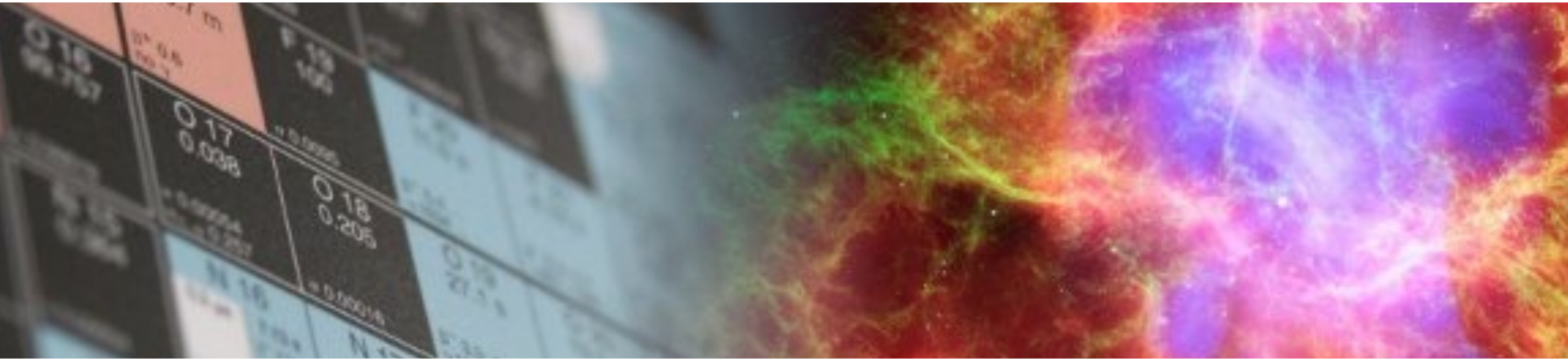
Ab initio advances for open-shell and heavy nuclei

Achim Schwenk

TECHNISCHE UNIVERSITÄT DARMSTADT

EMMI

MAX-PLANCK-INSTITUT FÜR KERNPHYSIK HEIDELBERG



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Outline

Chiral effective field theory for nuclear forces

In-medium similarity renormalization group

Global calculations and advances to heavy nuclei

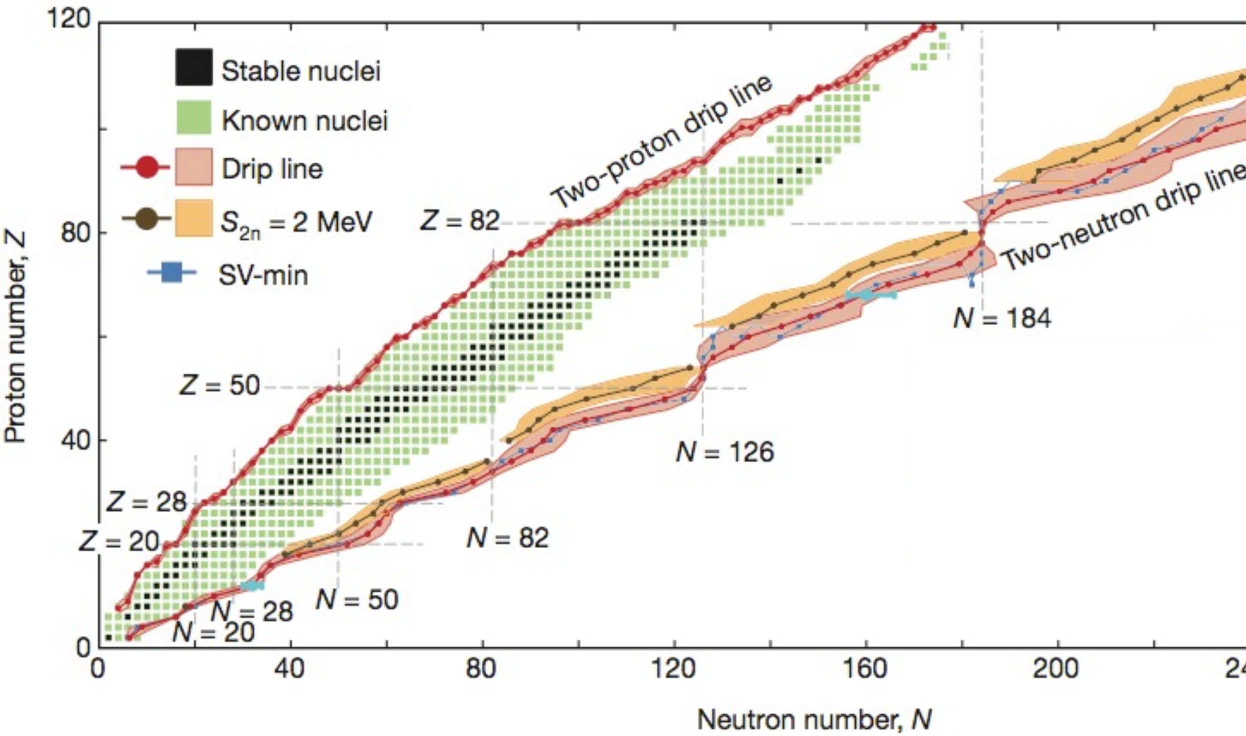
New development for open-shell nuclei:
Density matrix renormalization group

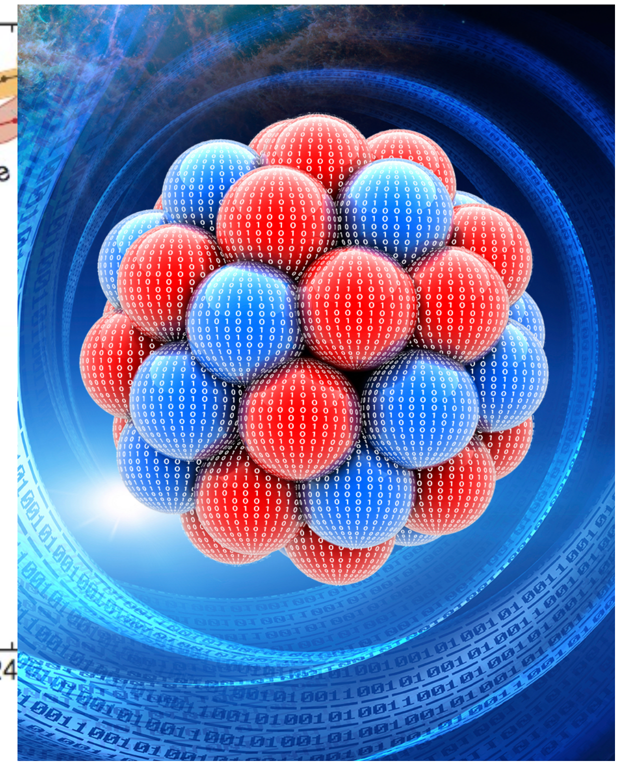
Nuclei bound by strong interactions

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]‡





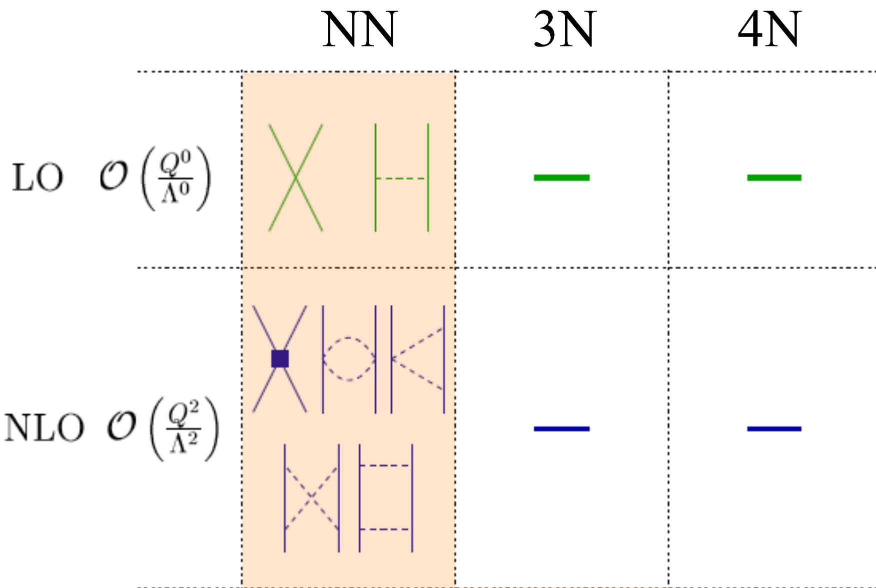
How does the nuclear chart emerge from the strong interaction?

Lattice QCD and **effective field theories of the strong interaction**

for few nucleons for all nuclei

Chiral effective field theory for nuclear forces

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



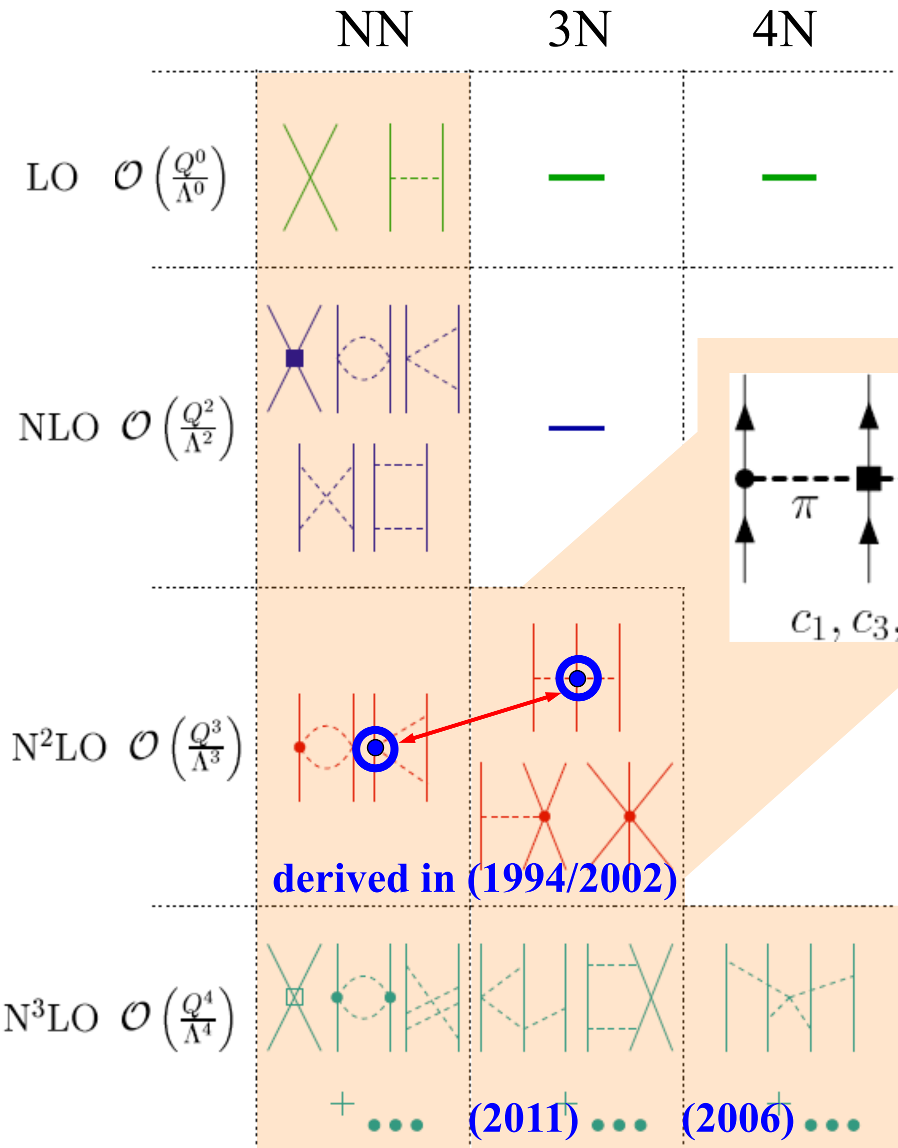
based on symmetries of strong interaction (QCD)

long-range interactions governed by pion exchanges

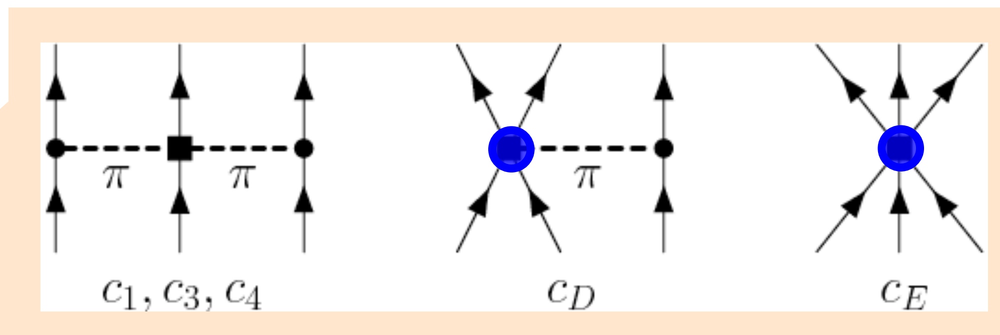
Weinberg (1990,91)

