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

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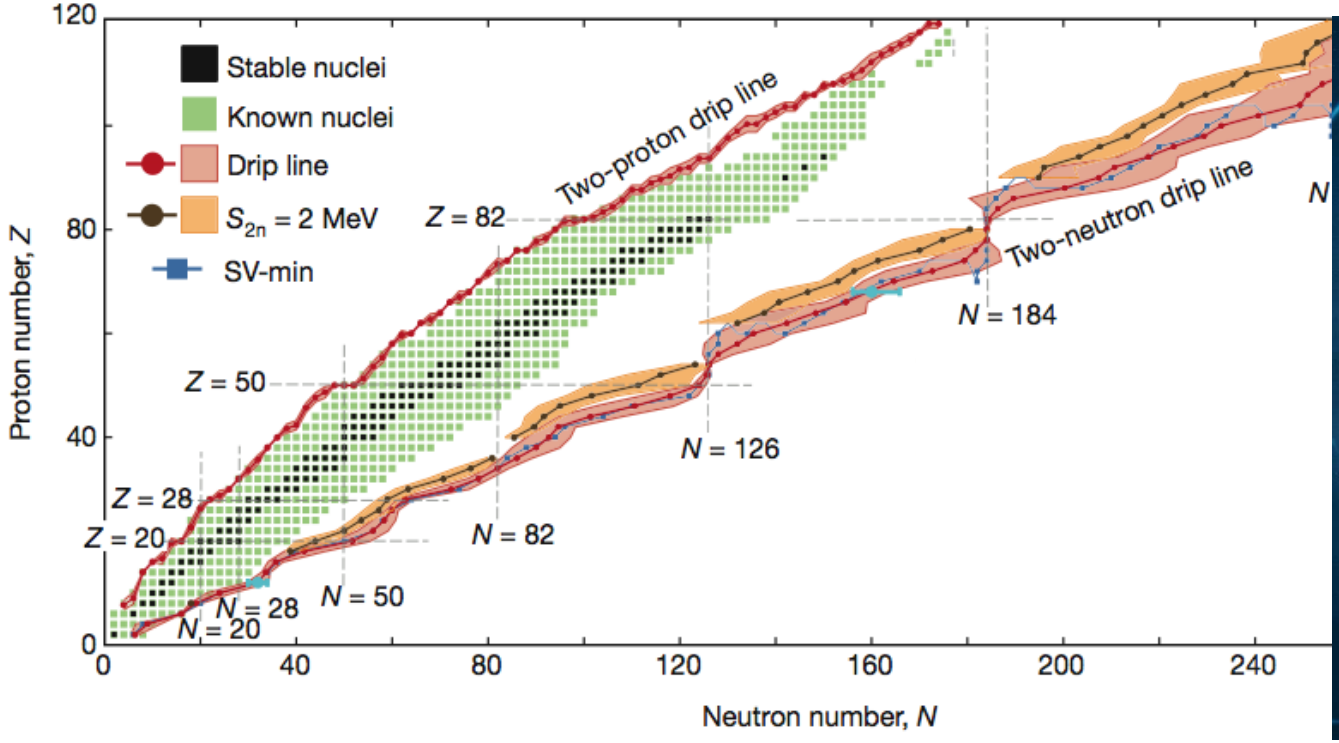
Structure of nuclei and dense matter in neutron stars

