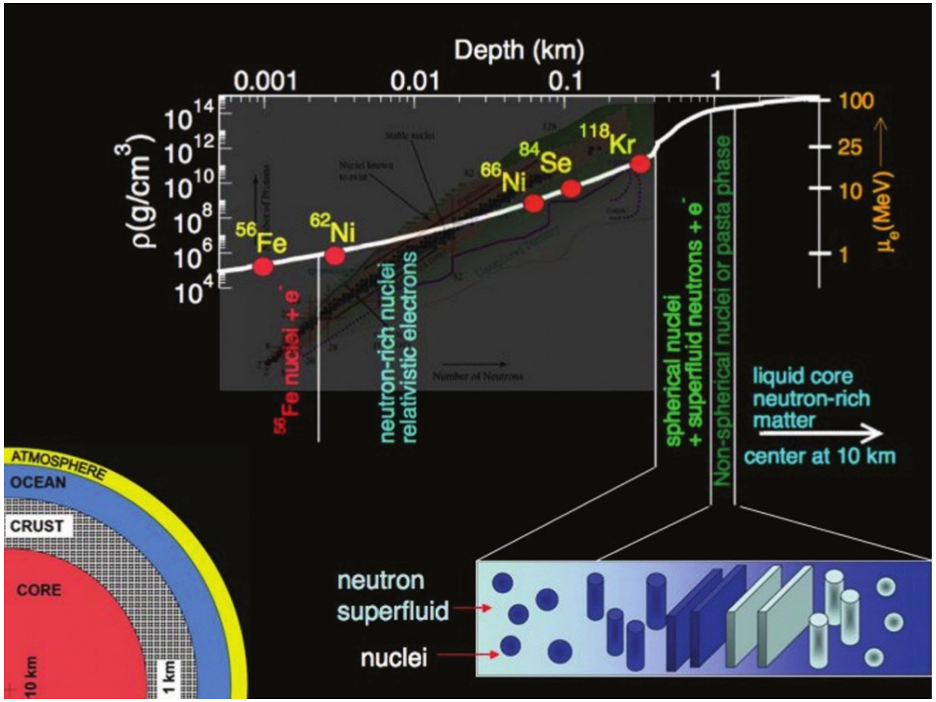
EOS of neutron star matter
at N^{2}LO and N^{3}LO,
no indication of EFT breakdown

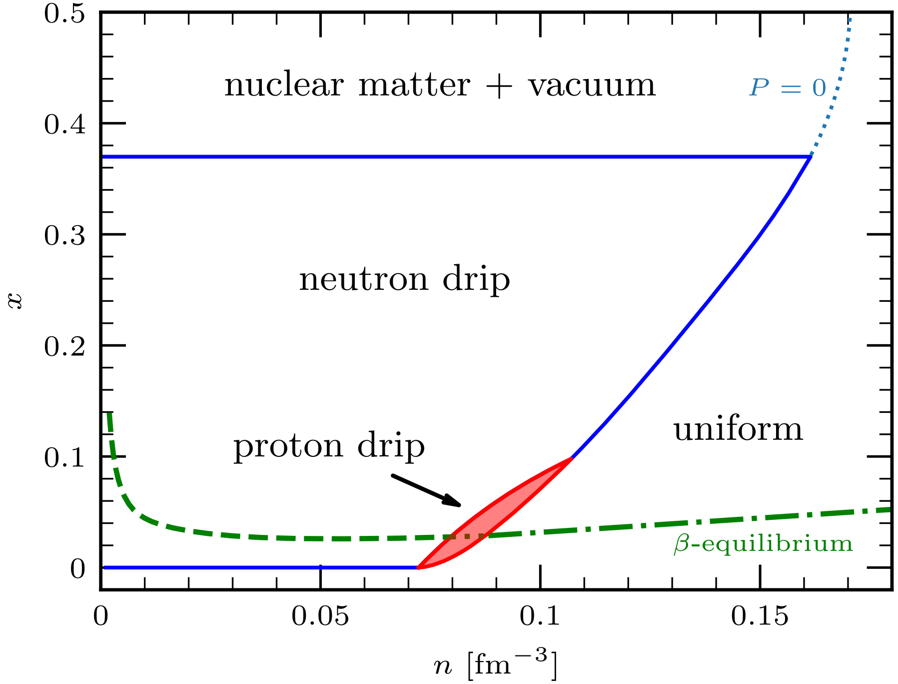
N^{3}LO band prefers higher pressures, improvement over older calculations

Subnuclear phase diagram of neutron star matter

~ 5% proton fraction in denser neutron matter

below ~ 0.5 n_0 possible pasta phases: clusters/structures of high density surrounded by neutron (and proton) gas: neutron (proton) drip