Chiral effective field theory for nuclear forces

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



powerful approach for many-body interactions



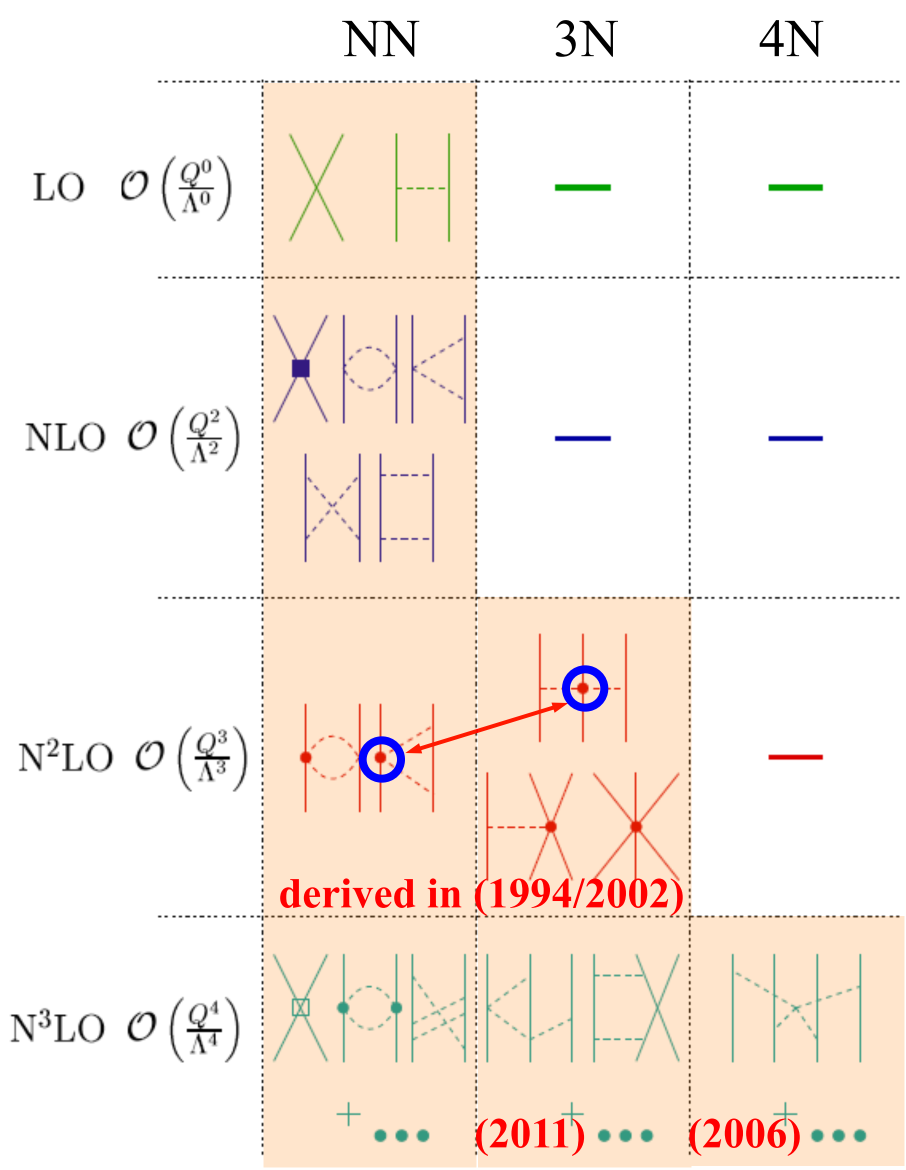
only 2 new couplings at N²LO

all 3- and 4-neutron forces predicted to N³LO

Hebeler, AS (2010), Tews, Krüger et al. (2013)

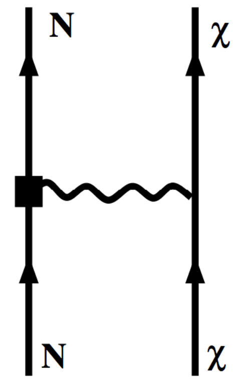
Weinberg, van Kolck (1992-1994), Kaplan, Savage, Wise, Bernard, Epelbaum, Kaiser, Meissner,…

Chiral EFT for coupling to electroweak interactions

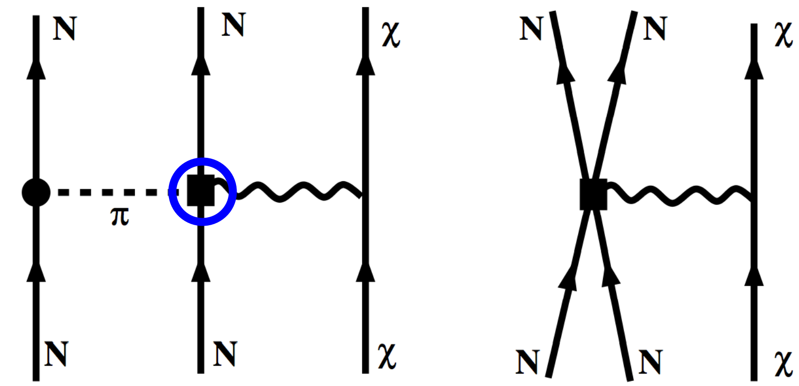


axial-vector currents (beta decays)

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



+ two-body currents at Q^3



same couplings in forces and currents!

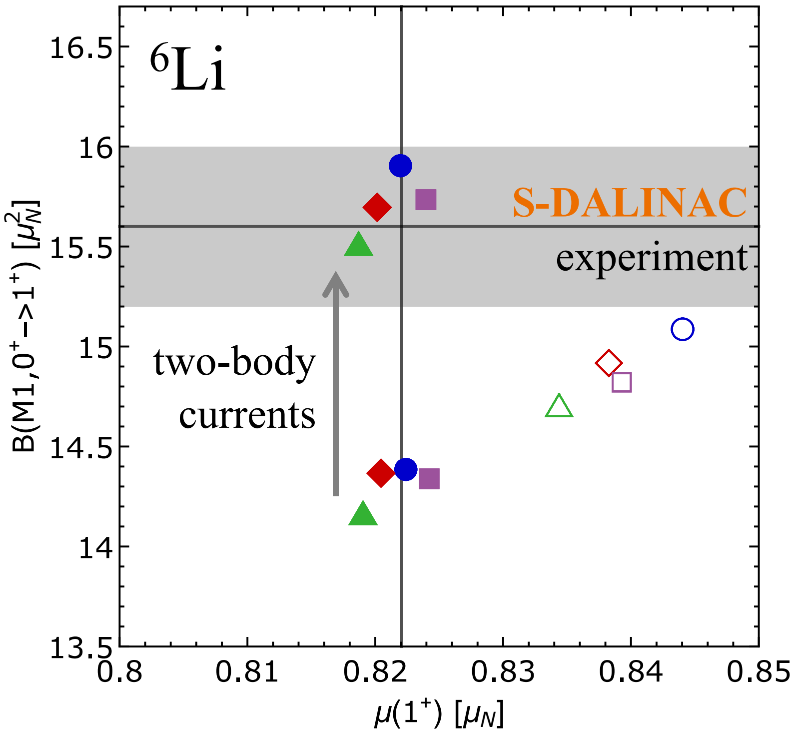
Chiral EFT for coupling to electroweak interactions

consistent electroweak one- and two-body currents

magnetic properties of light nuclei

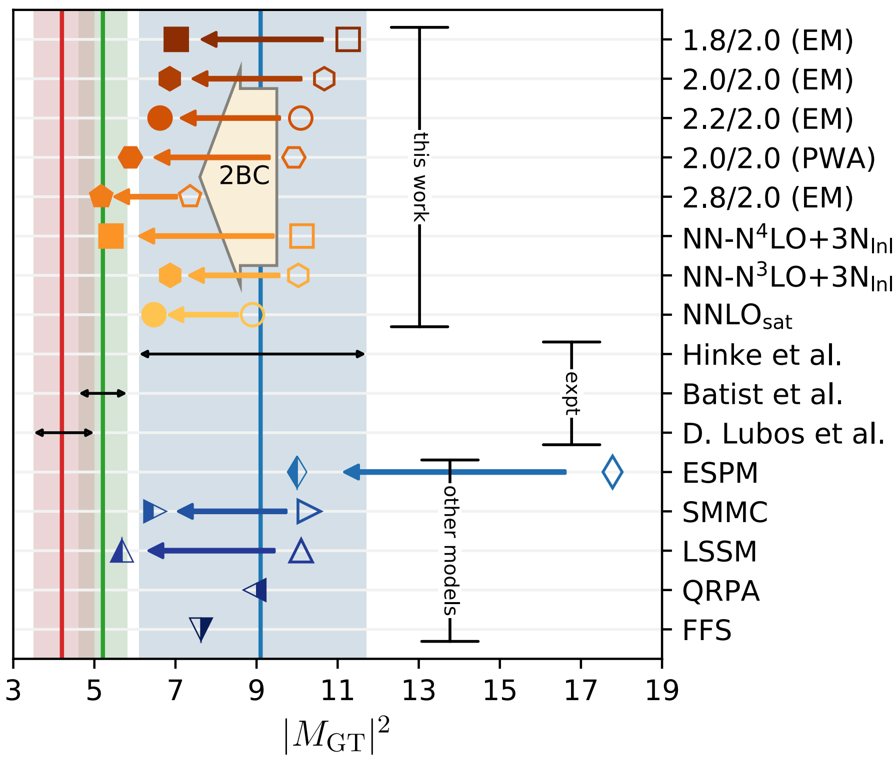
Pastore et al. (2012-)

B(M1) of ^{6}Li Gayer et al., PRL (2021)