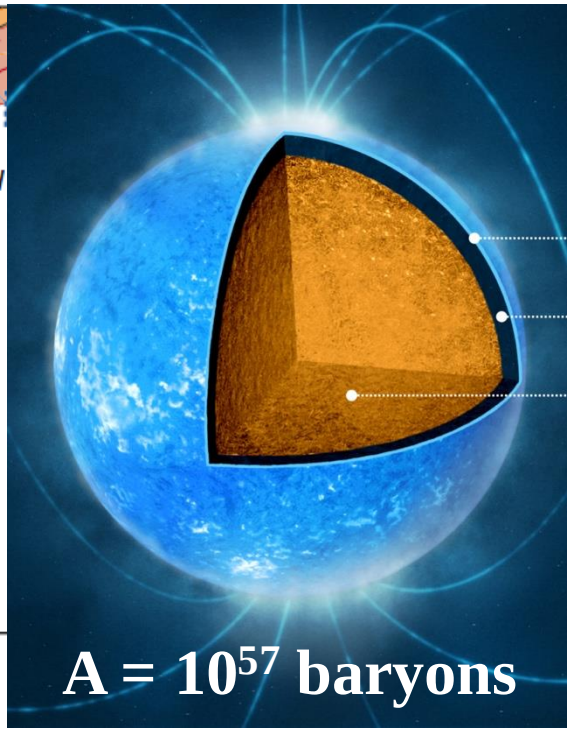
doi:10.1038/nature11188

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

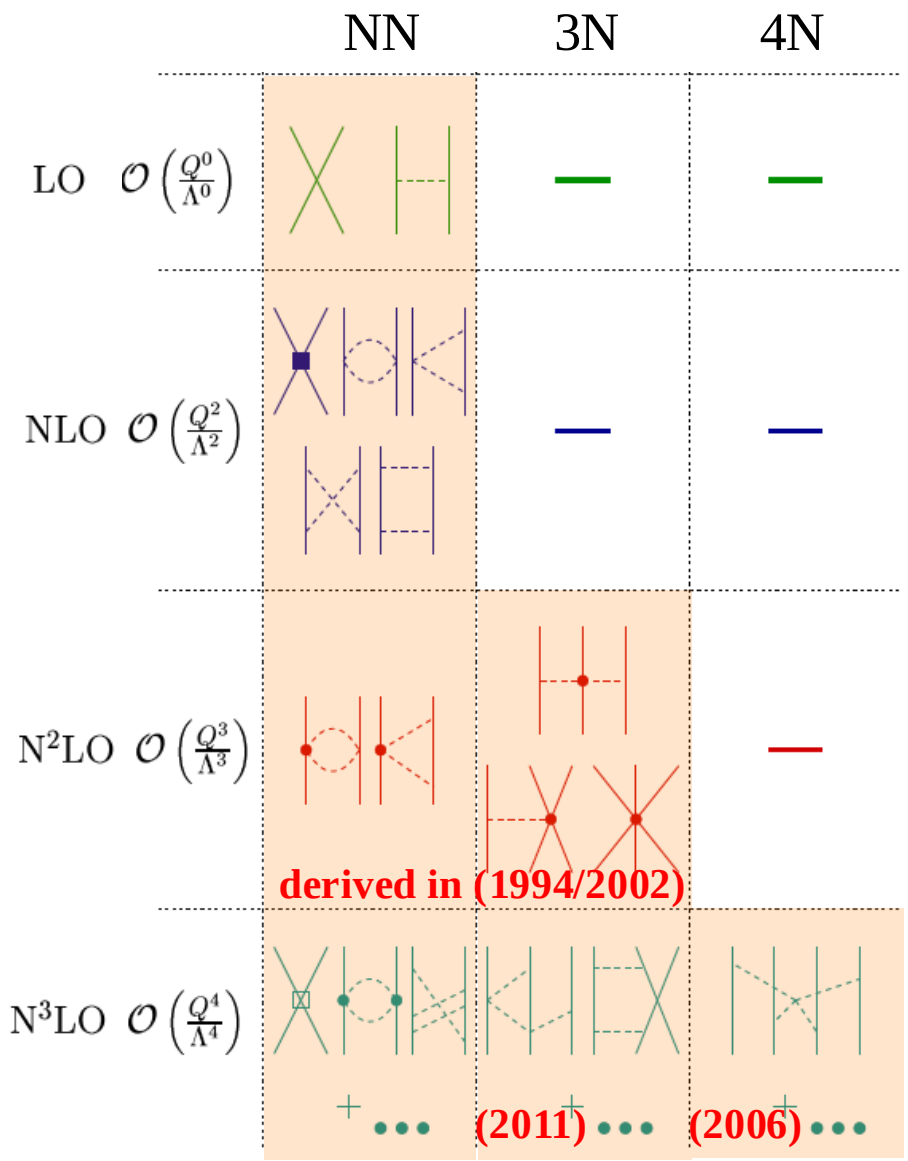




Extreme neutron-rich matter in neutron stars

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

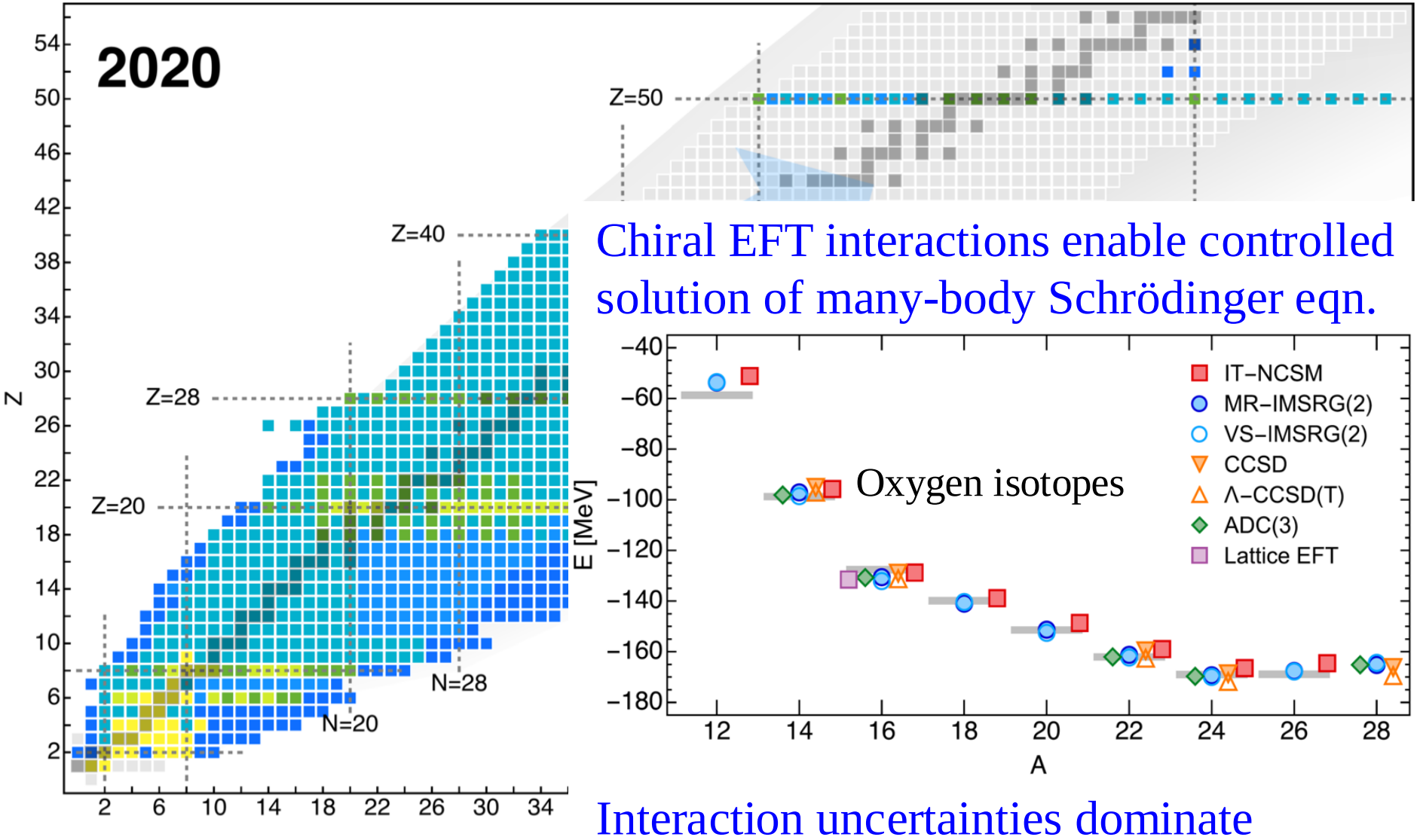
powerful approach for many-body interactions

all 3- and 4-neutron forces predicted to N³LO

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.

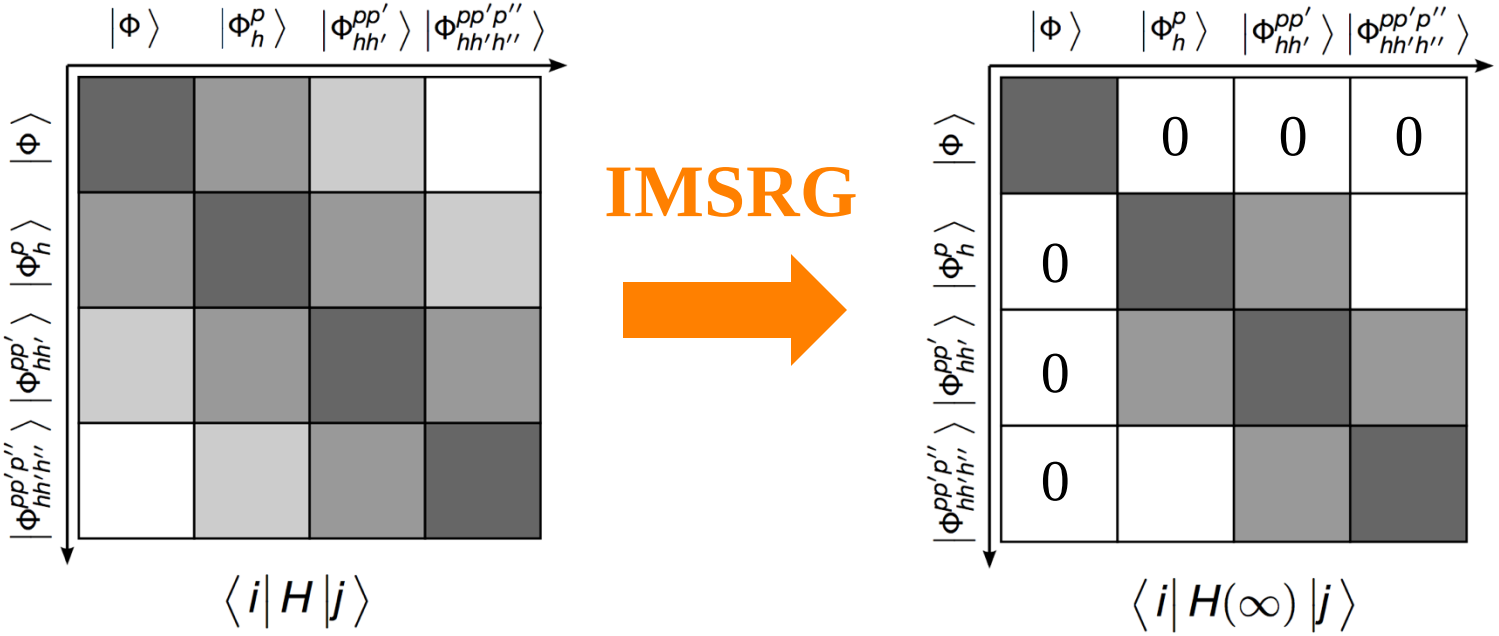
Interaction uncertainties dominate

figures from Hergert (2020)

In-medium similarity renormalization group (IMSRG)

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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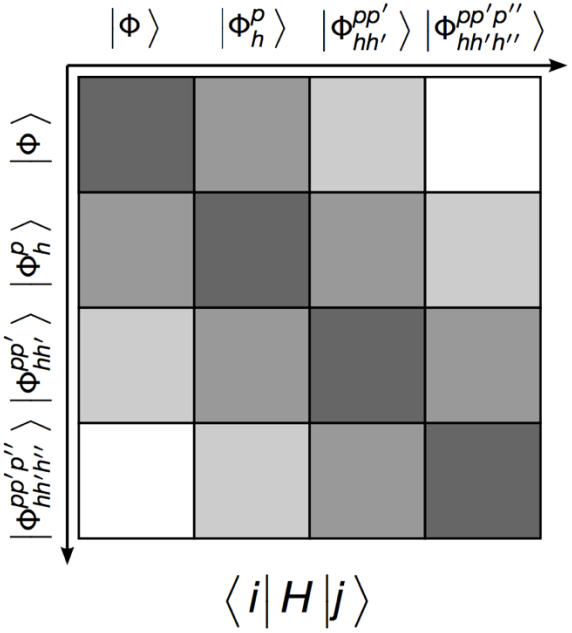
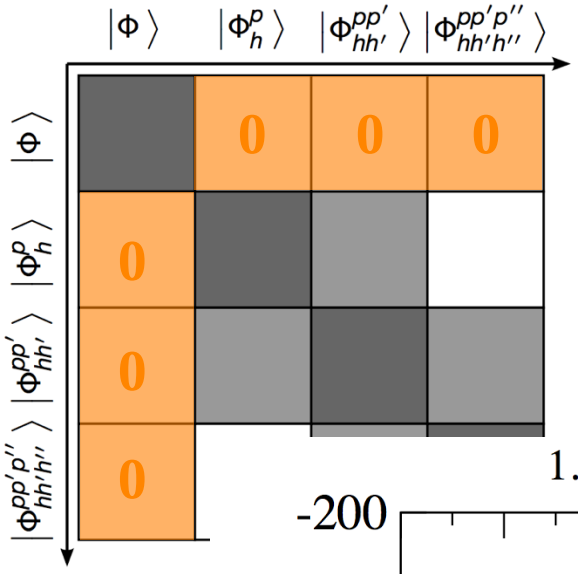