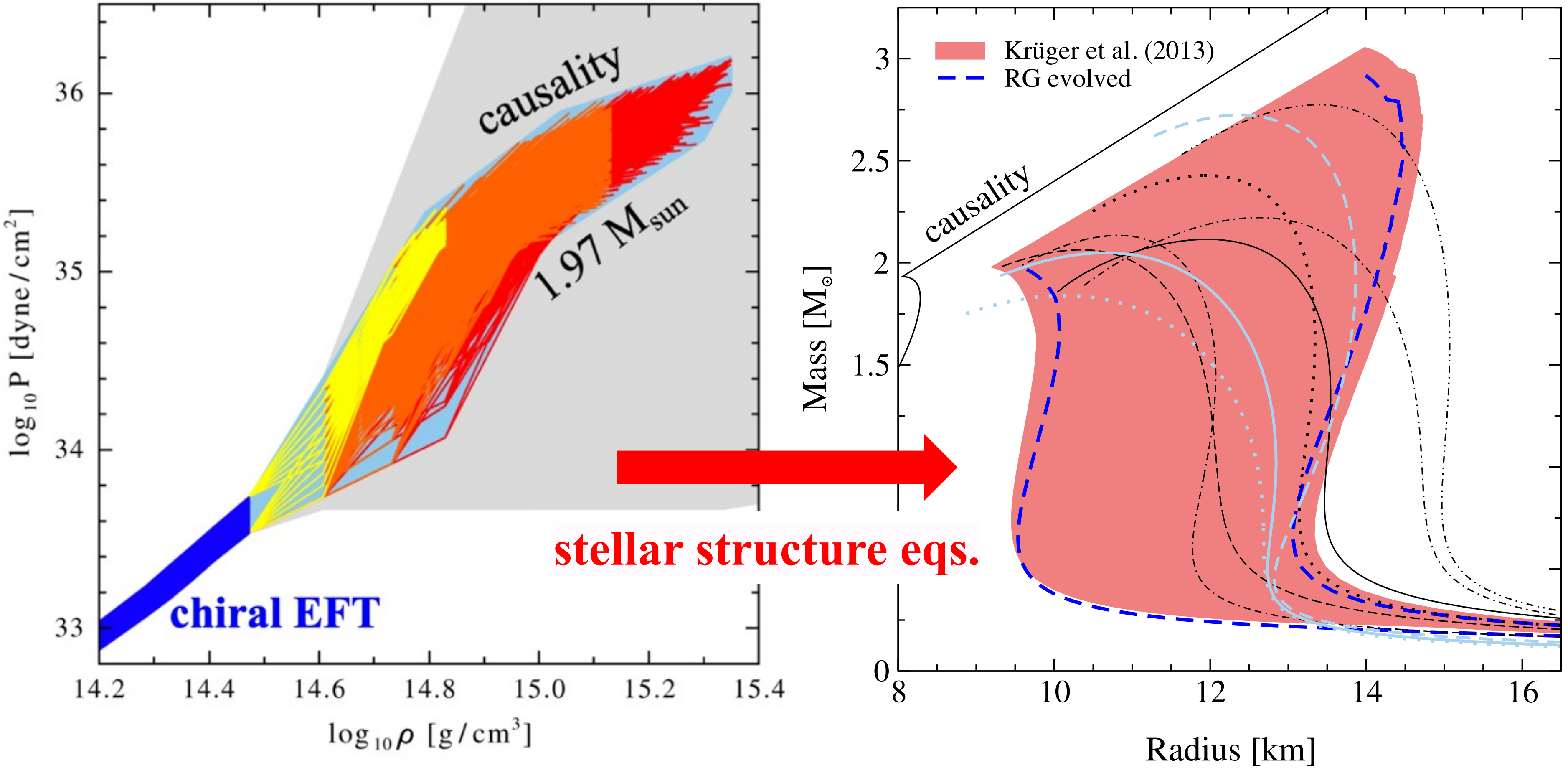
Keller, Hebeler, Pethick, AS, PRL (2024)

Challenging problem for uncertainty quantification due to correlated quantities, derivatives with larger mb uncertainties,…

Impact on neutron stars

Hebeler, Lattimer, Pethick, AS, PRL (2010), ApJ (2013)

constrain high-density EOS by causality, require to support 2 M_{sun} star



stellar structure eqs.