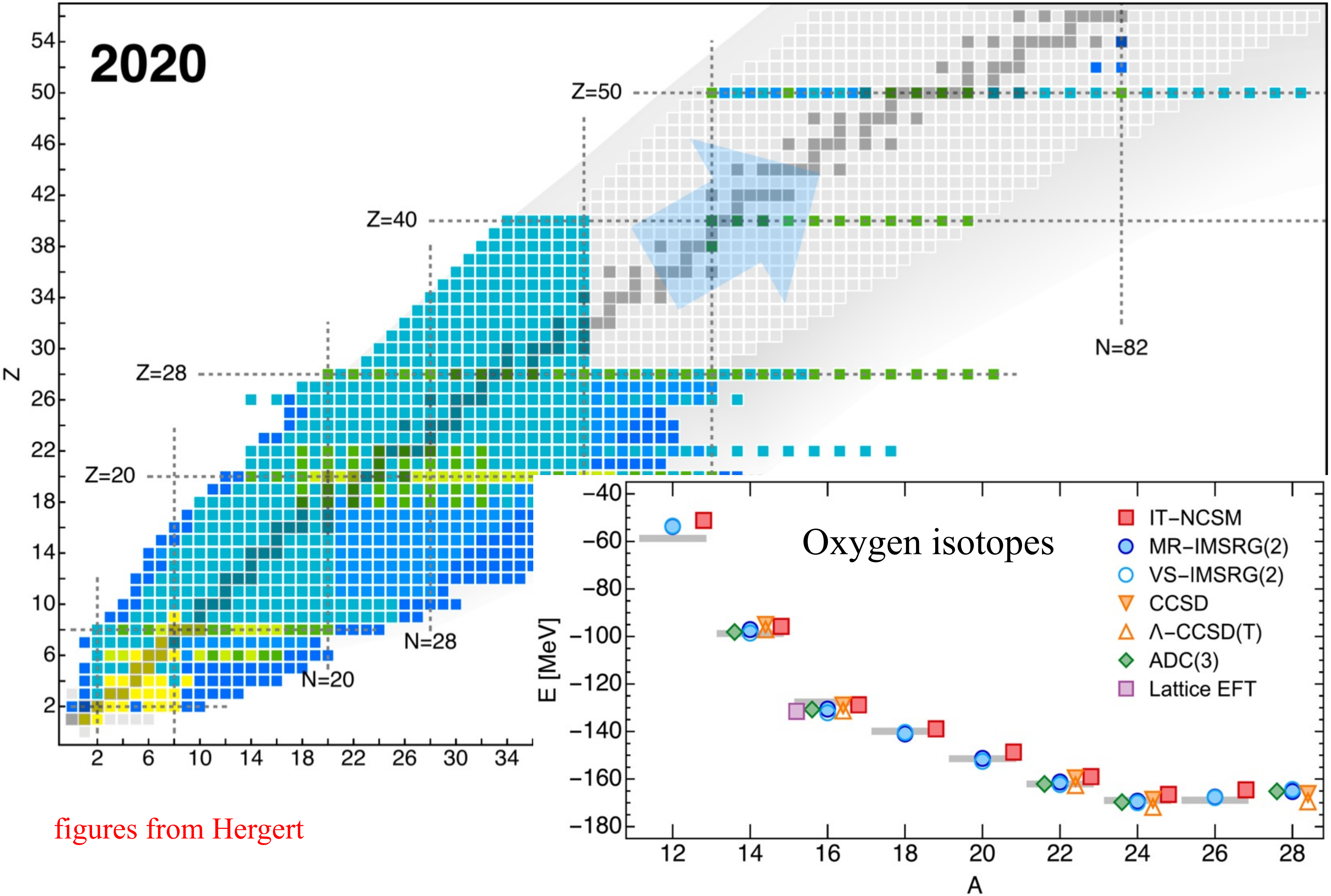
Gamow-Teller beta decay of ^{100}Sn

Gysbers et al., Nature Phys. (2019)



two-body currents (2BC) key for quenching puzzle of beta decays

Great progress in ab initio calculations of nuclei



figures from Hergert

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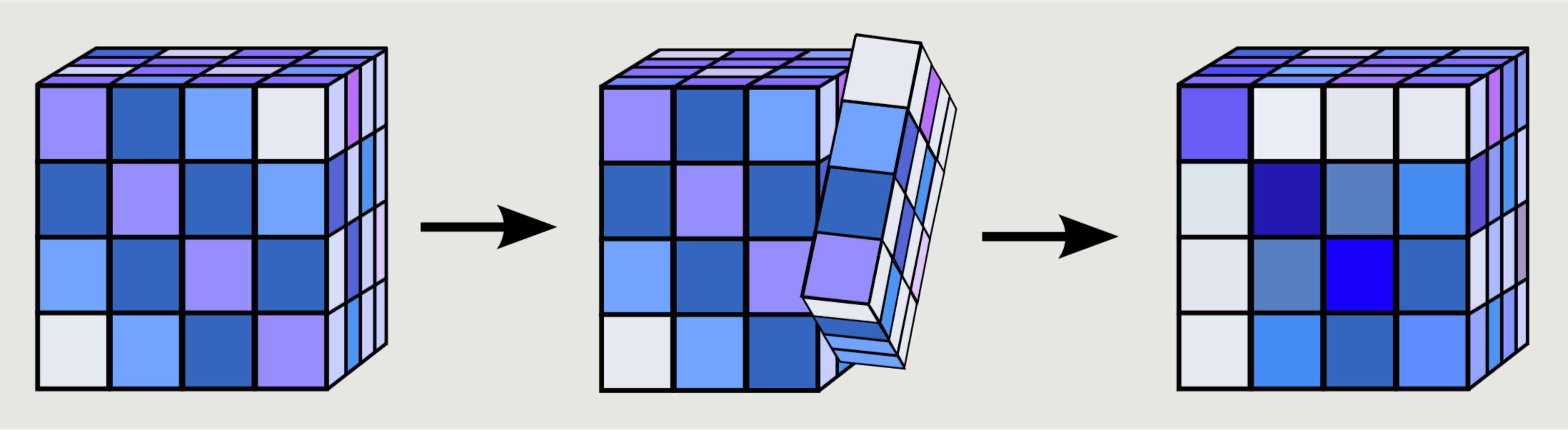
In-medium similarity renormalization group

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

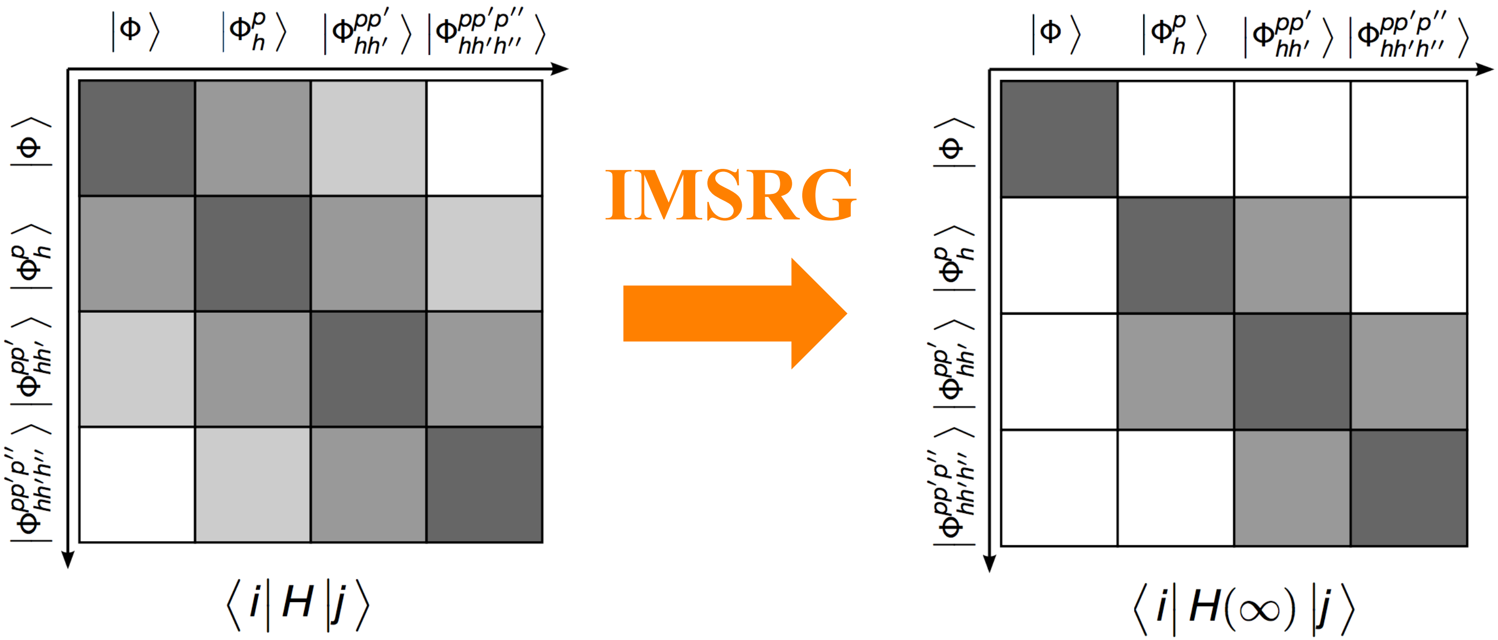
continuous transformation to block-diagonal form (→ decoupling)



In-medium similarity renormalization group

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

flow equations to decouple higher-lying particle-hole states



s = 0

s = ∞

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

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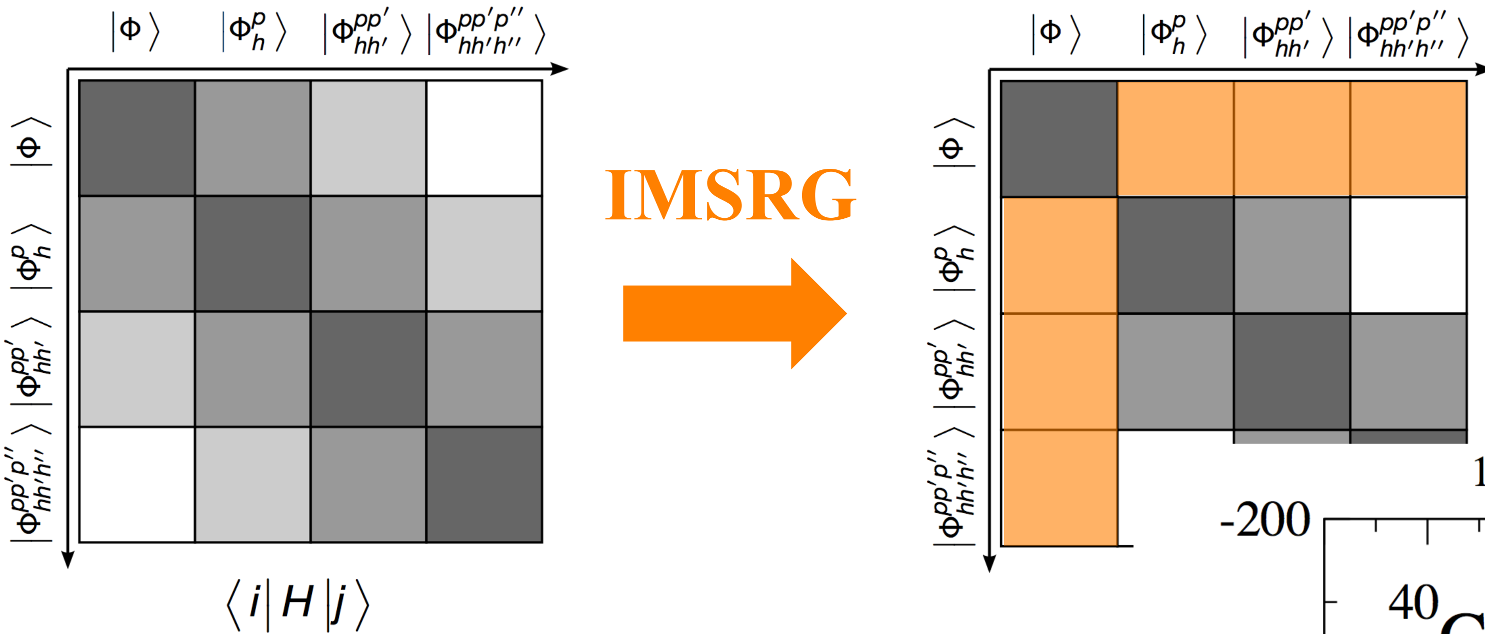
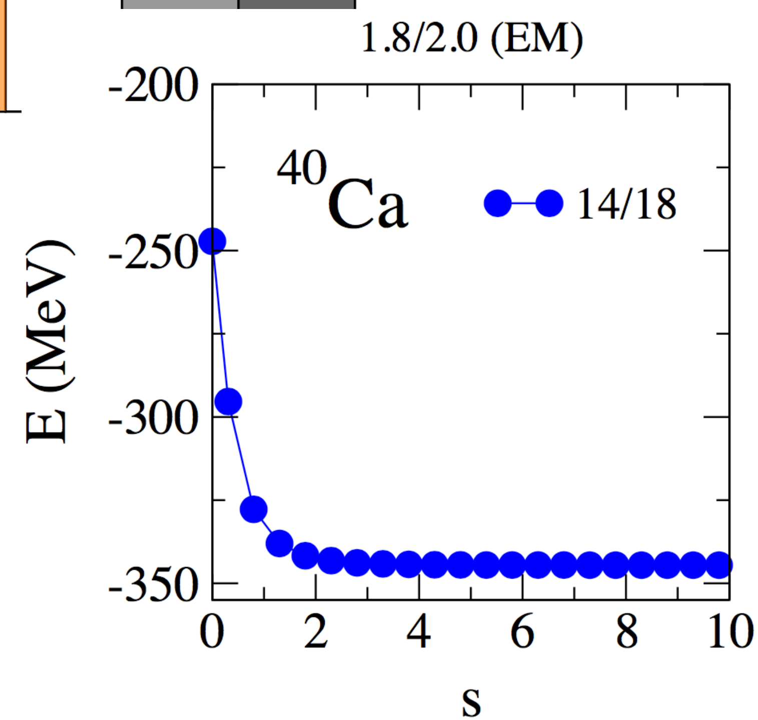