IMSRG

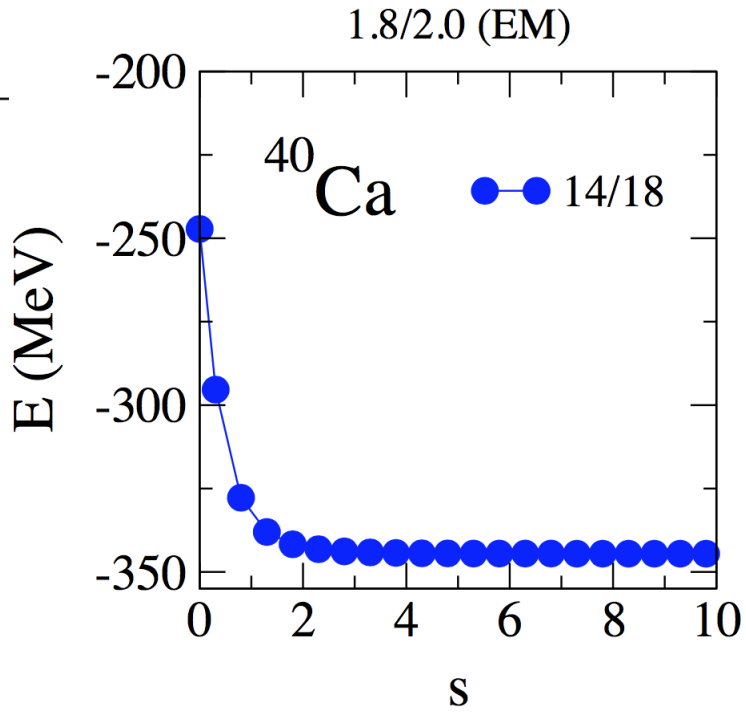


s = 0

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

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

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



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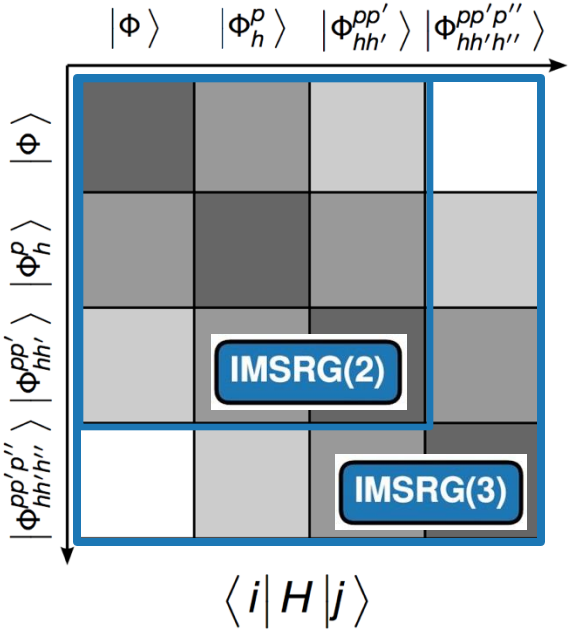
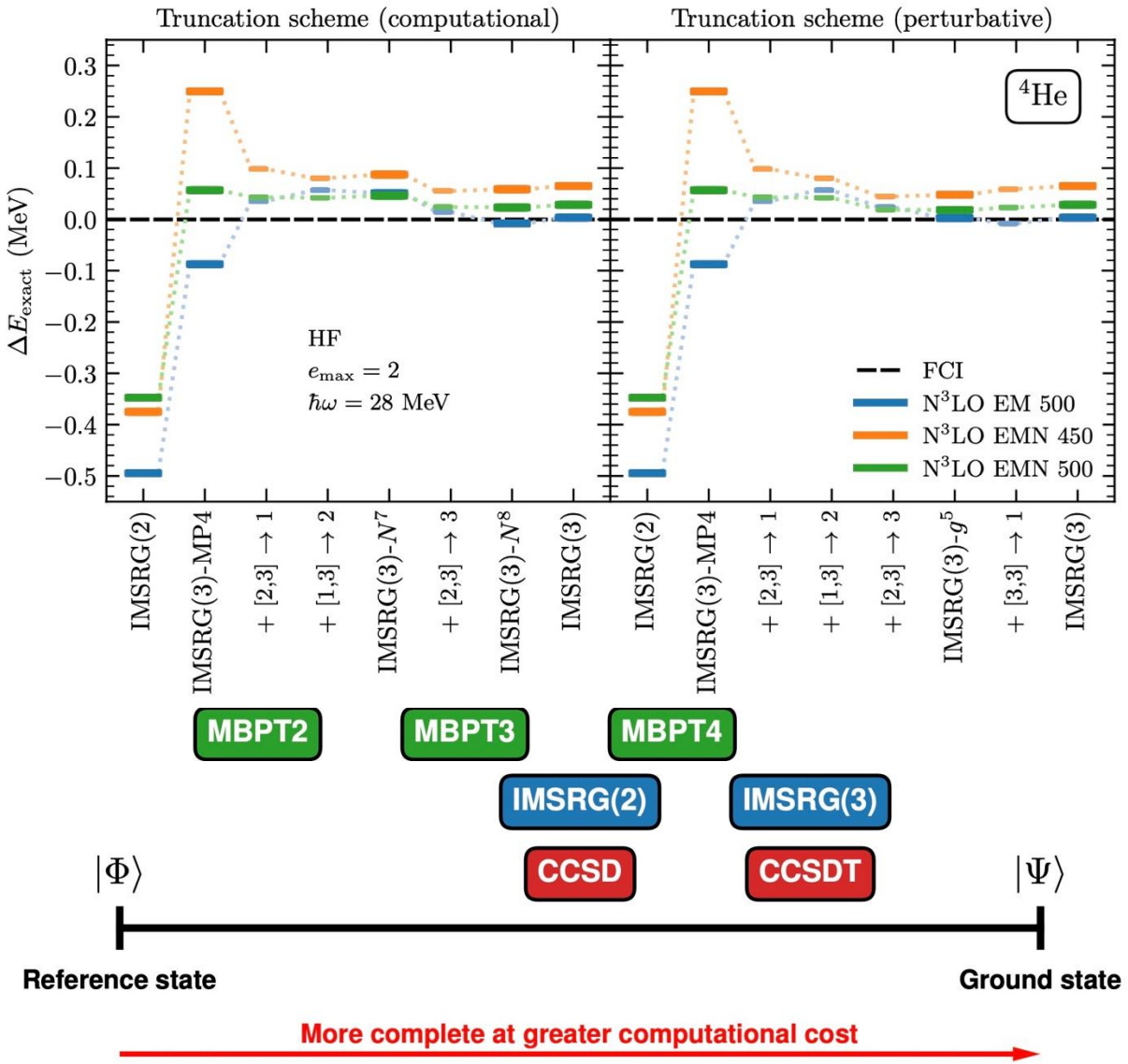


Standard truncation of IMSRG flow equations at normal-ordered 2-body level: IMSRG(2)

First IMSRG(3) results

Heinz et al., PRC (2021)



Outline

New chiral low-resolutions interactions

Pierre Arthuis, Hebeler, AS, arXiv:2401.06675

Probing nuclear structure with nonlinear King plots in ytterbium isotopes

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

Uncertainty quantification for low-resolution interactions

Tom Plies, Matthias Heinz, AS, preliminary

New chiral low-resolution interactions

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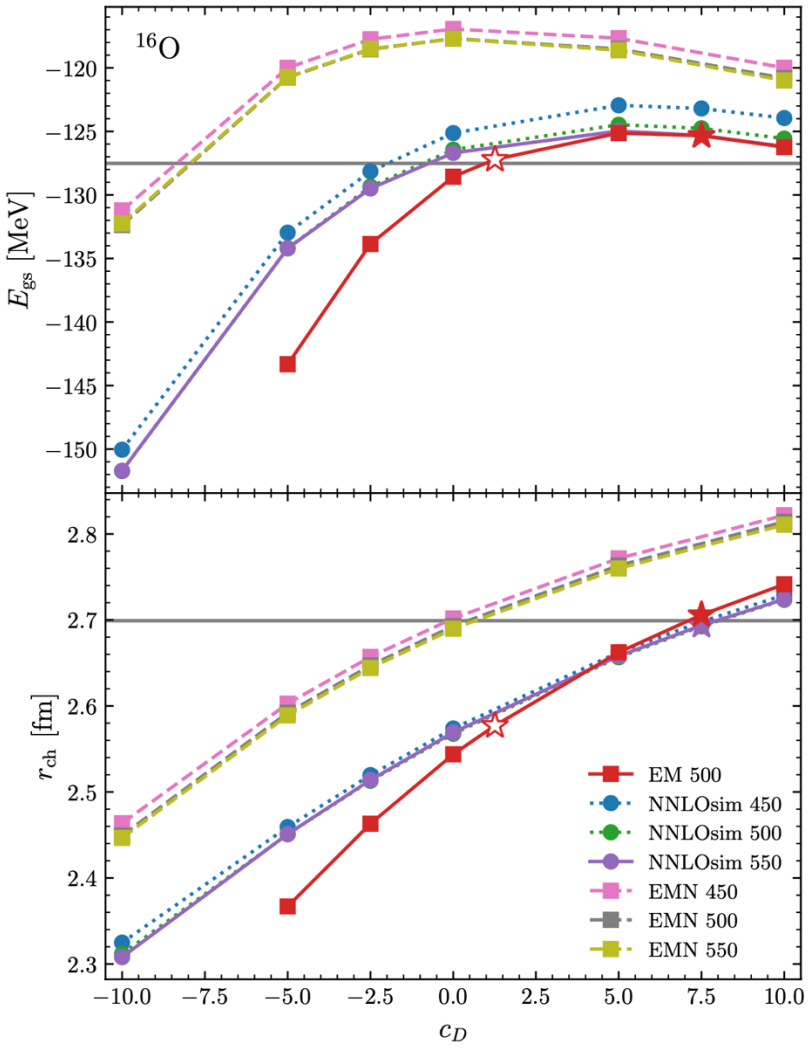
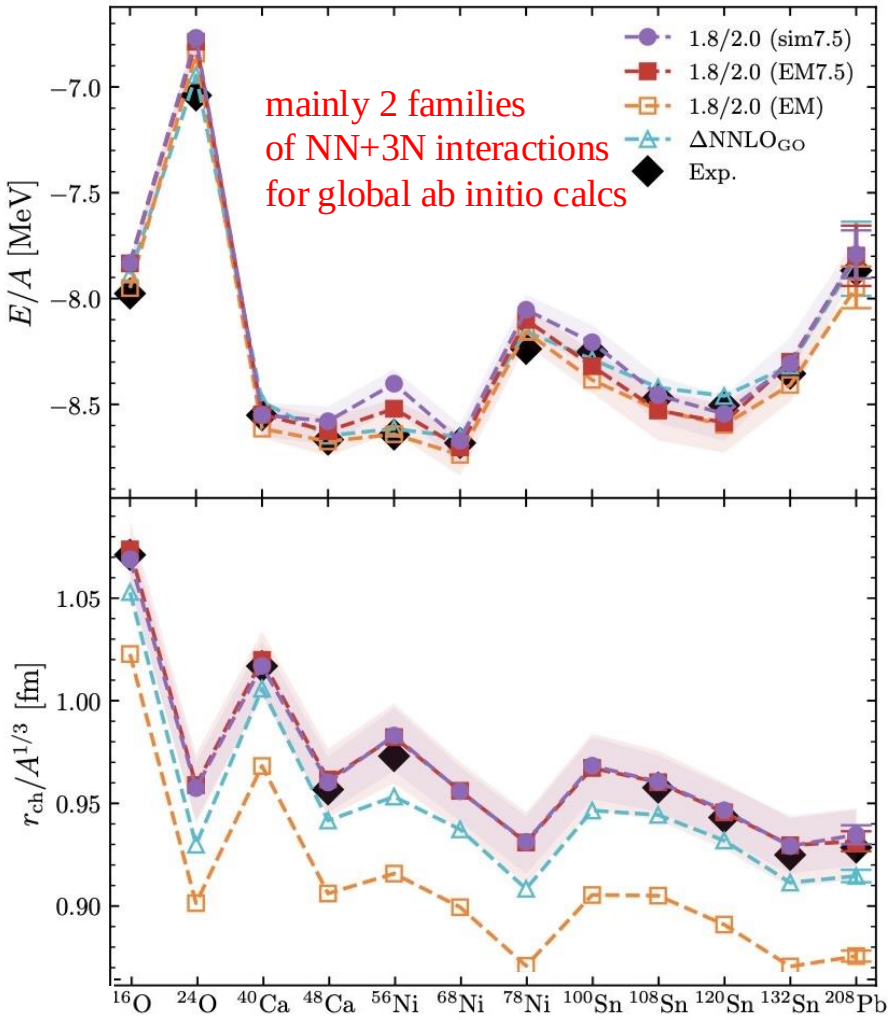
based on SRG-evolved NN interactions, 3N couplings fit to ^{3}H and ^{16}O