predicts neutron star radius: 9.7 - 13.9 km for M=1.4 M_{sun}

1.8 - 4.4 n_0 modest central densities

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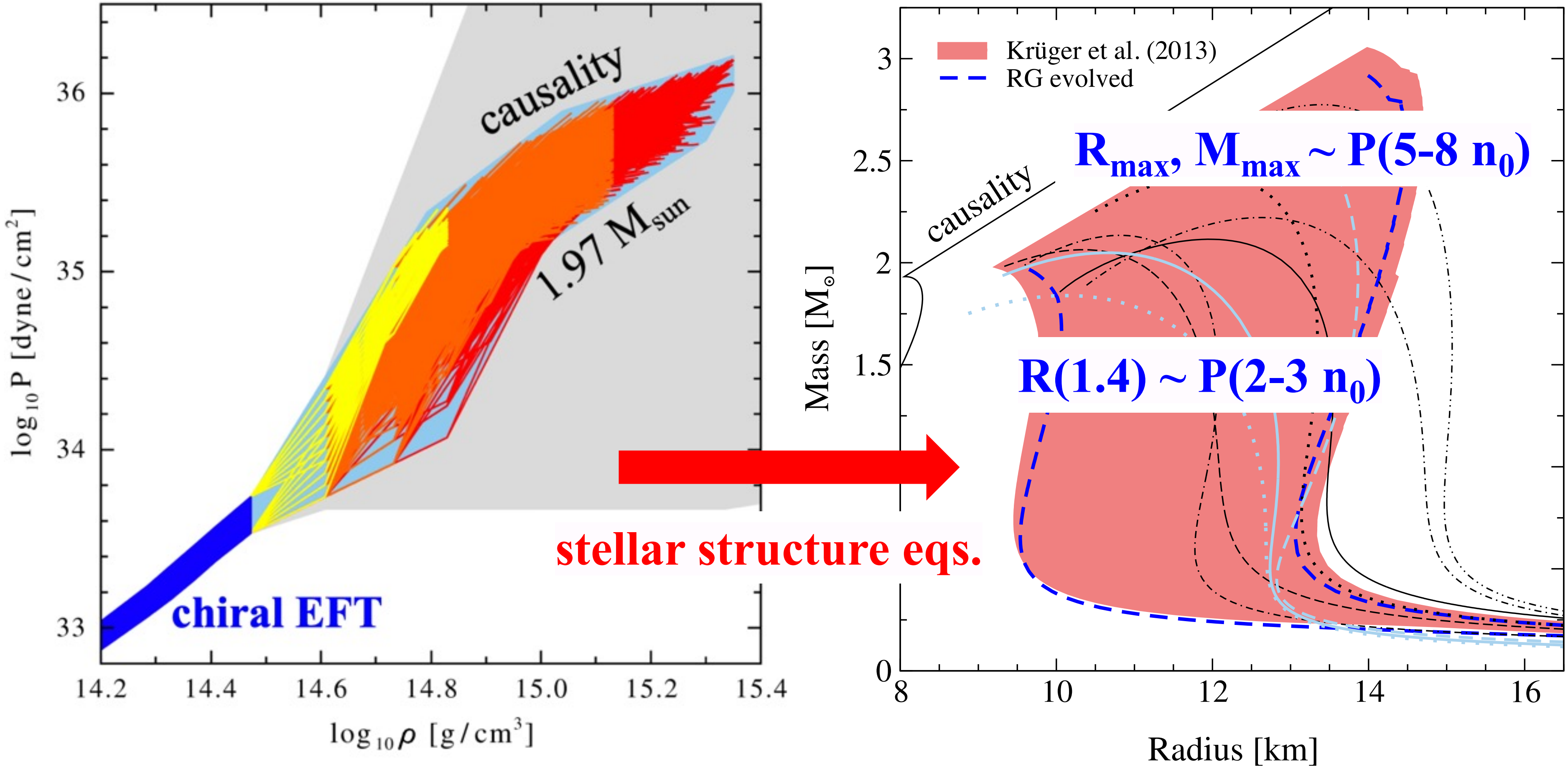


chiral EFT

stellar structure eqs.