s = 0

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

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

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



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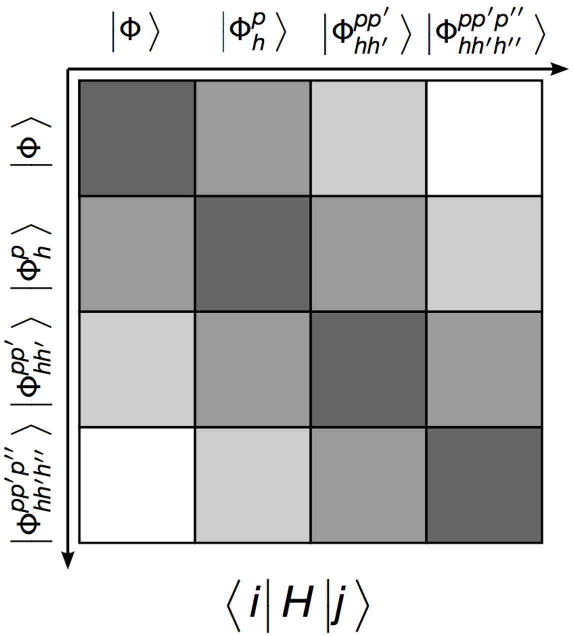
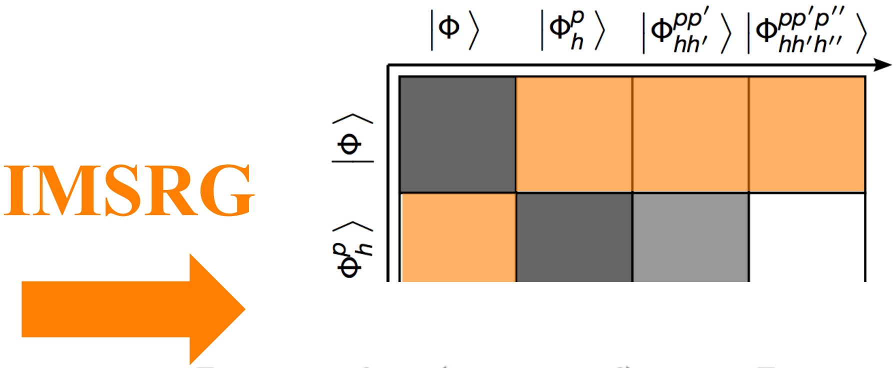
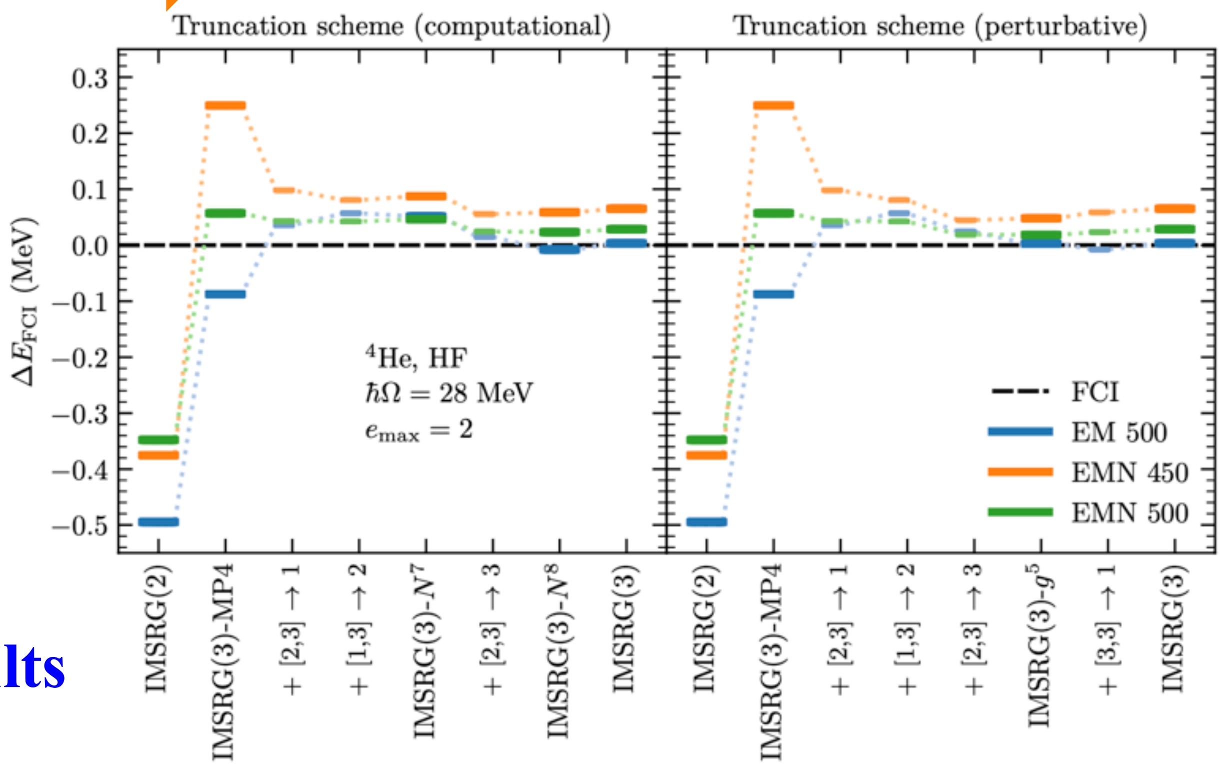


IMSRG





First IMSRG(3) results

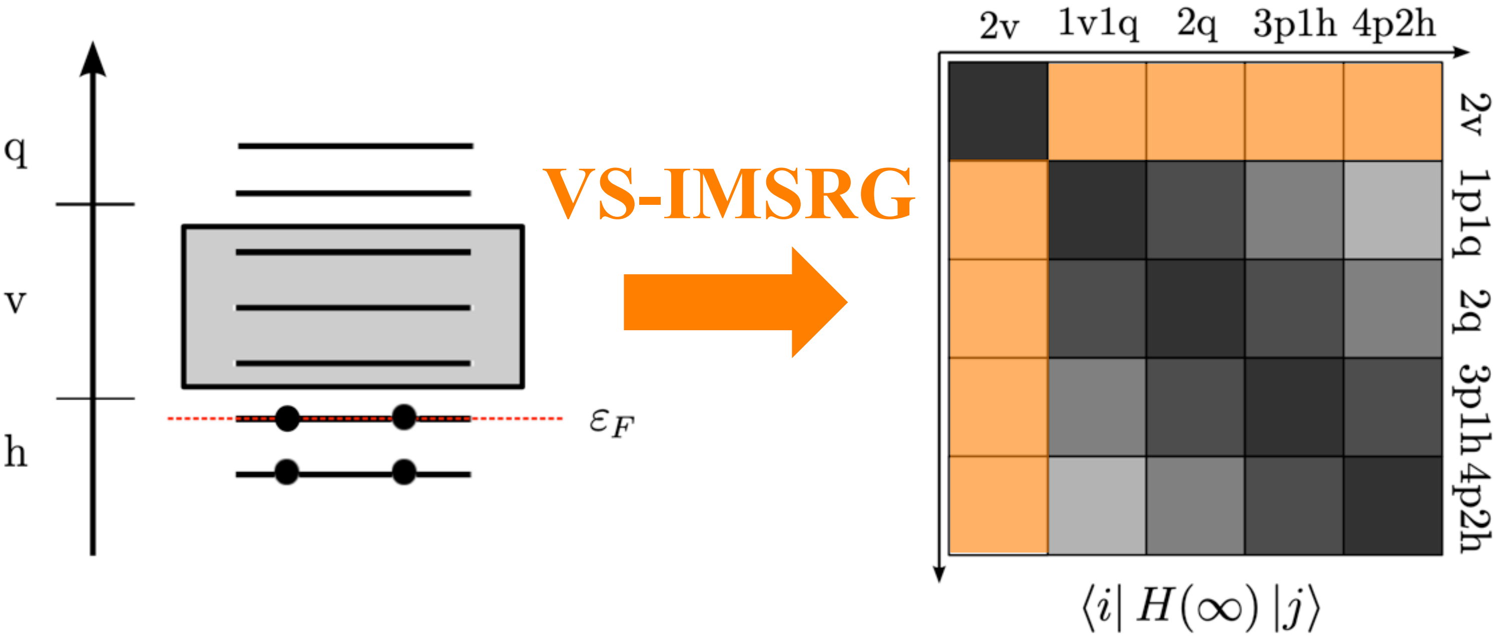
Heinz et al. (2021)

Valence-space IMSRG

Tsukiyama et al. (2012); Bogner et al., PRL (2014); Stroberg et al., PRL (2016), PRL (2018)

decouple valence space of few particles

followed by exact diagonalization in valence space



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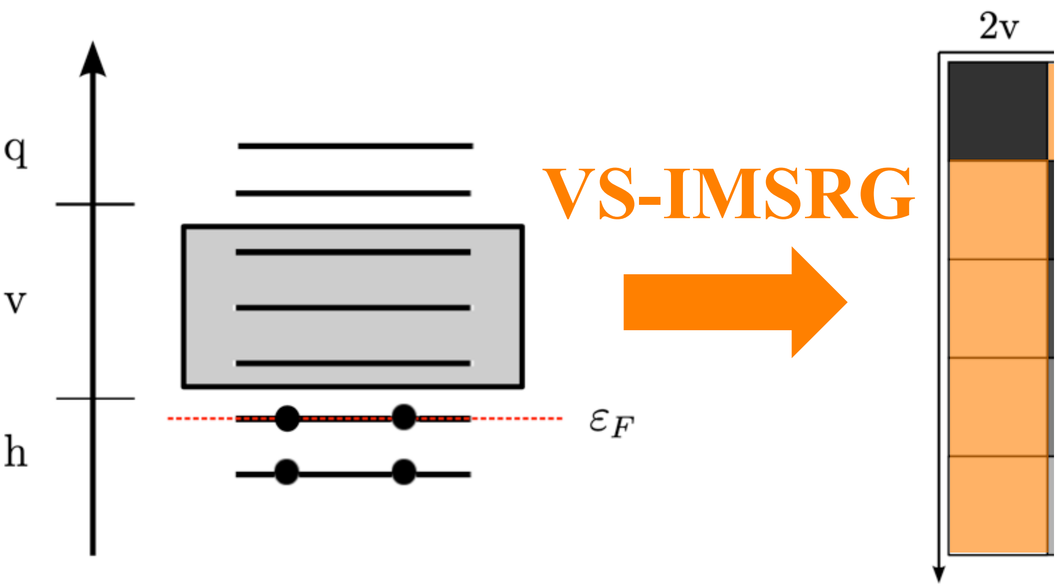