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





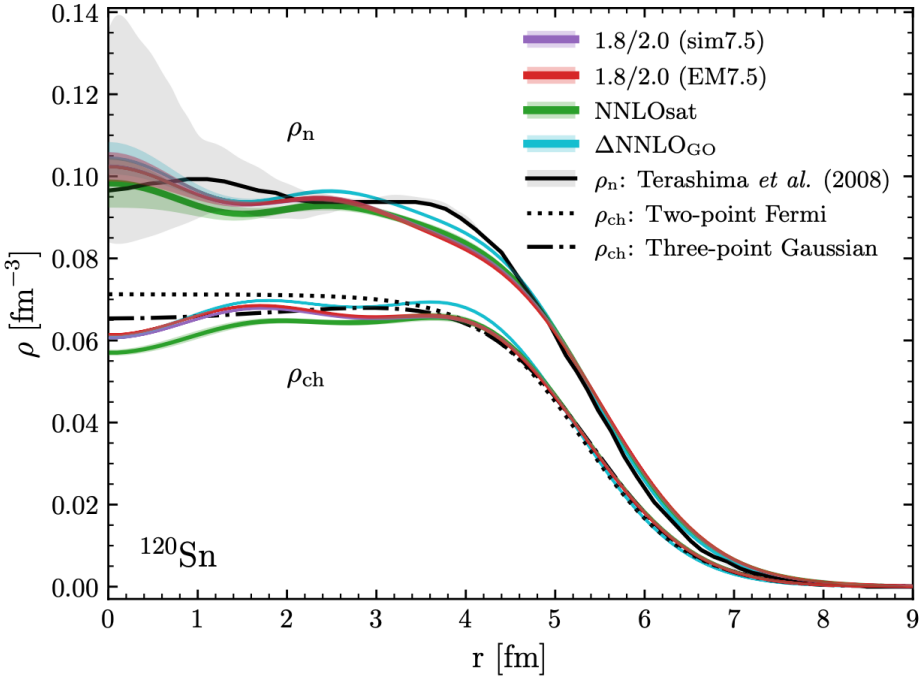
Neutron/proton density distributions in medium-heavy nuclei

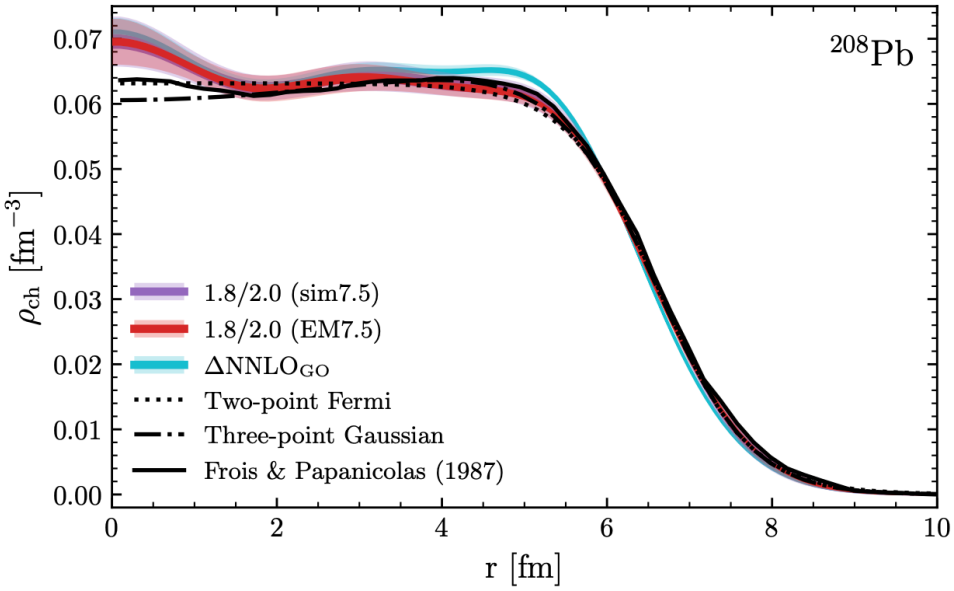
Arthuis, Hebeler, AS, arXiv:2401.06675

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



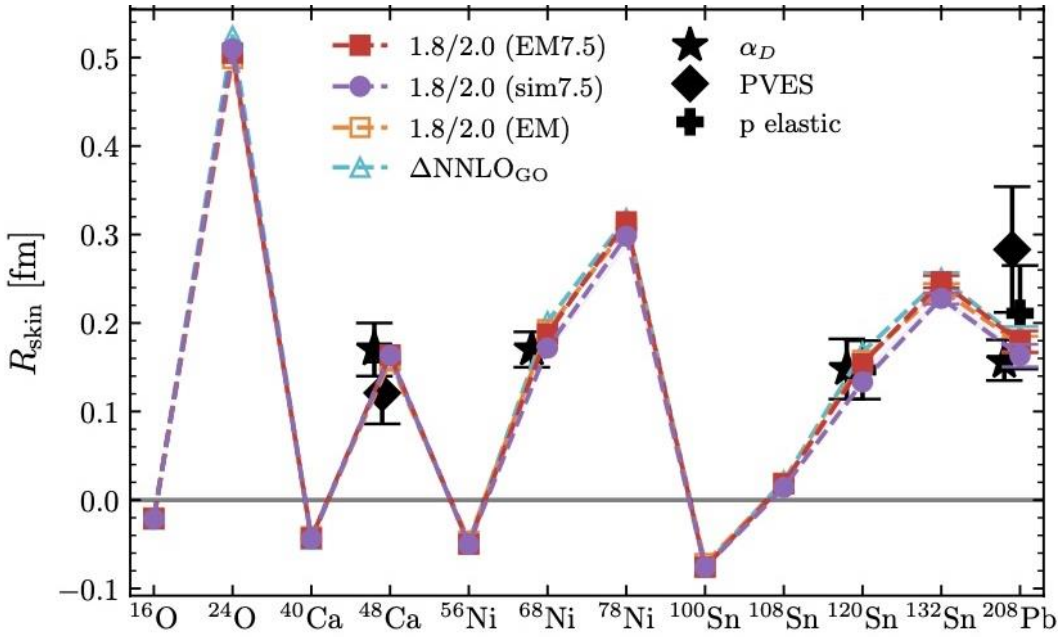


Neutron skins

Arthuis, Hebeler, AS, arXiv:2401.06675

very model independent

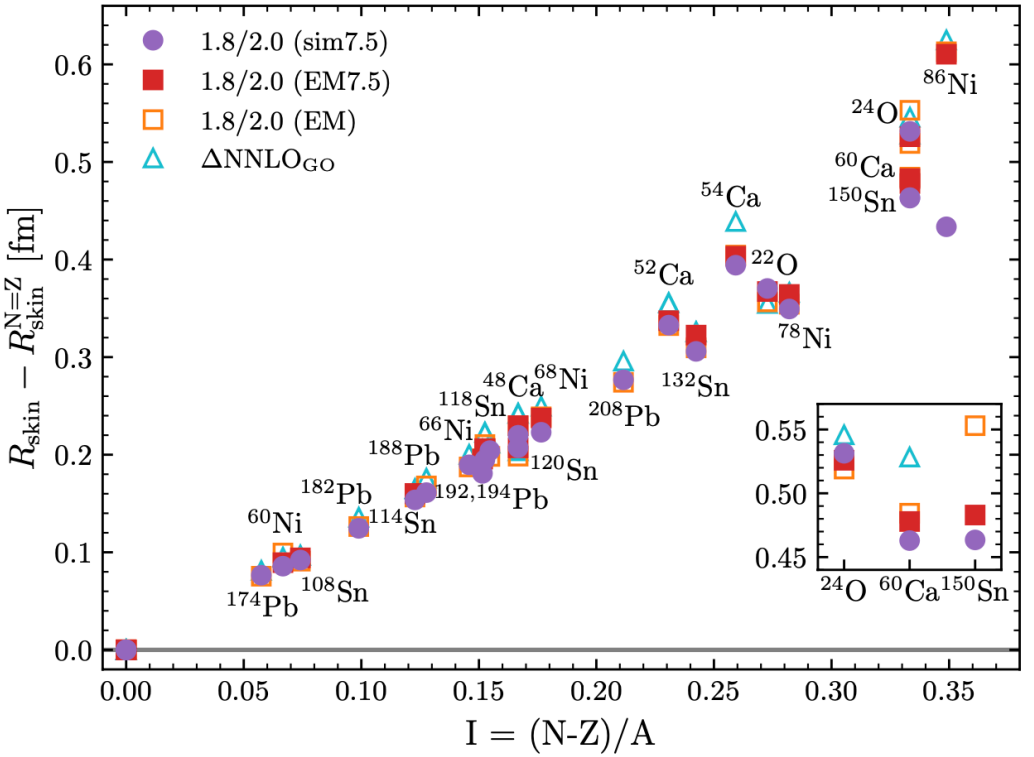
based on new (and previous) chiral NN+3N interactions