R_{max}, M_{max} ~ $P(5\text{-}8\ n_0)$

$R(1.4)$ ~ $P(2\text{-}3\ n_0)$

predicts neutron star radius: 9.7 - 13.9 km for M=1.4 M_{sun}

1.8 - 4.4 n_0 modest central densities

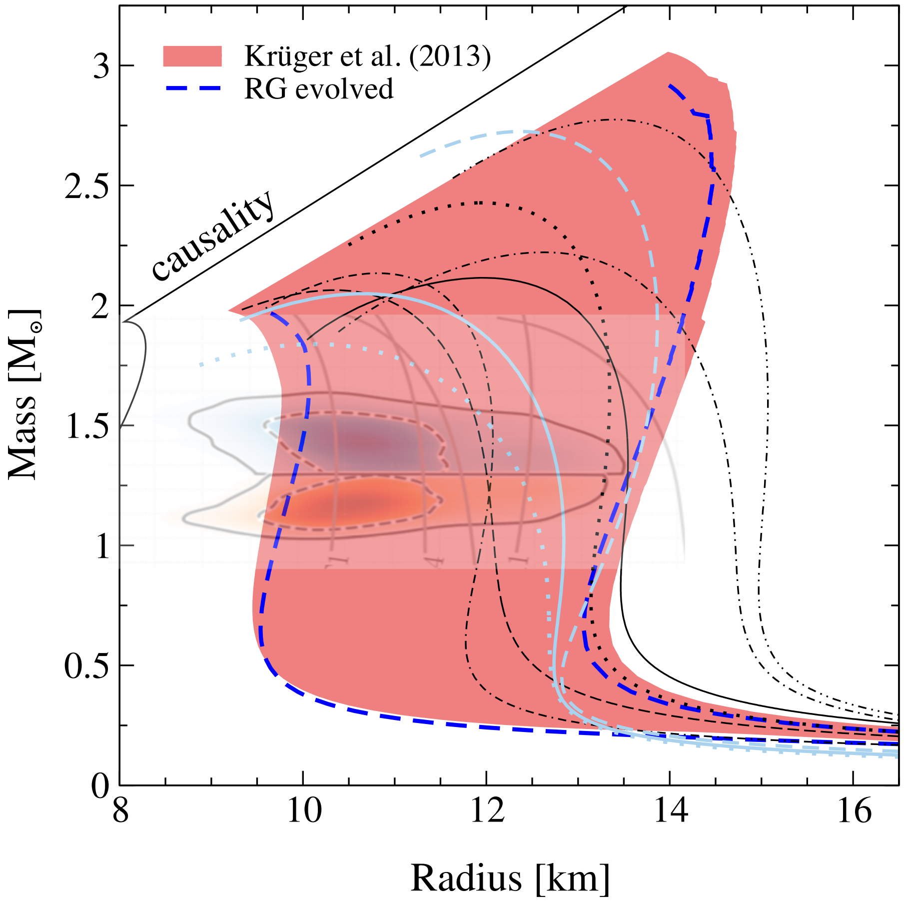
Neutron star radius

chiral EFT + general EOS extrapolation based on causality + 2 M_{sun} stars

predicted neutron star radii: 9.7 - 13.9 km for $M=1.4\ M_{sun}$

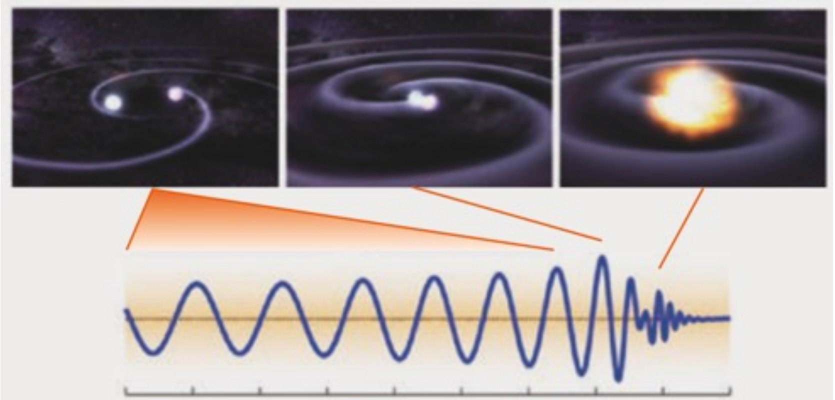
Hebeler, Lattimer, Pethick, AS, PRL (2010), ApJ (2013)