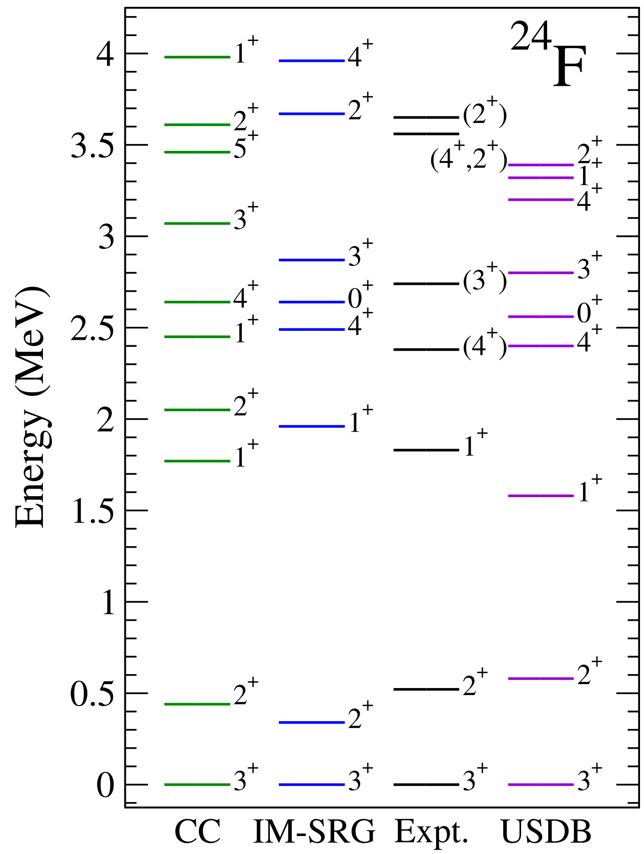

Cáceres et al., PRC (2015)

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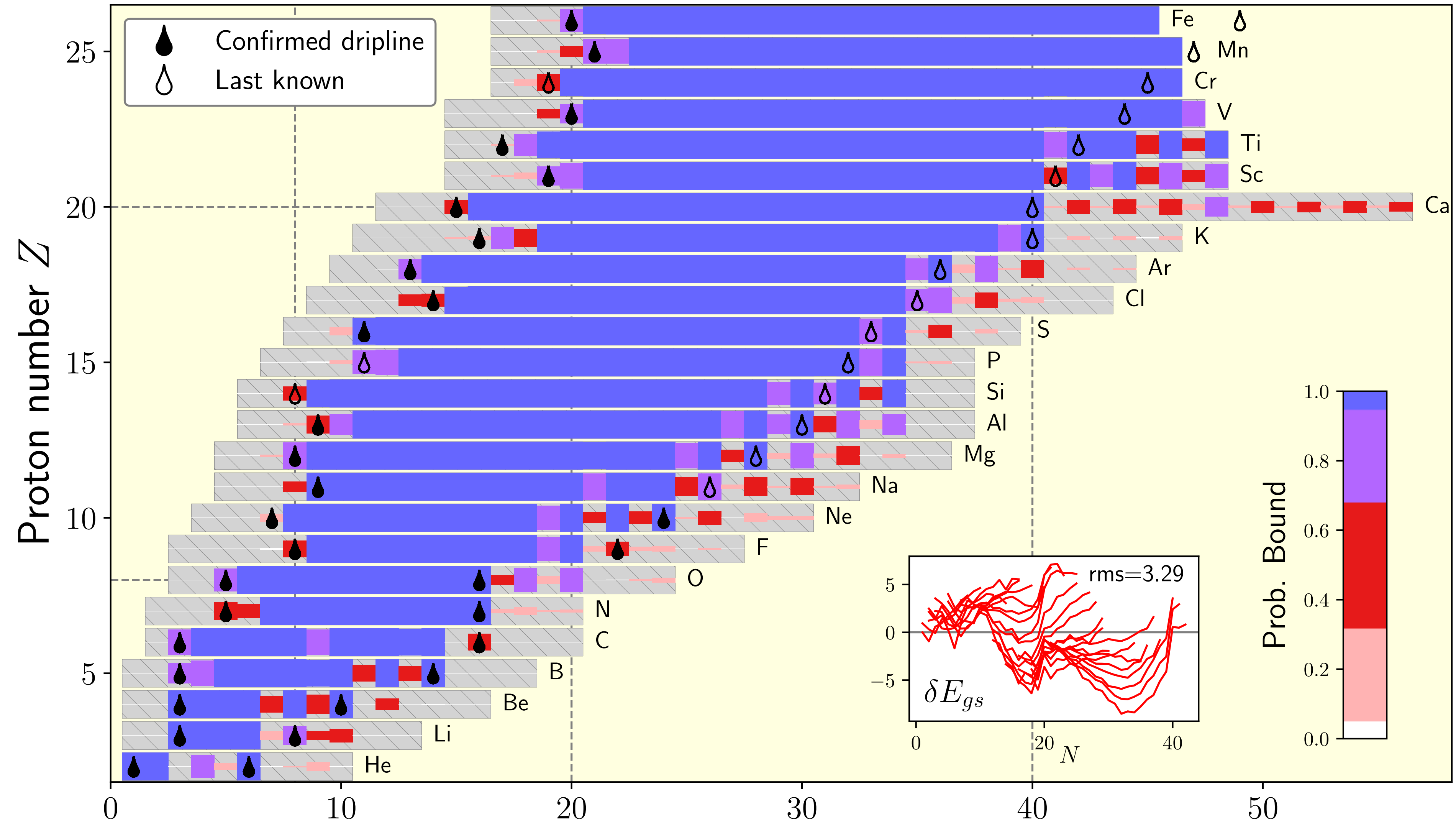
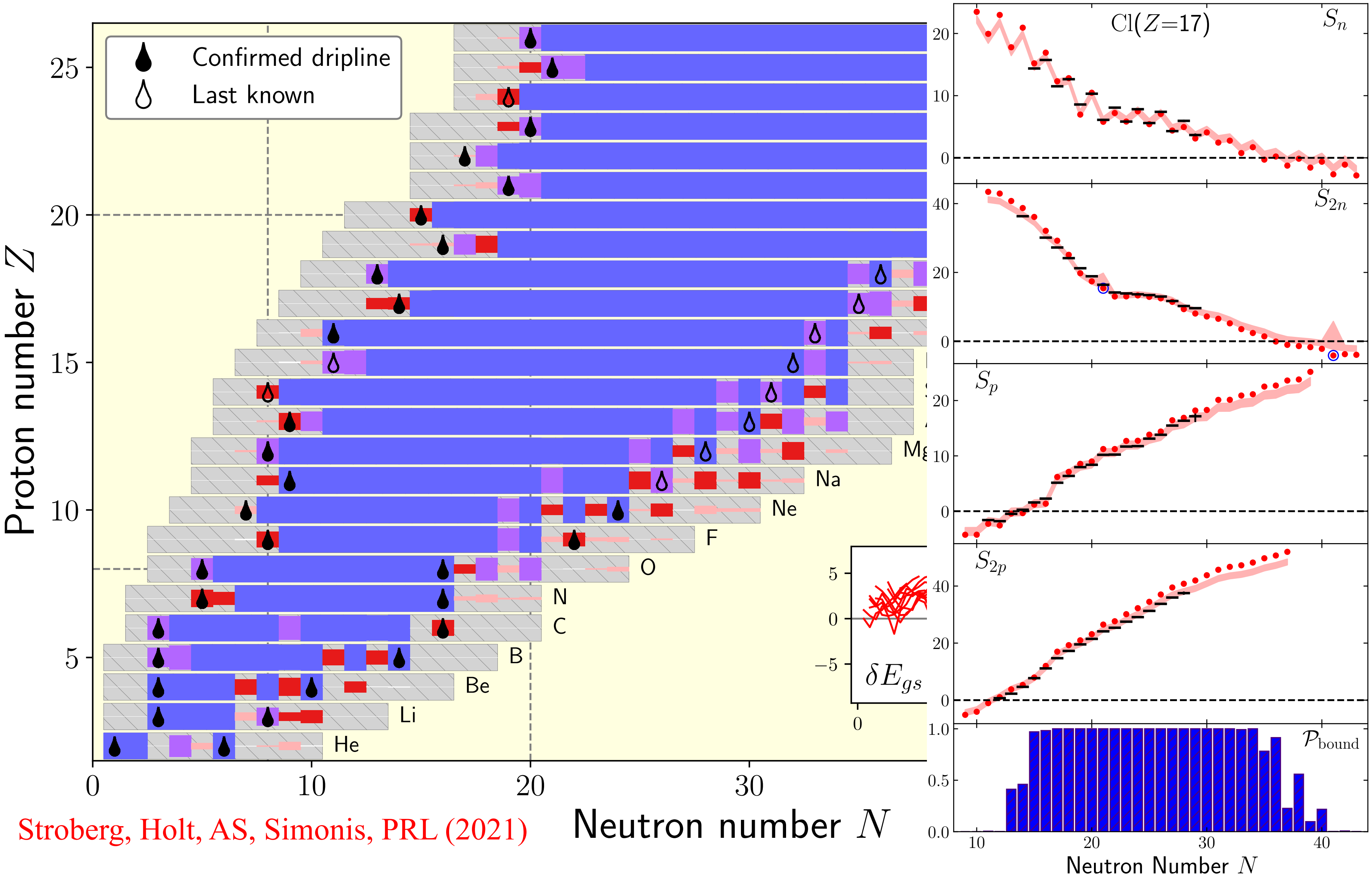
Nuclear landscape based on a chiral NN+3N interaction



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)

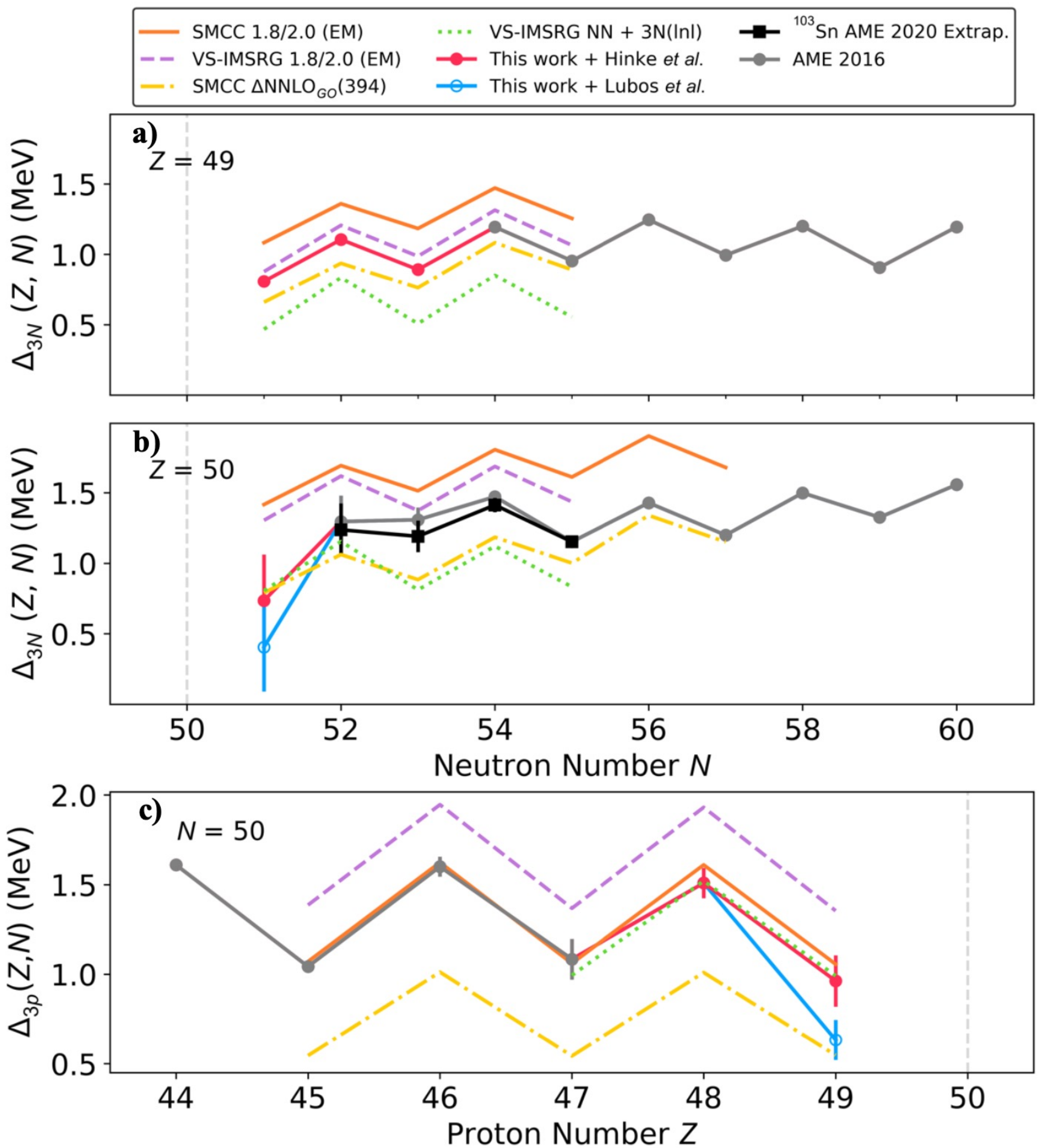
ab initio is advancing to global theories, limitations due to input NN+3N