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



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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

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

mass shift — field shift

leading terms give linear King plot

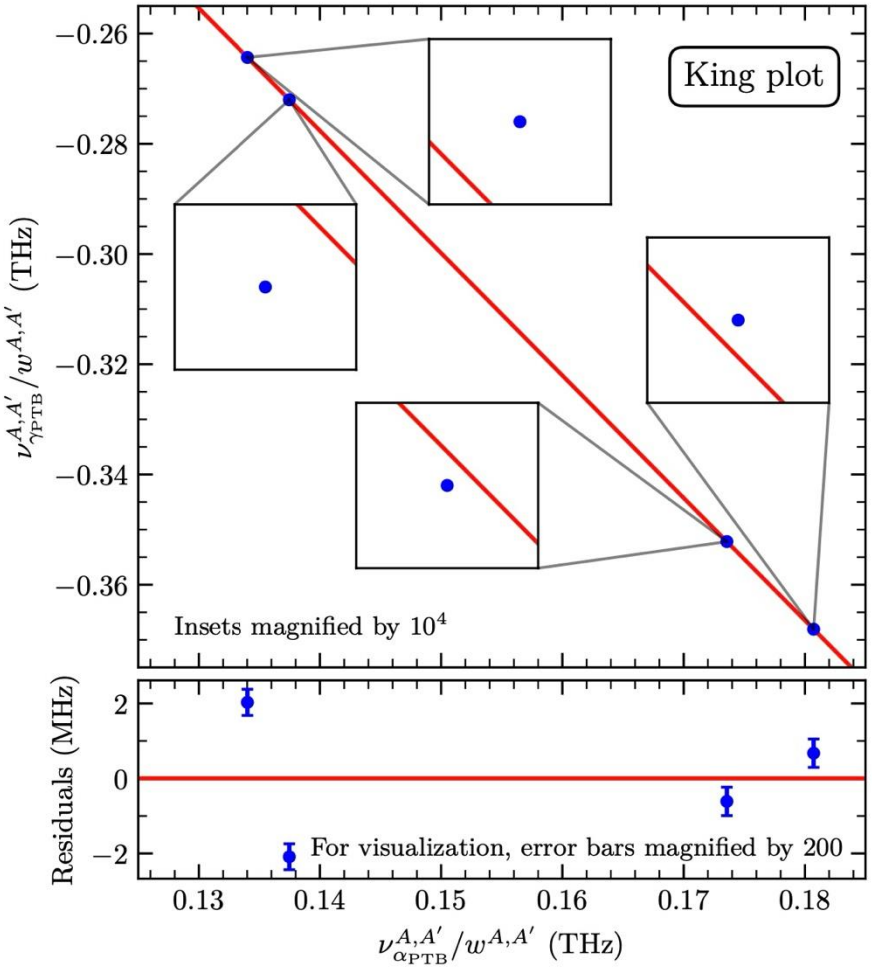
nonlinearities from higher-order Standard Model and BSM

$$\nu_{\tau,\text{nonlin.}}^{A,A'} = G_\tau^{(2)}(\delta\langle r^2\rangle^2)^{A,A'} + G_\tau^{(4)}\delta\langle r^4\rangle^{A,A'}$$

higher-order nuclear structure

$$+\frac{\alpha_{\text{NP}}}{\alpha_{\text{EM}}} D_\tau h^{A,A'} + \ldots$$

possible new boson



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

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

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nonlinearity decomposition suggests one dominant contribution

$$\nu^{A,A'}_{\tau,\text{nonlin.}} = G^{(2)}_\tau (\delta\langle r^2\rangle^2)^{A,A'} + G^{(4)}_\tau \delta\langle r^4\rangle^{A,A'}$$

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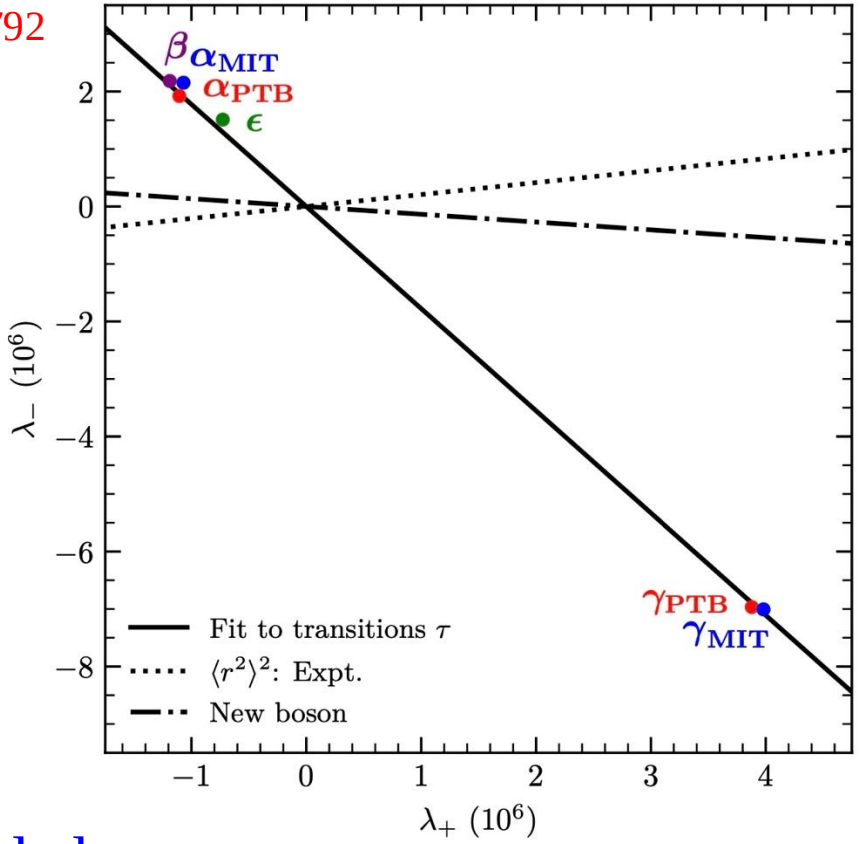
$$+ \frac{\alpha_{\text{NP}}}{\alpha_{\text{EM}}} D_\tau h^{A,A'} + \ldots$$

possible new boson

→ not quadratic field shift

→ not new boson



theory predictions of quartic radius needed

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higher-order nuclear structure