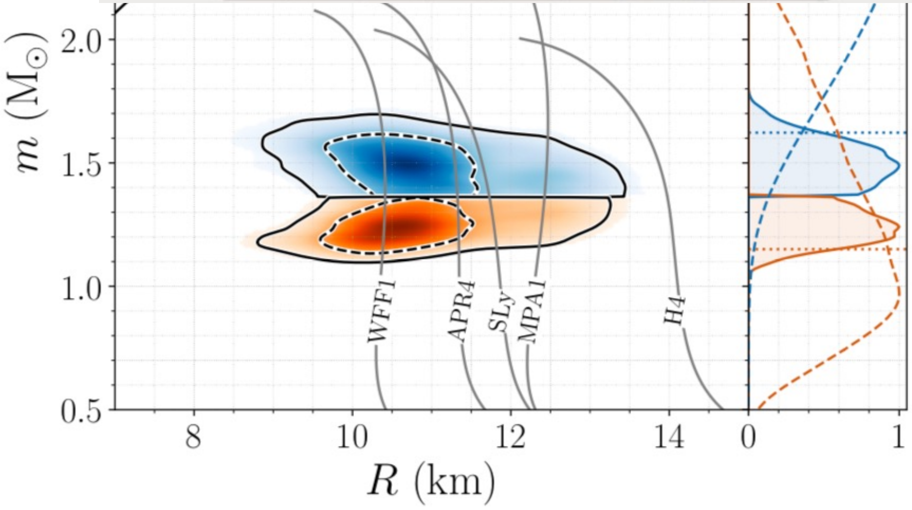
consistent with LIGO/Virgo



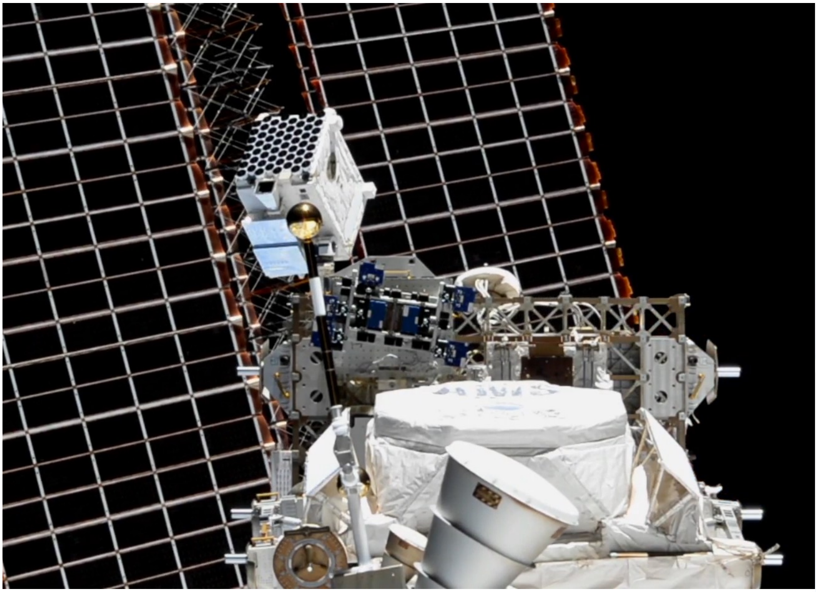
GW170817: Measurements of neutron star radii and equation of state

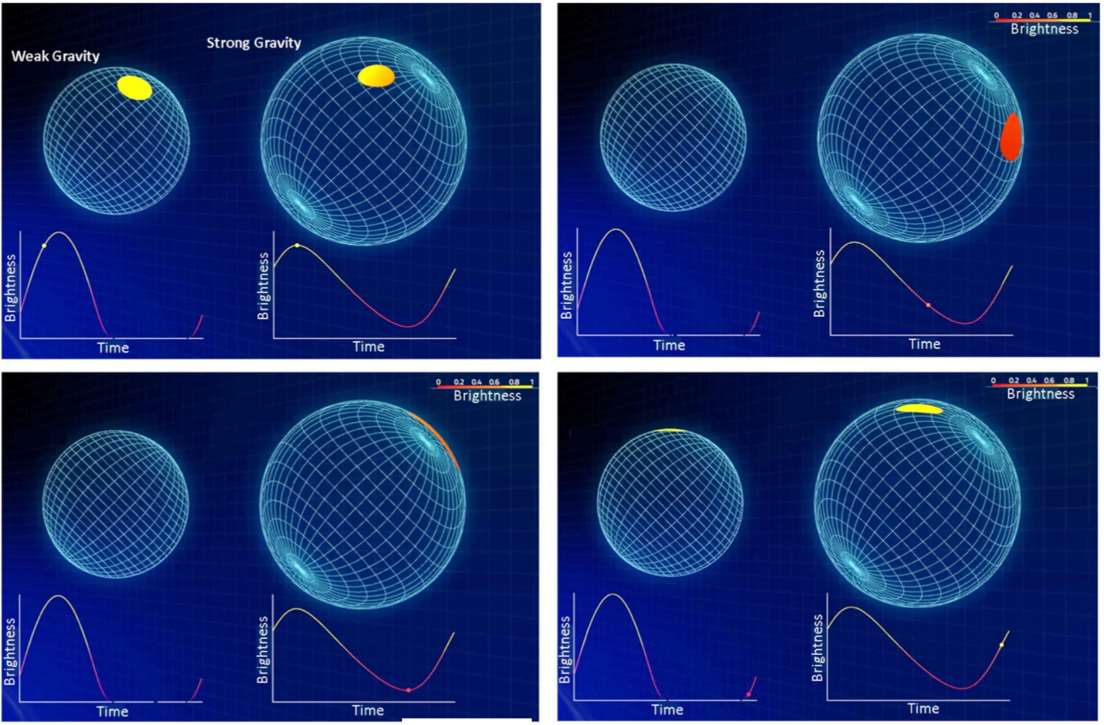
The LIGO Scientific Collaboration and The Virgo Collaboration