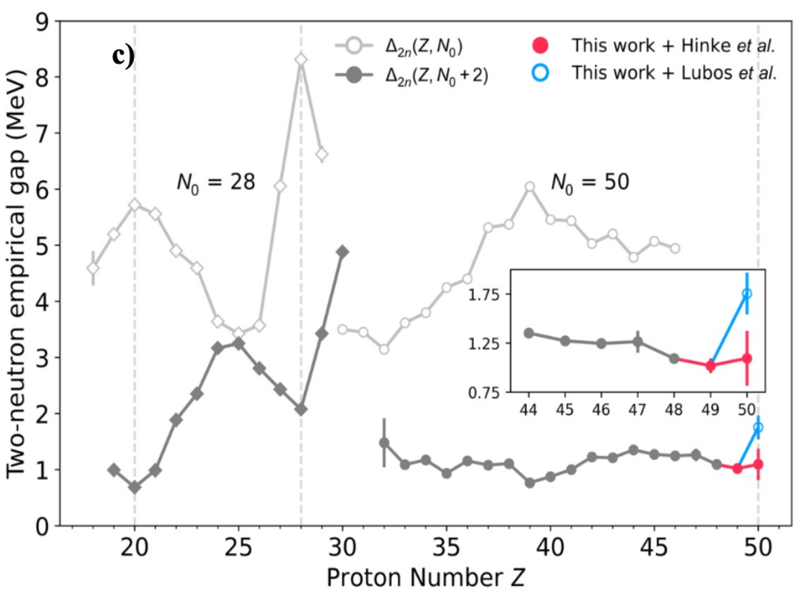
Indium mass measurements

ISOLTRAP mass measurements of $^{99\text{-}101}$In Mougeot et al., Nature Phys. (2021)

odd-even staggering consistent with all calculations

helps to constrain Q-value for beta decay of ^{100}Sn, more consistent with Hinke et al.

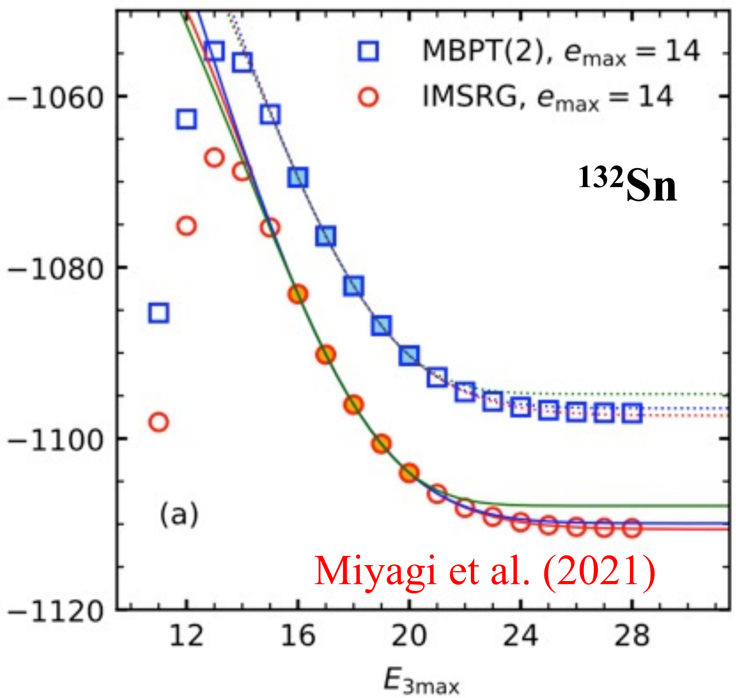




First ab initio calculations of ^{208}Pb

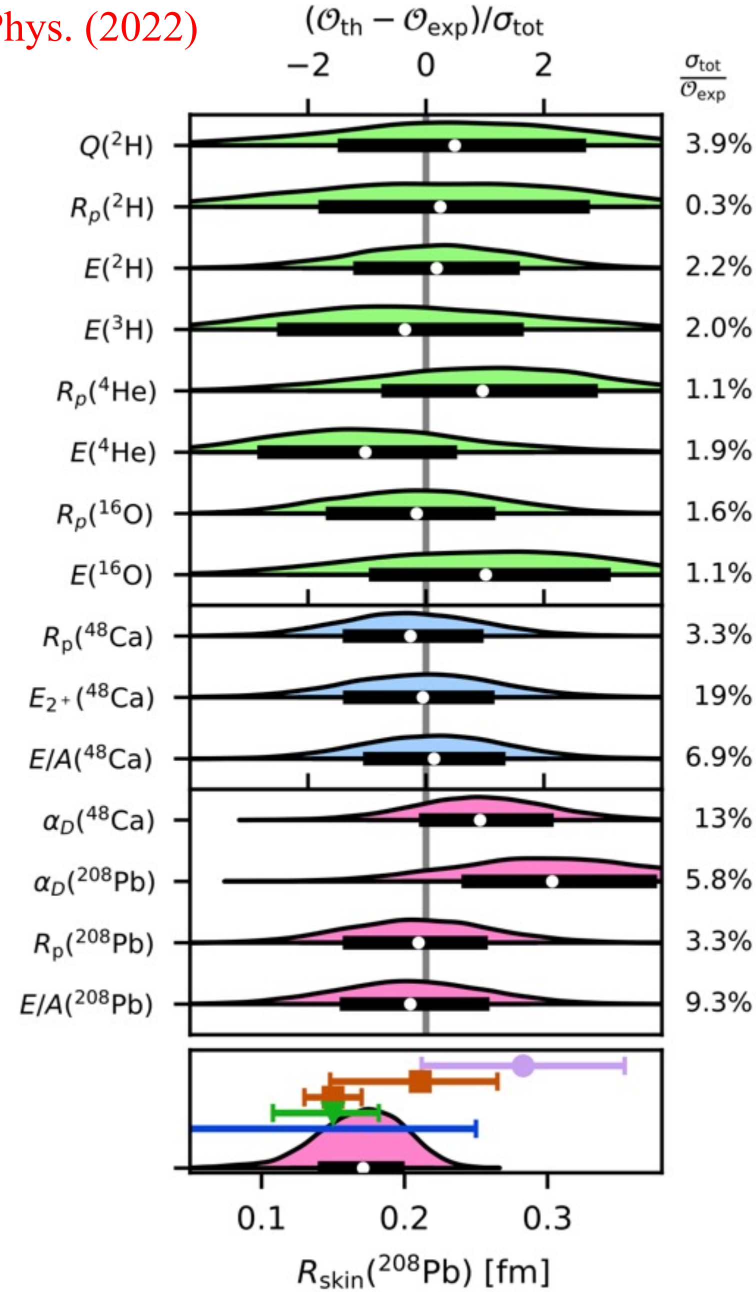
Hu, Jiang, Miyagi et al. [Chalmers, ORNL, TRIUMF], Nature Phys. (2022)

enabled by 3N advances



history matching to explore uncertainties in NN+3N interactions

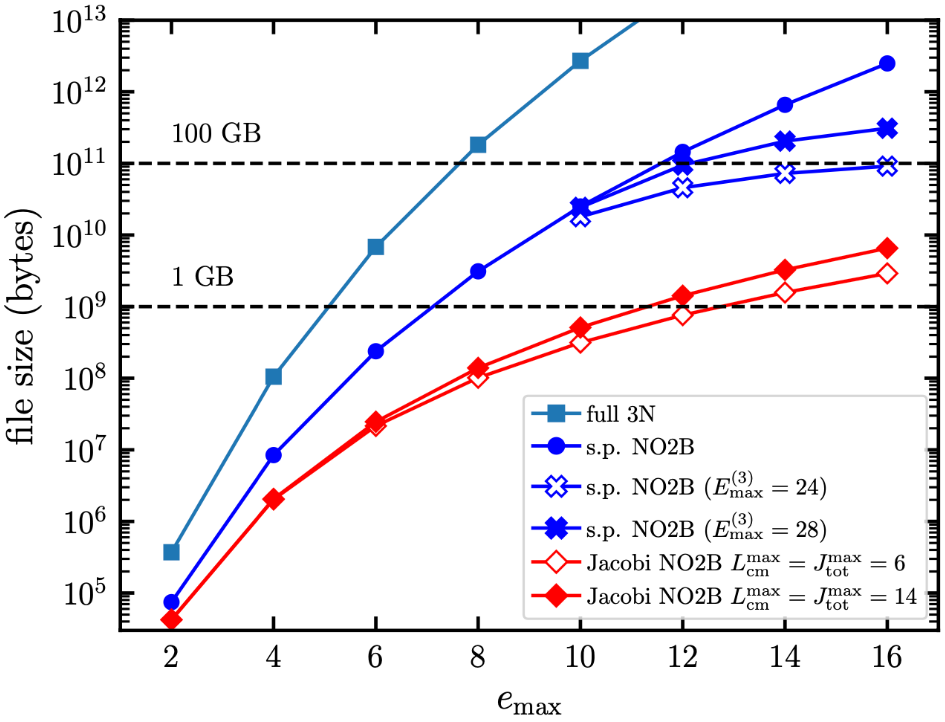
range for **neutron skin of ^{208}Pb**



Novel Jacobi normal ordering for 3N interactions

Hebeler, Durant, Hoppe et al., arXiv:2211.16262

normal ordering in Jacobi basis
circumvents costly storage of
single-particle 3N matrix elements