$$+ \frac{\alpha_{\text{NP}}}{\alpha_{\text{EM}}} D_\tau h^{A,A'} + \ldots$$

possible new boson

→ not quadratic field shift

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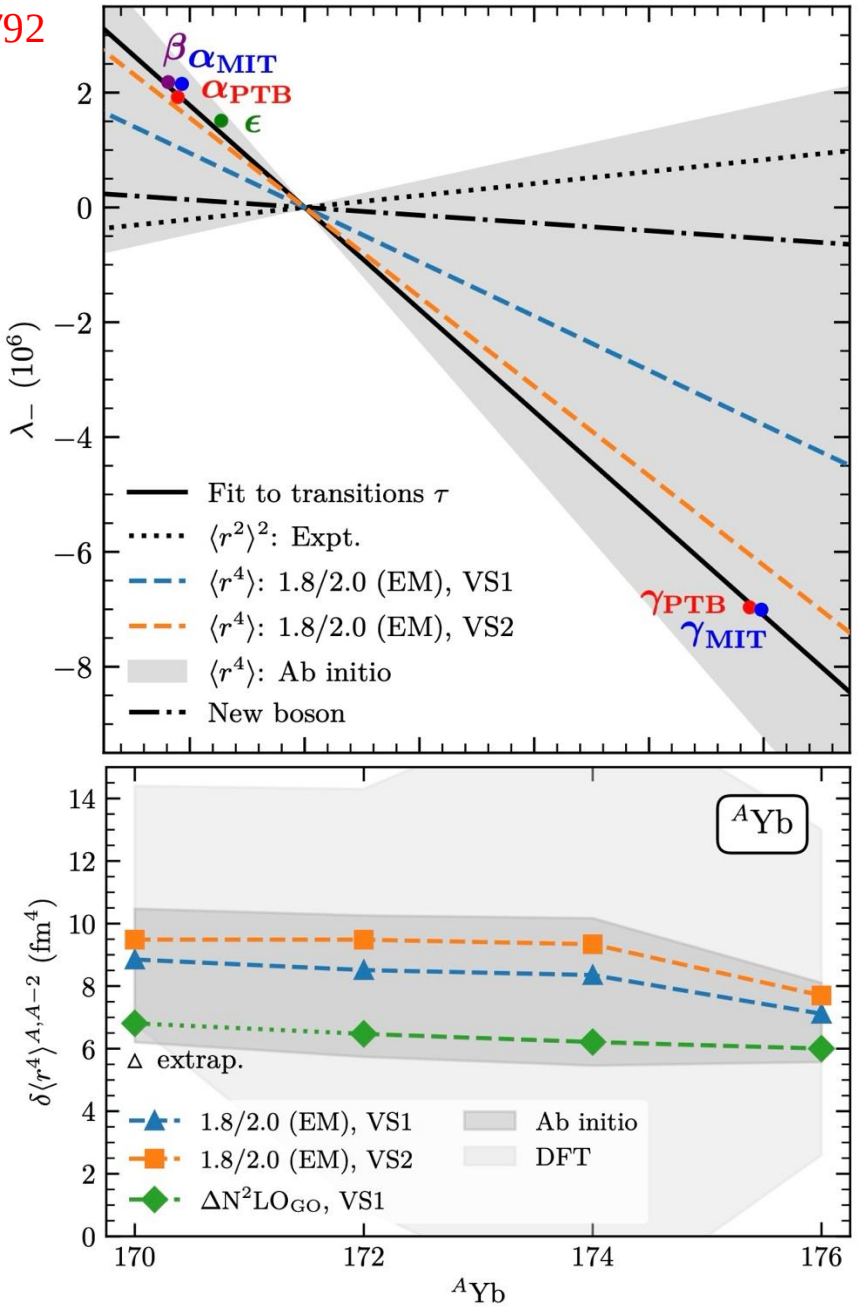
theory predictions of quartic radius:
VS-IMSRG calculations,
uncertainty estimates from:
1.8/2.0 (EM), ΔN^2LO_{GO} interactions,
two valence spaces,
many-body estimated from IMSRG(3)



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

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nonlinearity decomposition suggests one dominant contribution

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

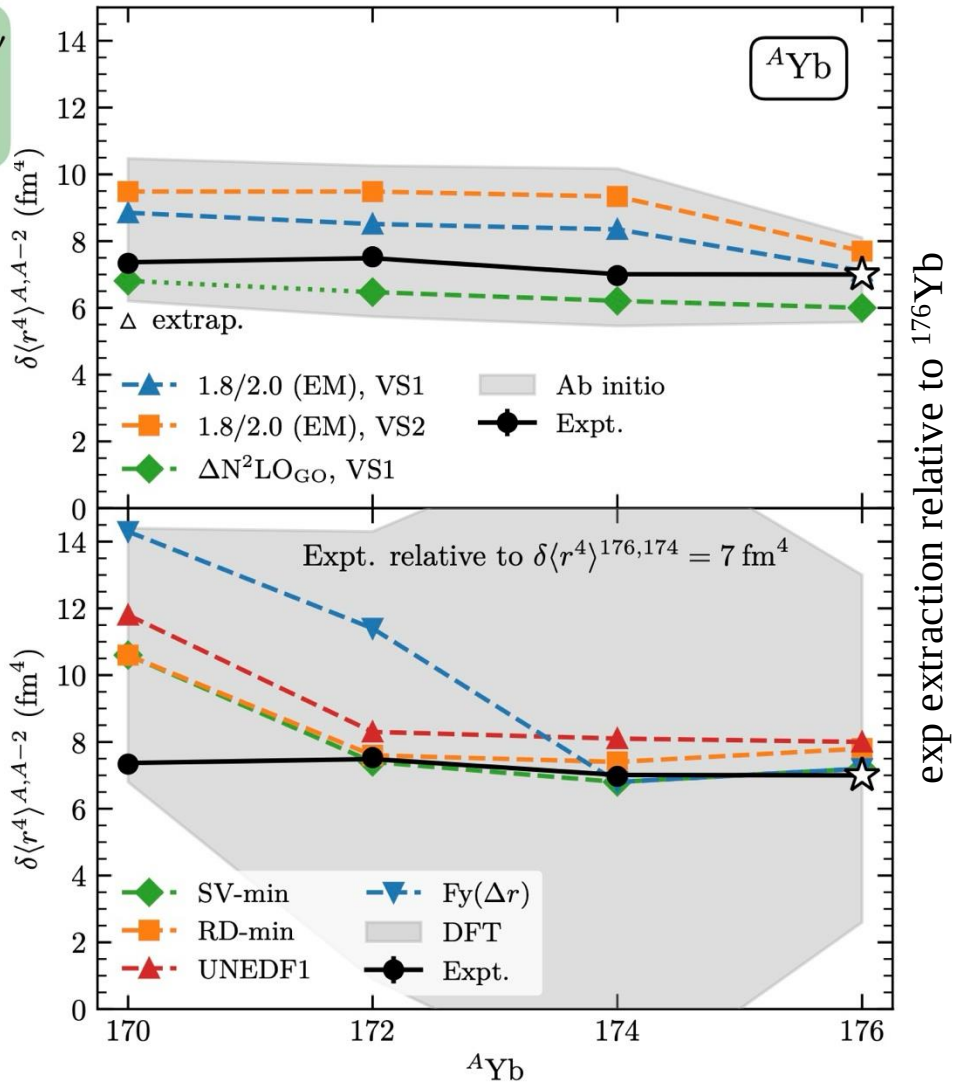
→ not quadratic field shift

→ 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



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Uncertainty quantification for low-resolution interactions

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EFT uncertainties for SRG-evolved interactions

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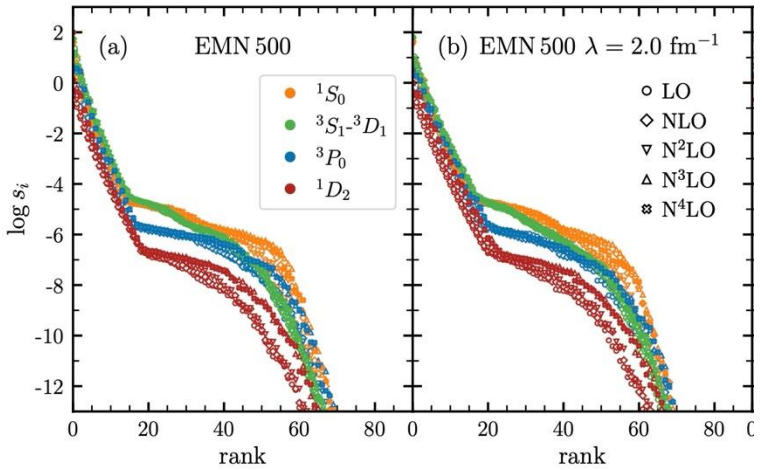
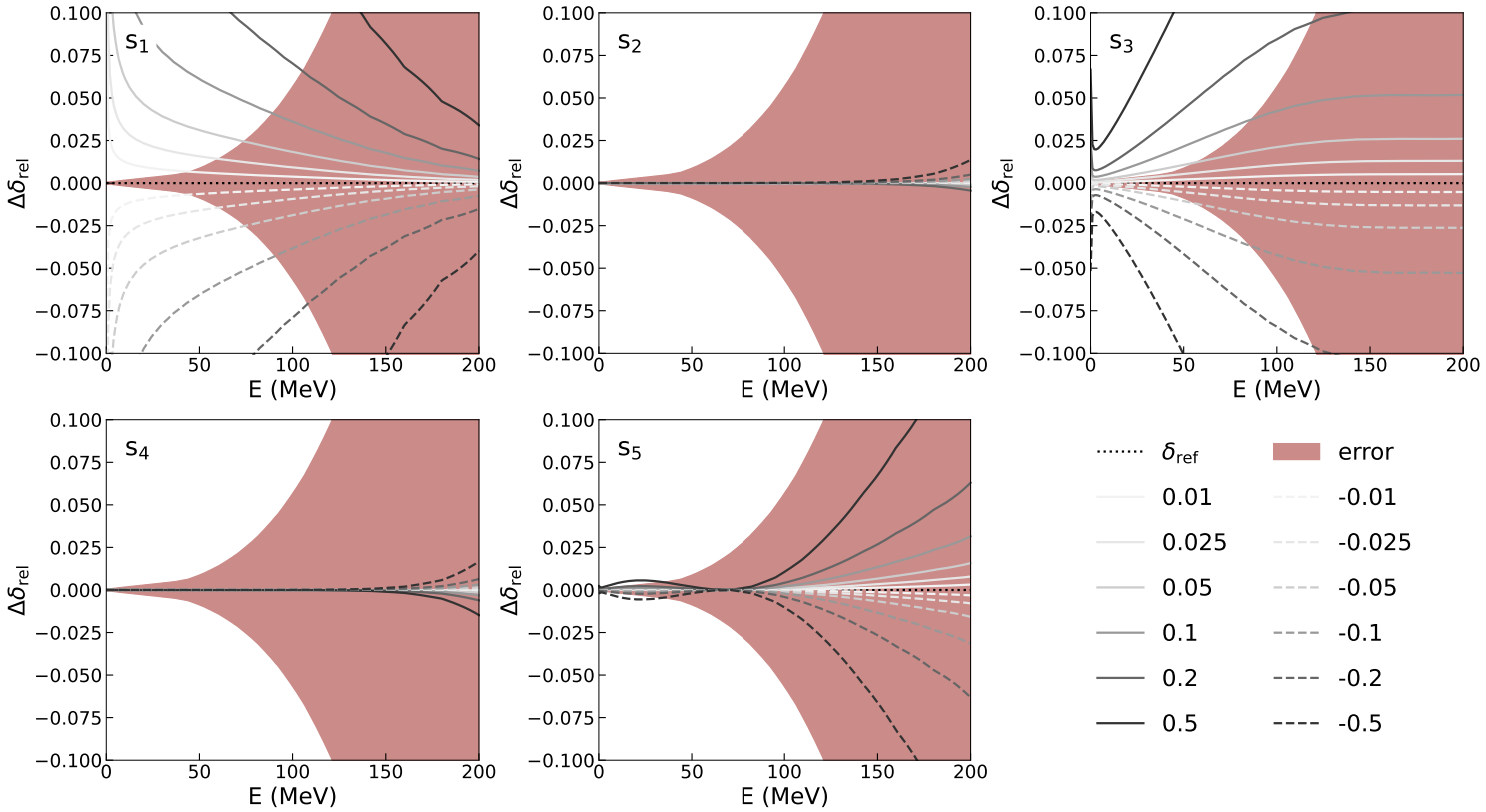
use singular value decomposition (SVD) as operator basis see Tichai et al., PLB (2021)