New NICER results for J0437

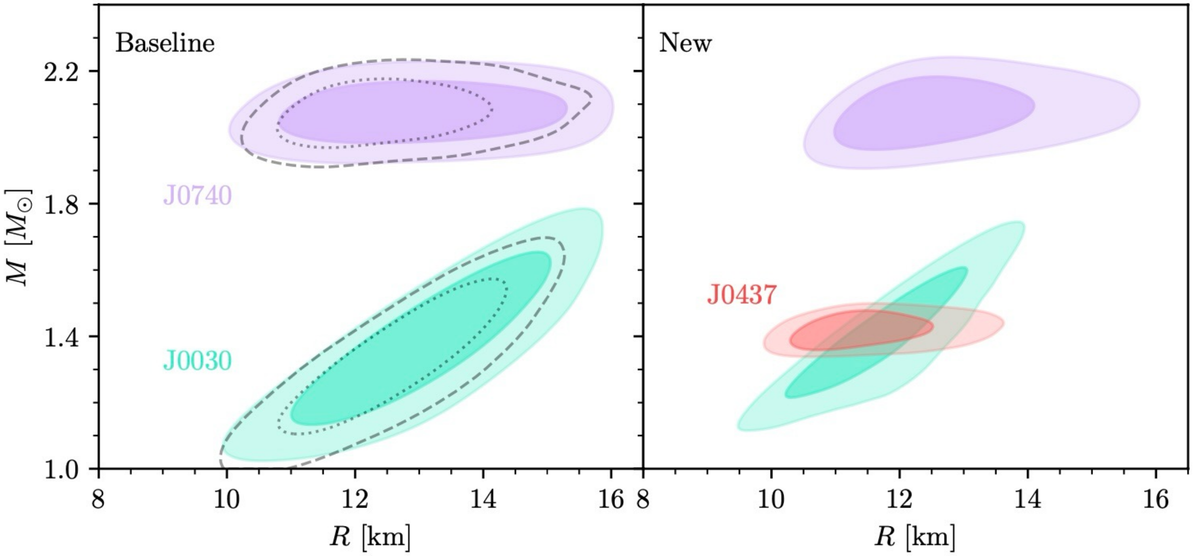




Neutron star radius from pulse profile modeling

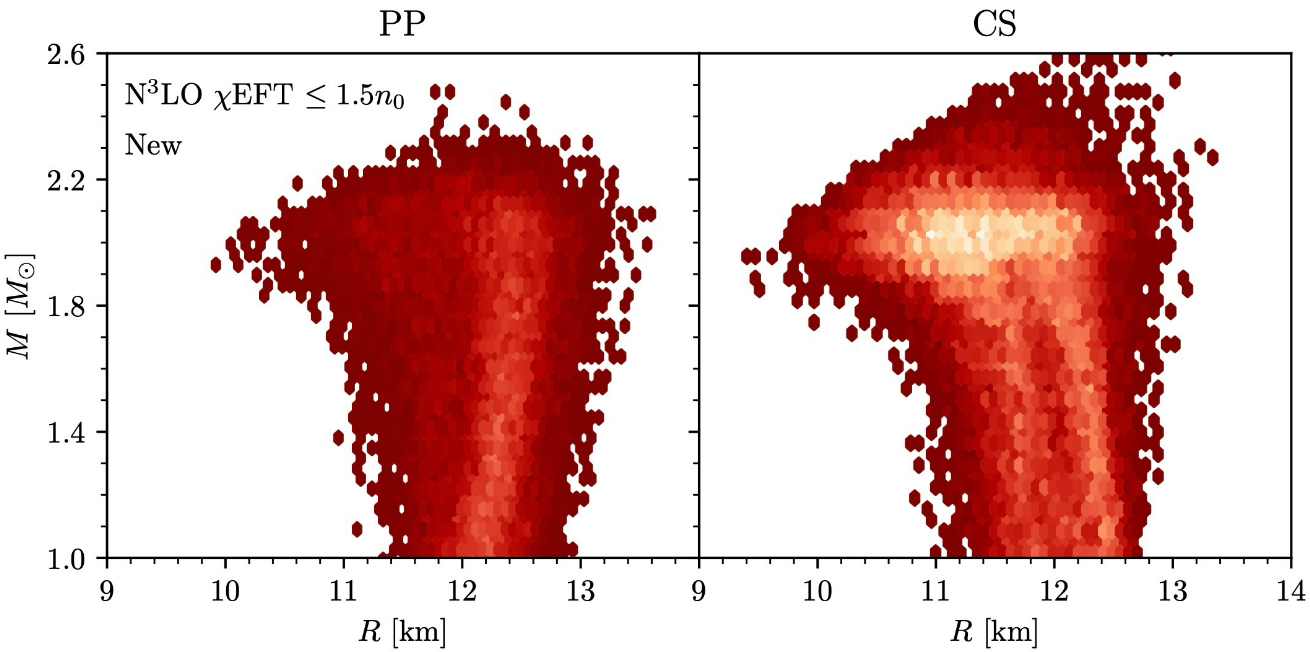
here: Amsterdam analysis
ApJL (2019), (2021), submitted (2024)

J0030 and J0740
similar results from
Illinois-Maryland analysis
ApJL (2019), (2021)