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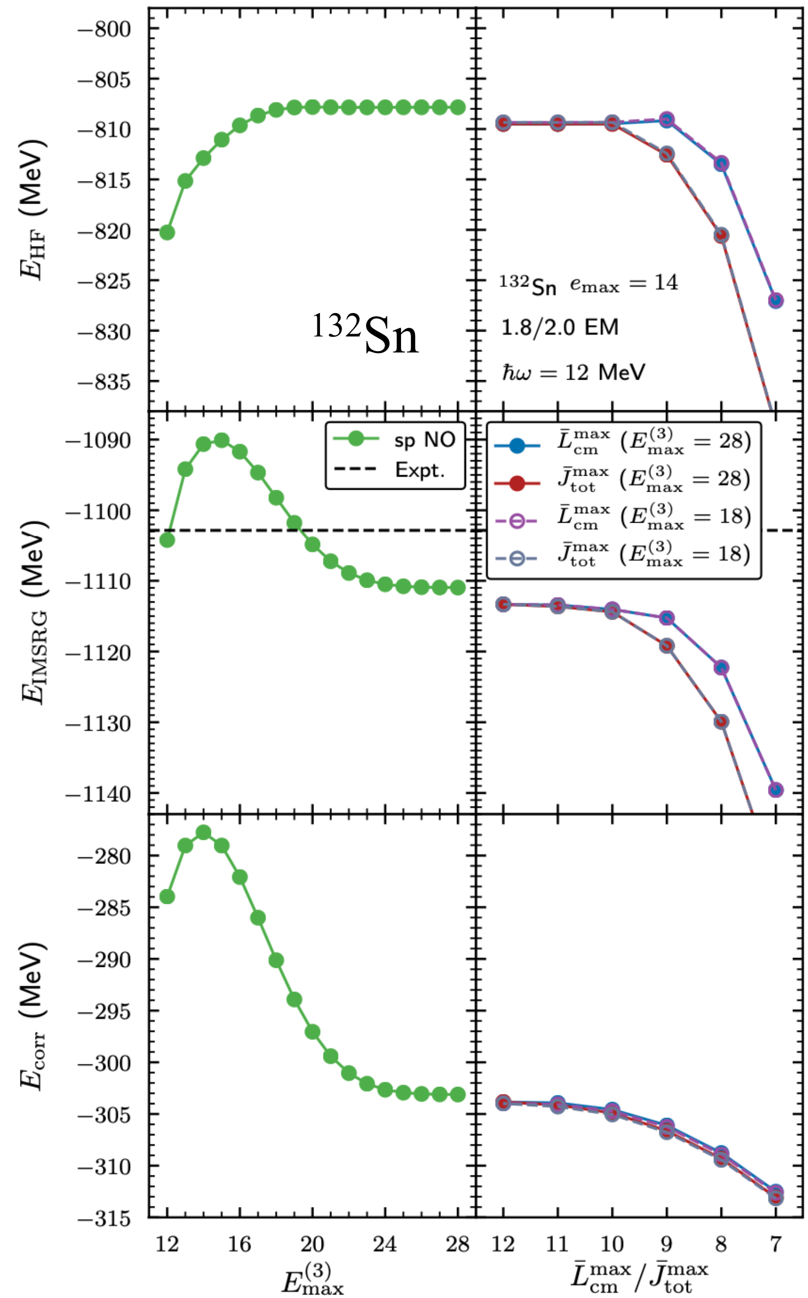
agrees with traditional normal ordering with 0.1% differences due to numerical precision and antisymmetrization

	E_{HF} (MeV)	E_{IMSRG} (MeV)
Antisymmetrization in Jacobi HO basis		
single precision	-806.11	-1109.02
$J^{\mathrm{max}} = l^{\mathrm{max}} = 5$ truncation	-808.79	-1111.83
half precision	-807.84	-1110.49
Antisymmetrization in Jacobi momentum-space basis		
single precision	-807.19	-1110.27
$J^{\mathrm{max}} = l^{\mathrm{max}} = 5$ truncation	-809.05	-1112.29
Jacobi normal ordering		
$\bar{L}_{\mathrm{cm}}^{\mathrm{max}} = \bar{J}_{\mathrm{tot}}^{\mathrm{max}} = 13$	-809.49	-1113.33



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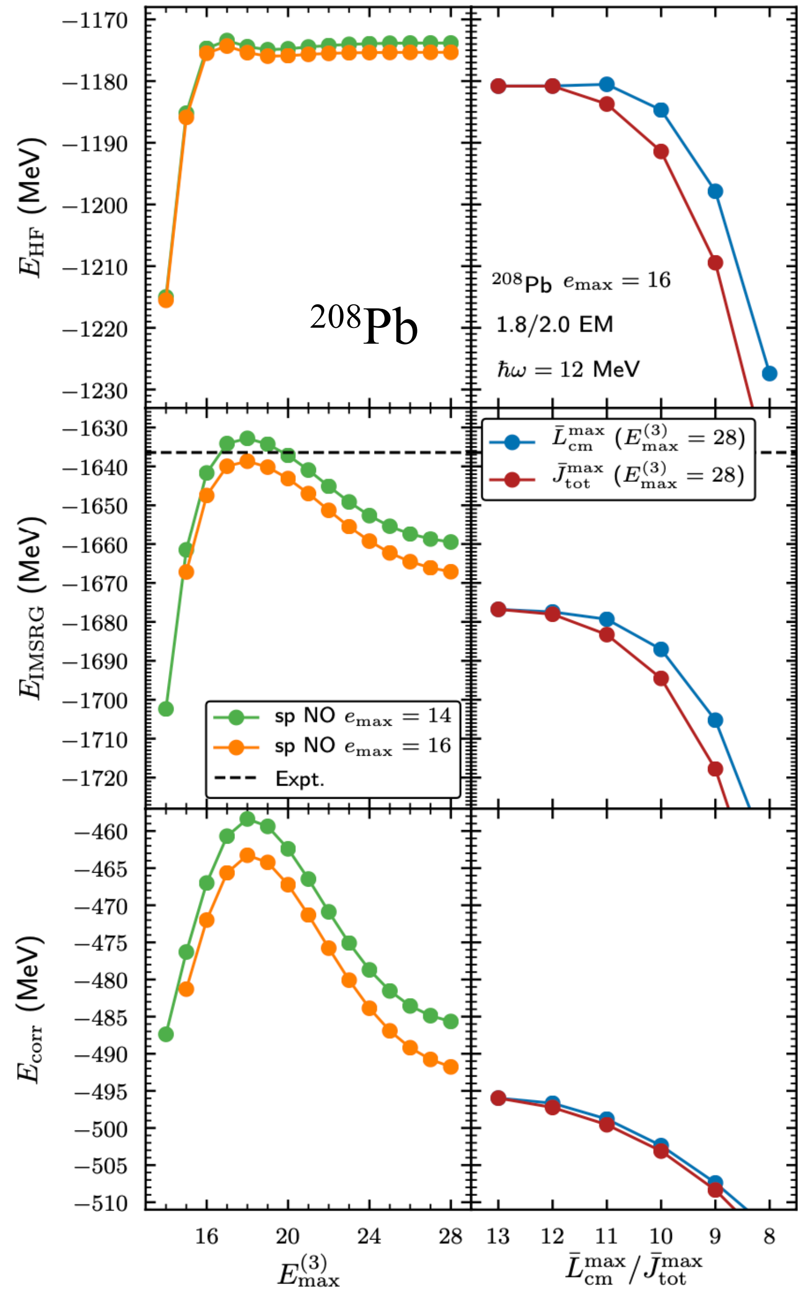
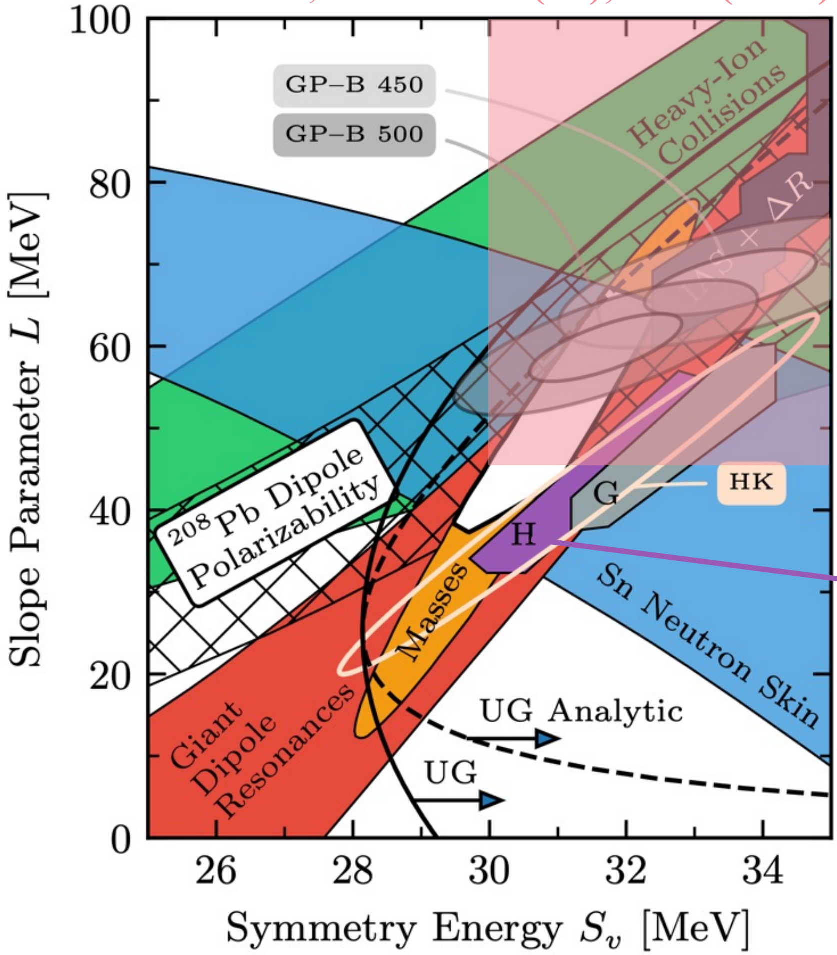
results up to ^{208}Pb

advantage: improved radial dependence without E_{3max} cut



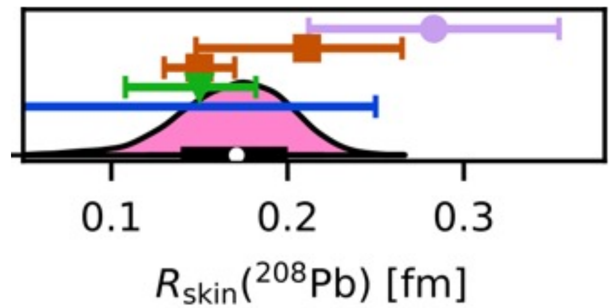
Symmetry energy vs. L parameter based on Lattimer, Lim, ApJ (2013)

PREX II, Reed et al. (2σ), PRL (2021)



Ab initio calc of ^{208}Pb neutron skin

Hu, Jiang, Miyagi et al., arXiv:2112.01125



Region H corresponds to ^{208}Pb neutron skin: 0.14-0.20 fm

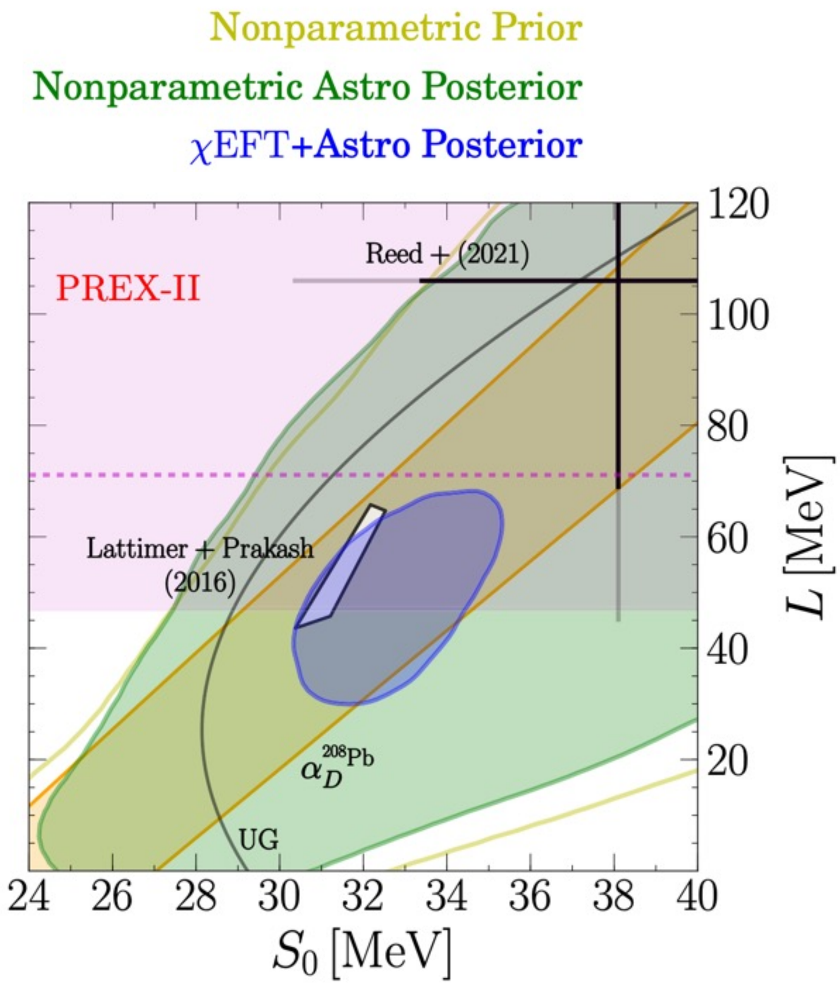
Hebeler, Lattimer, Pethick, AS, PRL (2010)

from Drischler, Holt, Wellenhofer, AS, ARNPS (2021)