consider lowest 5 singular values/operators

effectively 3 generate phase shift variation

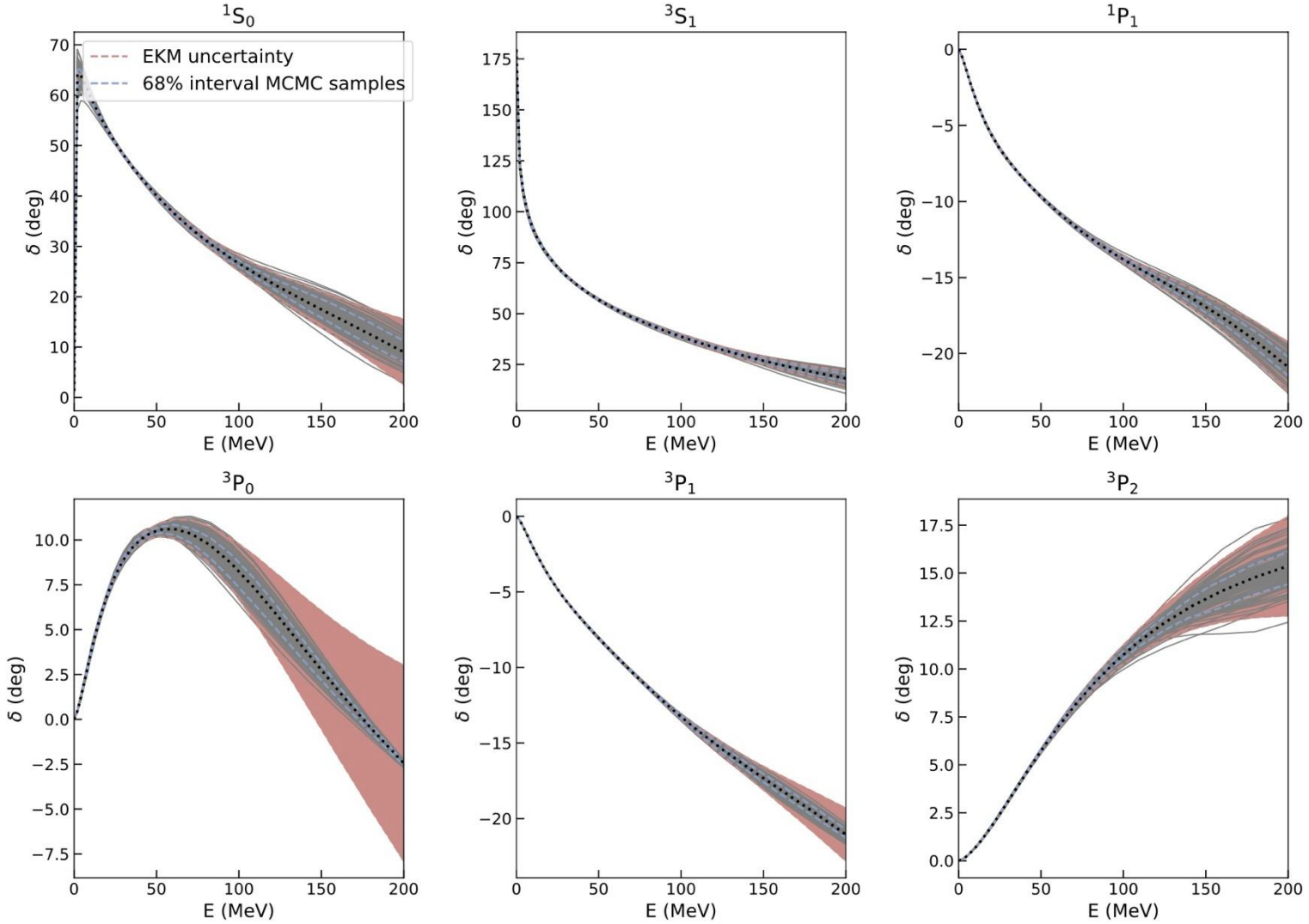




EFT uncertainties for SRG-evolved interactions

Tom Plies, Matthias Heinz, AS, preliminary

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



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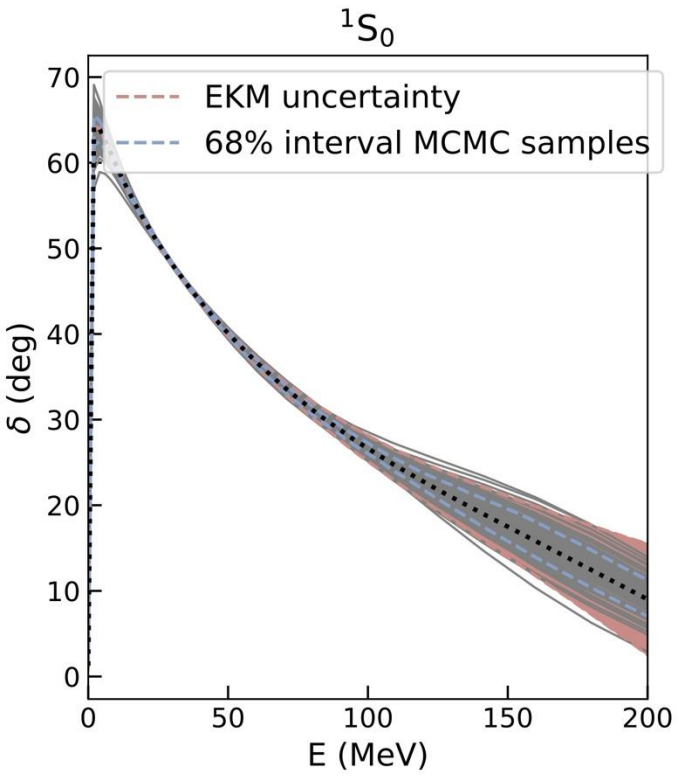
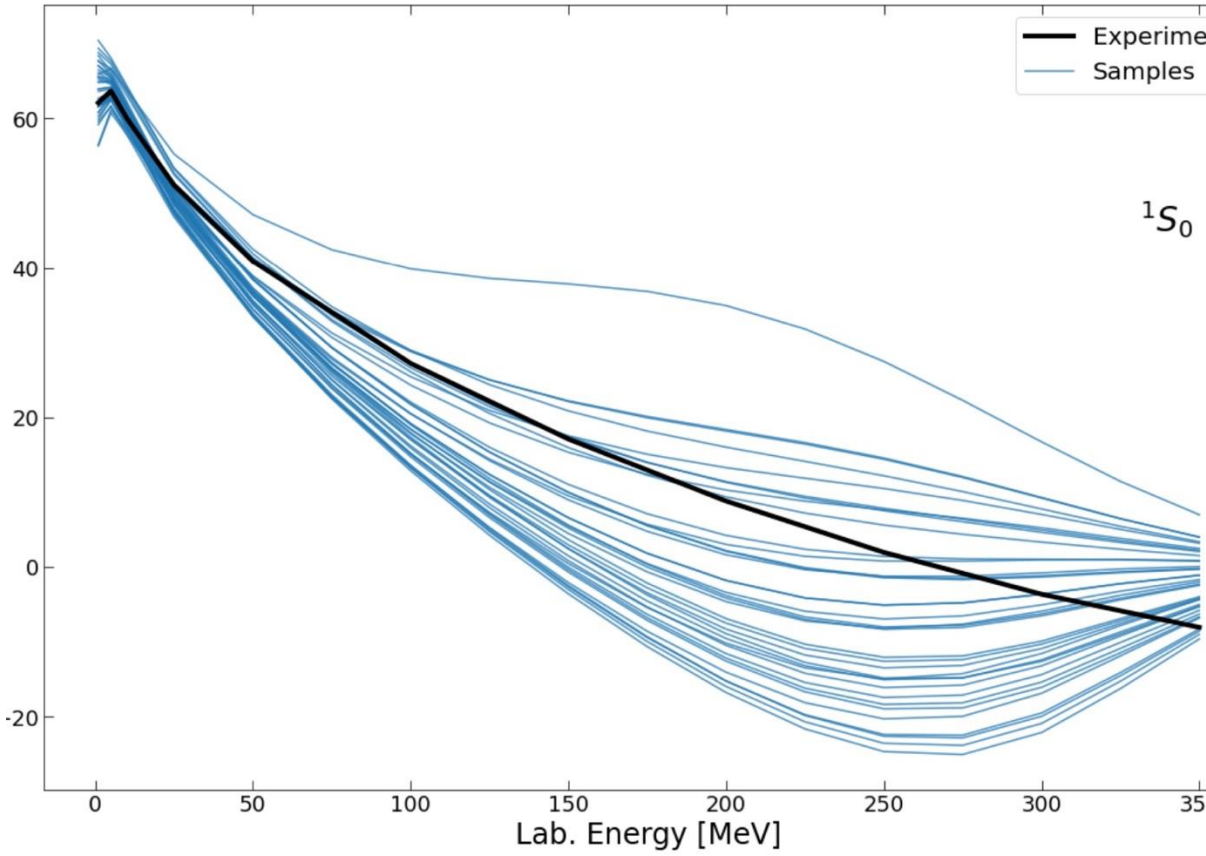