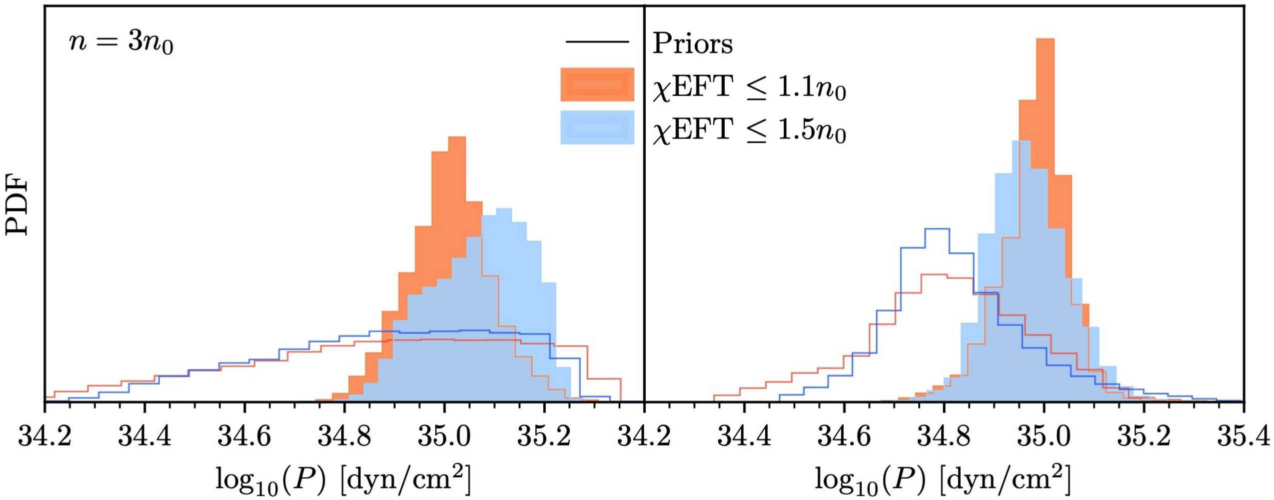


Combined LIGO/Virgo and NICER constraints

Raaijmakers et al., ApJL (2020), (2021), Rutherford, Mendes, Svensson et al., submitted (2024)



neutron star radius
~ 12±1 km



pressure posteriors
at 3 n_0
→ astro prefers
higher pressures

Summary

Thanks to: ab initio: **P. Arthuis**, K. Hebeler, H. Hergert, **M. Heinz**, **J. Hoppe**, J.D. Holt, **T. Miyagi**, **T. Plies,** R. Stroberg, **A. Tichai**
EOS: **Y. Dietz,** C. Drischler, **H. Göttling**, K. Hebeler, **S. Huth**, J. Lattimer, **J. Keller**, **M. Mendes**, C. Pethick, **G. Raaijmakers**, **N. Rutherford**, **I. Svensson**, I. Tews, A. Watts

Chiral EFT interactions + powerful many-body methods
→ great progress for ab initio calcs of nuclei and dense matter

reliable EOS up to ~ 1-2 n_0 with controlled uncertainties
→ key for multimessenger era of neutron stars,
high-density constraints from astrophysics

Discussion points

Interaction uncertainties have focused on EFT truncation.
What about other systematic choices (such as regulators, fit choices,…)?

Status of A_y puzzle. Is this solved with EFT uncertainties?

Suite of few- and many-body observables for interaction optimization?

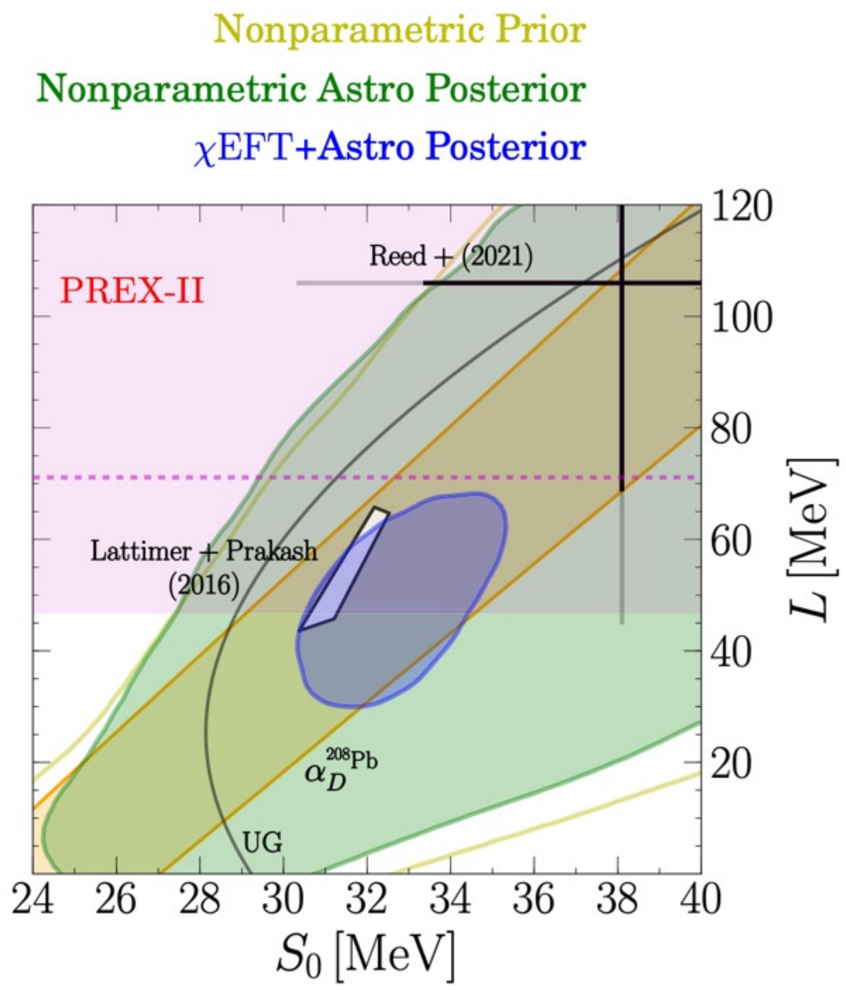
Many-body uncertainties beyond expert assessment.

More systematic exploration/development of accurate NN+3N needed.

EFT uncertainties for electroweak matrix elements/responses with external momentum.

Impact of PREX and ^{208}Pb dipole polarizability

Essick, Landry, AS, Tews, PRL, PRC (2021)



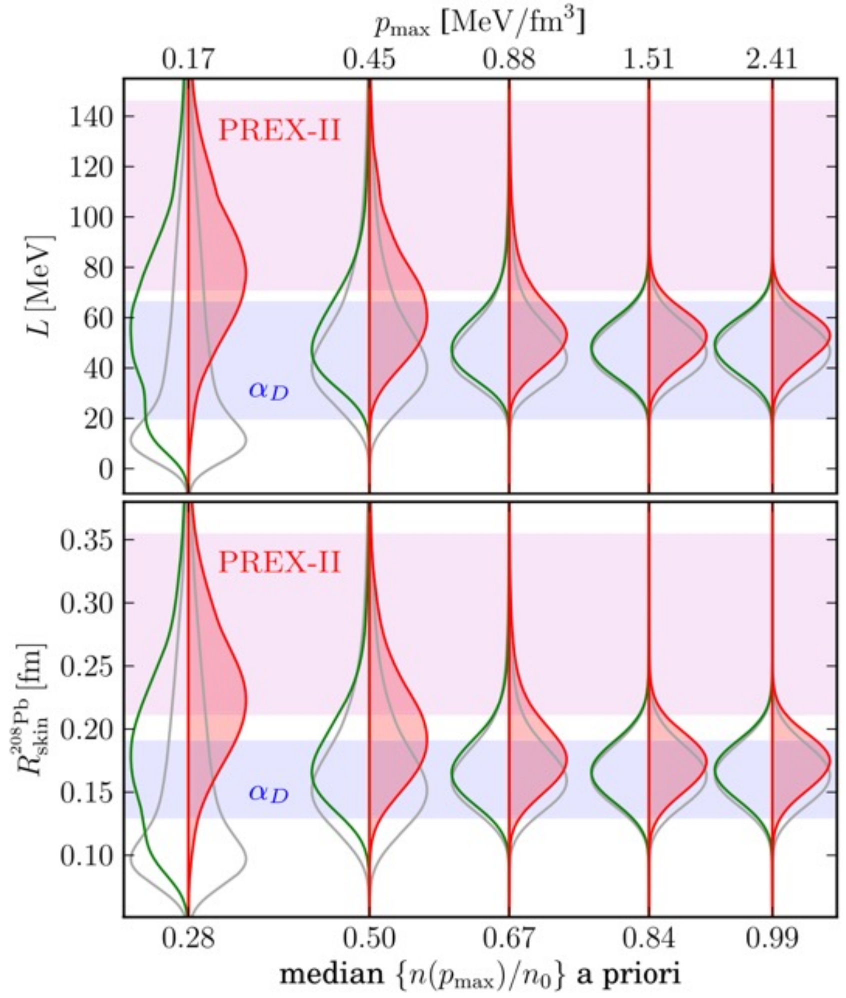


FIG. 2. Prior (gray, unshaded), Astro posterior (green, left-unshaded), and Astro + PREX-II posterior (red, right-shaded)

^{208}Pb dipole polarizability Tamii et al., PRL (2021)
very consistent with χEFT+Astro posterior