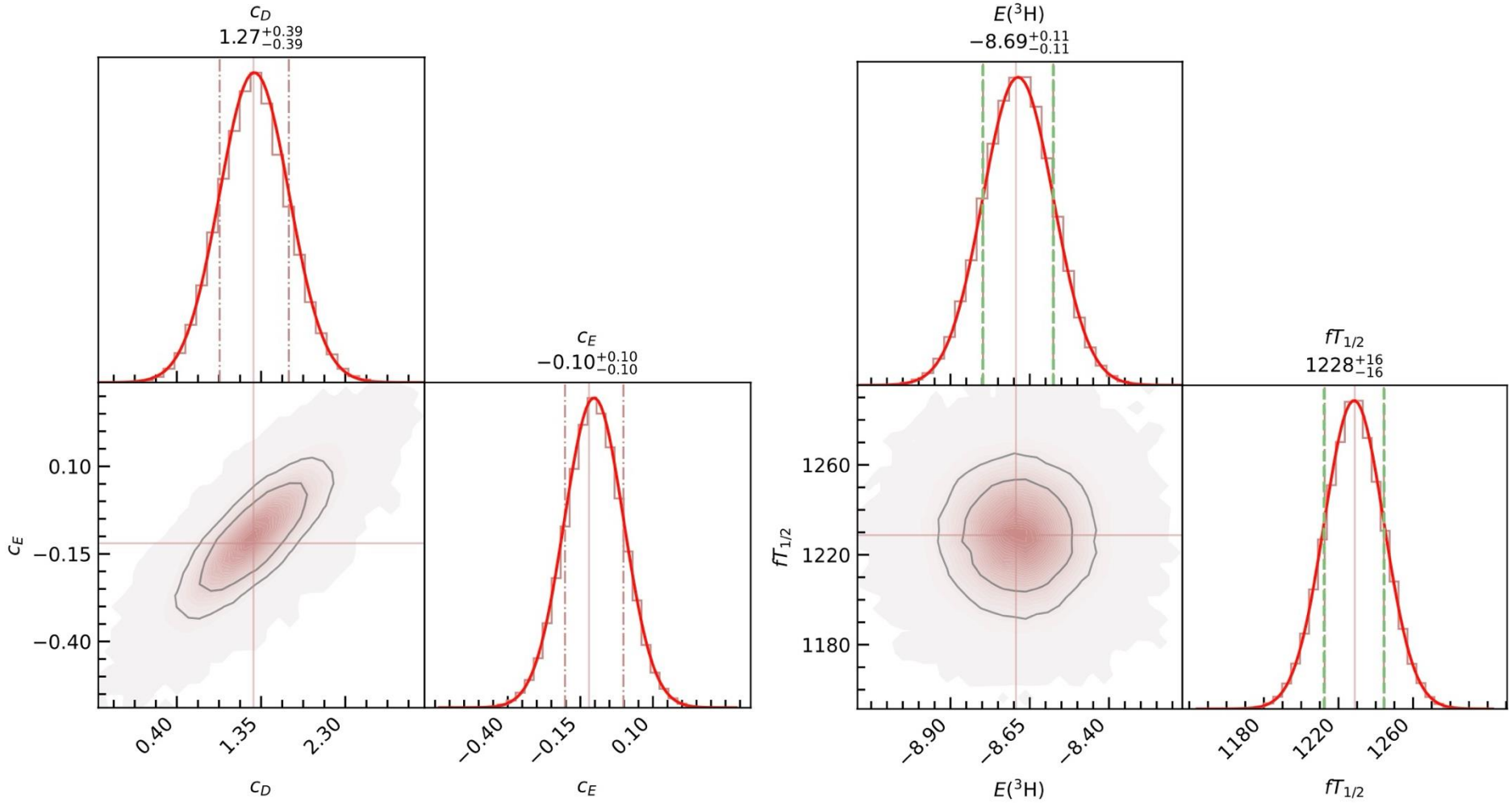


comparison to nonimplausible ΔN^2LO interactions Ekström, Forssen et al.

EFT uncertainties for SRG-evolved interactions

Tom Plies, Matthias Heinz, AS, preliminary

generate range of low-resolution NN+3N interactions
here: S and P waves, higher partial waves unvaried,
3N uncertainties from ^{3}H binding energy and half-life EFT uncertainties



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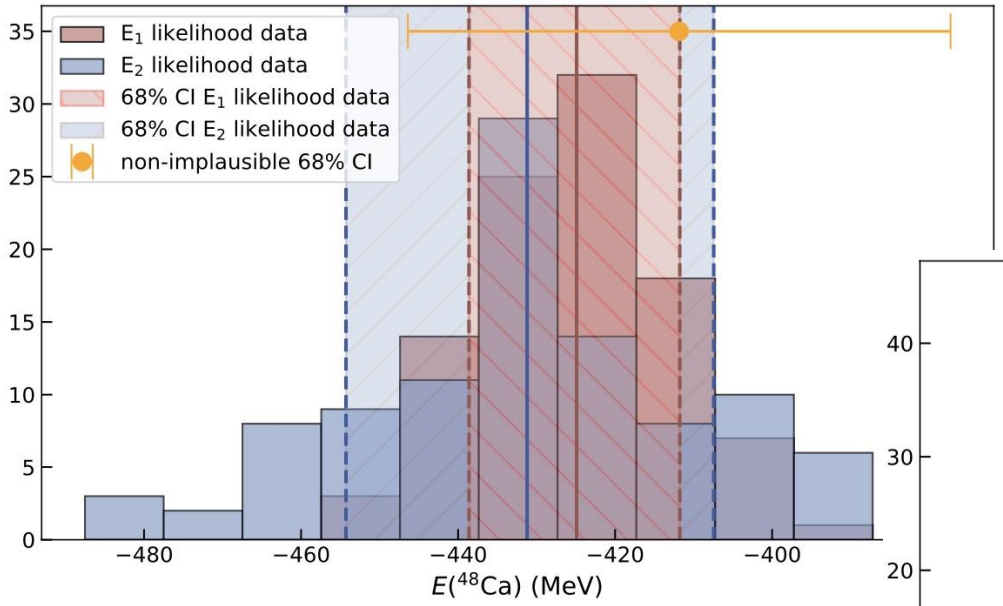
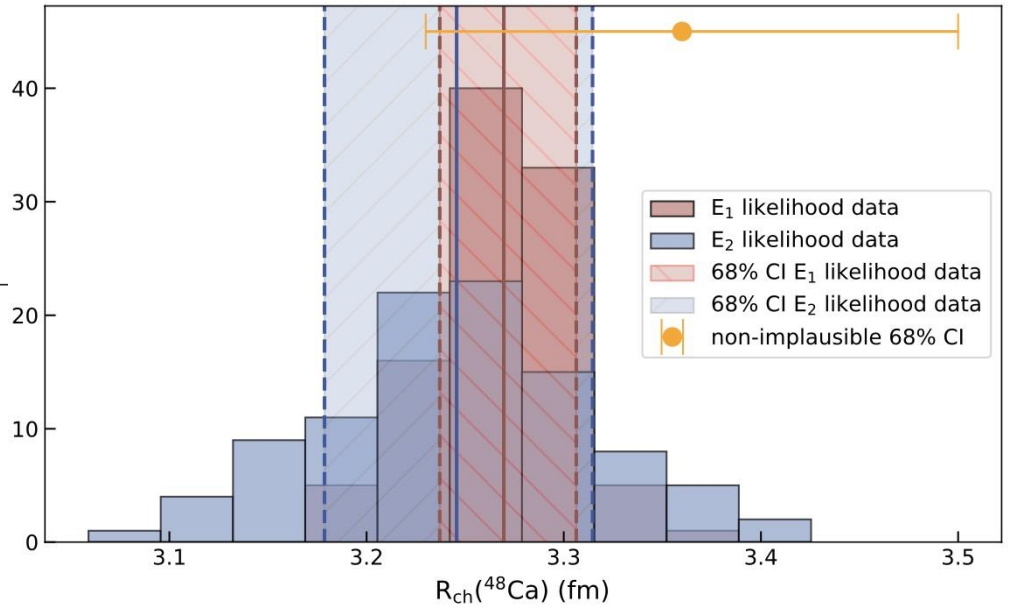
resulting posterior distributions for ^{48}Ca ground-state energy and radius





Summary

Chiral EFT interactions + powerful many-body methods

- great progress for ab initio calculations

New chiral low-resolutions interactions

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- neutron skins remarkably similar up to ^{208}Pb for chiral NN+3N

Probing nuclear structure with nonlinear King plots in ytterbium isotopes

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

- first extraction of δR_{ch}^4 from isotope shifts, evolution along heavy Yb isotopes in good agreement with IMSRG calculations

Uncertainty quantification for low-resolution interactions

Tom Plies, Matthias Heinz, AS, preliminary

- SVD basis to sample EFT uncertainties, first results for ^{48}Ca