Note: not all regions are at same saturation density

Impact of PREX and ^{208}Pb dipole polarizability

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



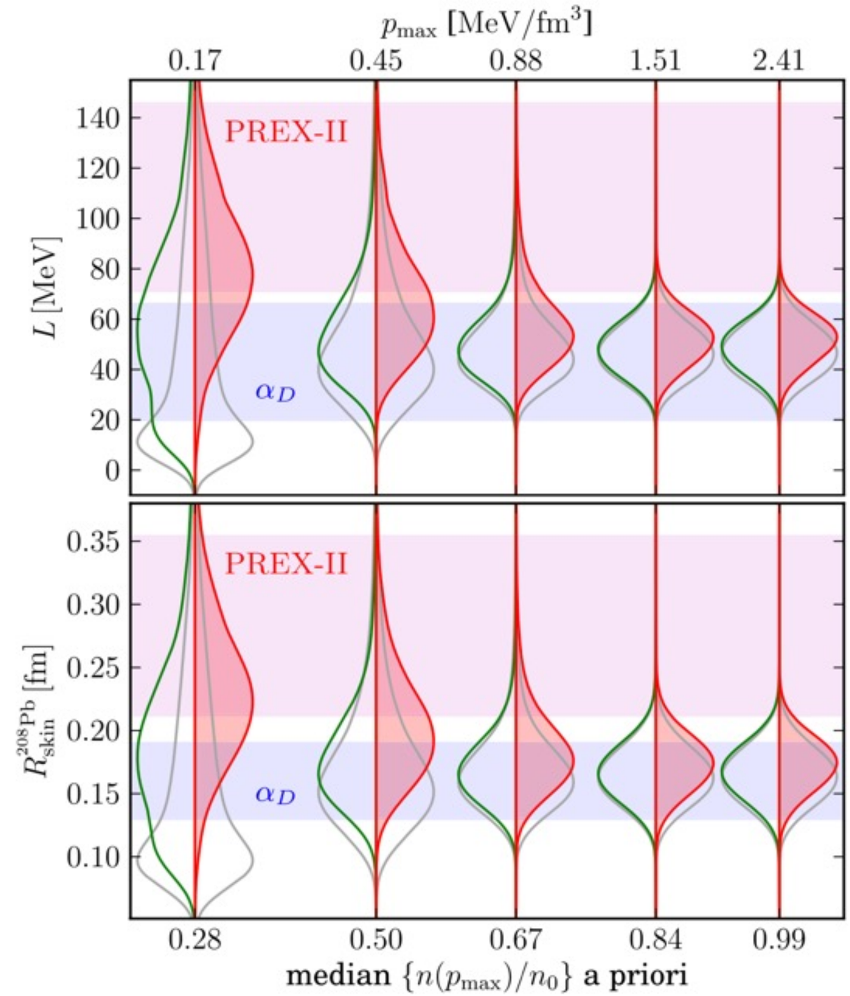


FIG. 2. Prior (gray, unshaded), Astro posterior (green, left-unshaded), and Astro + PREX-II posterior (red, right-shaded)

^{208}Pb dipole polarizability Tamii et al., PRL (2021)

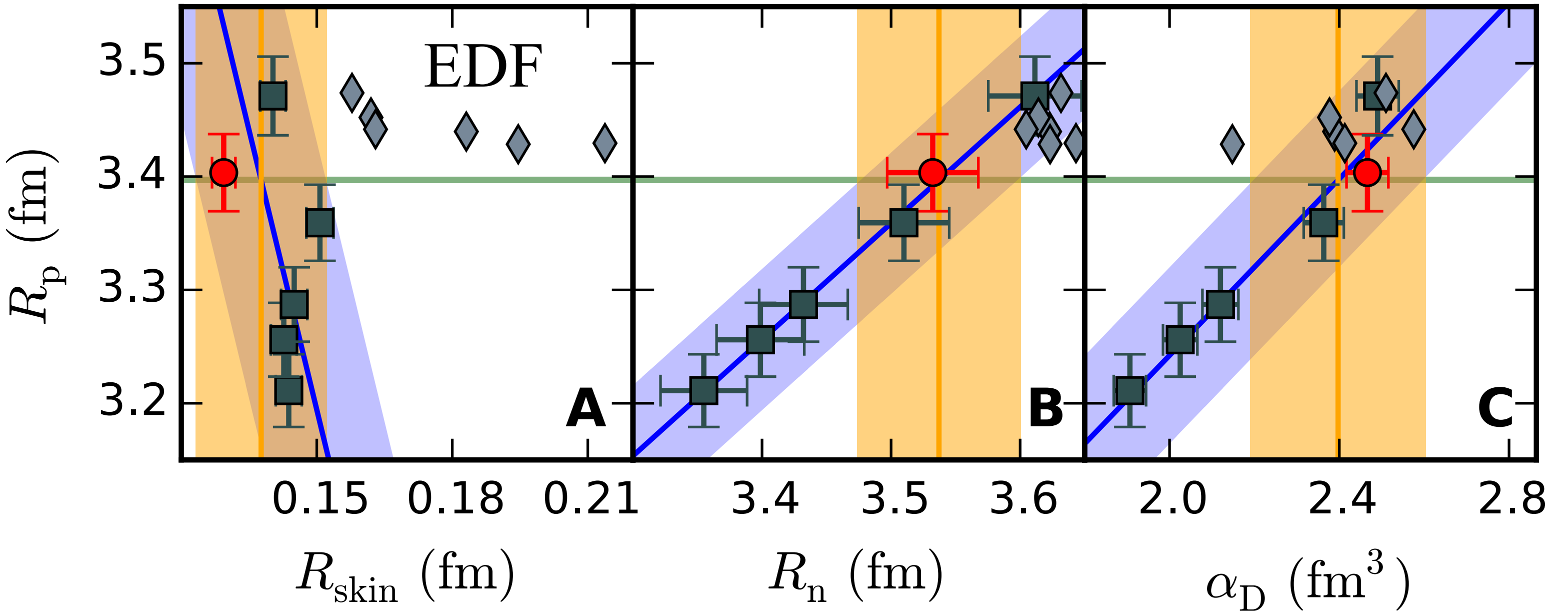
very consistent with χEFT+Astro posterior

Neutron skin and dipole polarizability of ^{48}Ca

Hagen et al., Nature Phys. (2015)

ab initio calculations lead to charge distributions consistent with exp,

predict **small neutron skin** **dipole polarizability α_D**



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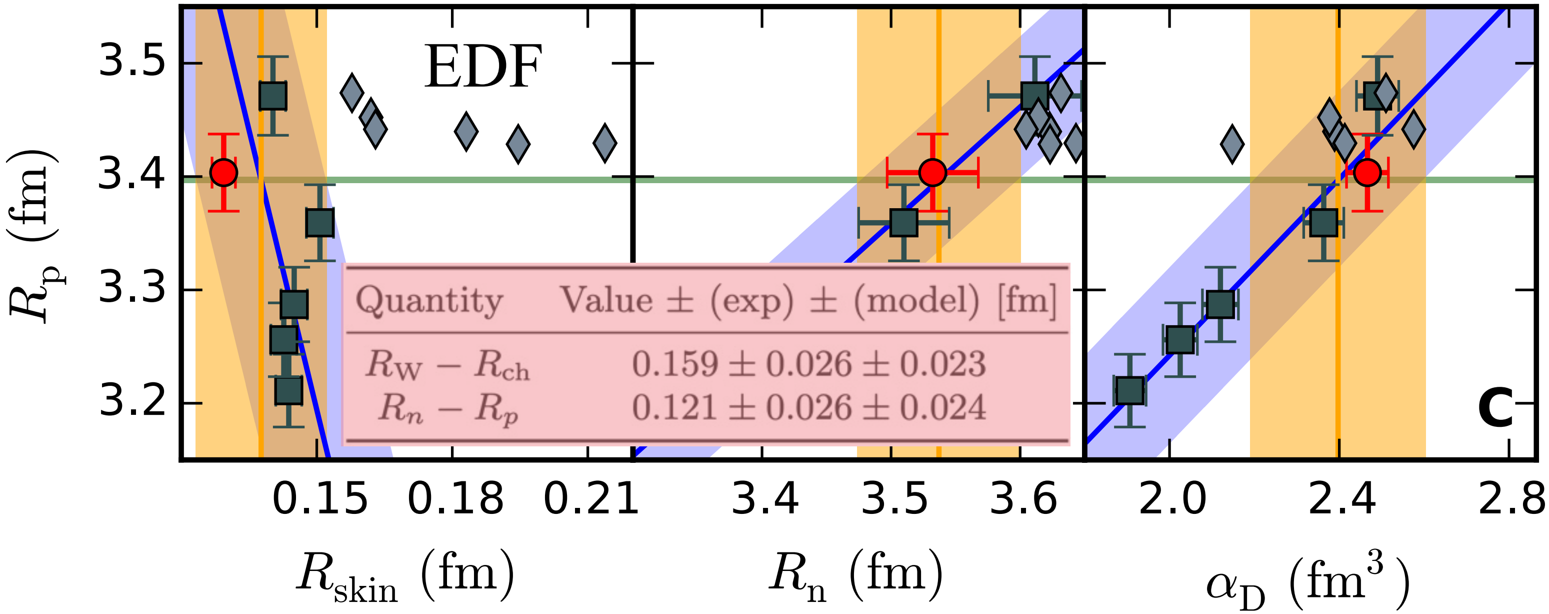
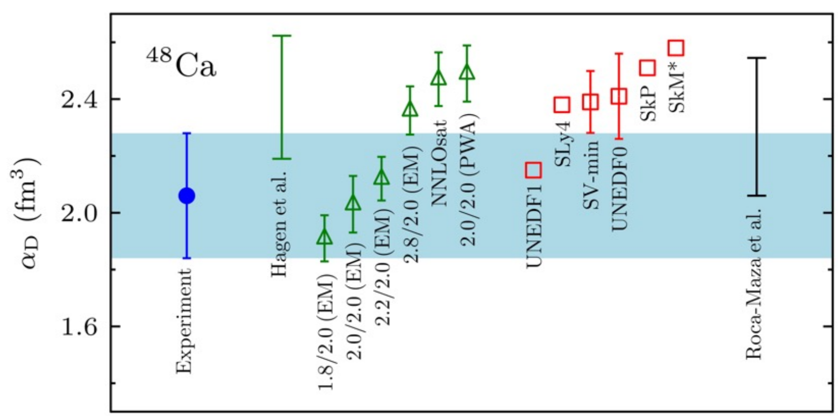


agrees with dipole polarizability from Darmstadt-Osaka exp Birkhan et al., PRL (2017)

+ with CREX result Adhikari et al., PRL (2022)



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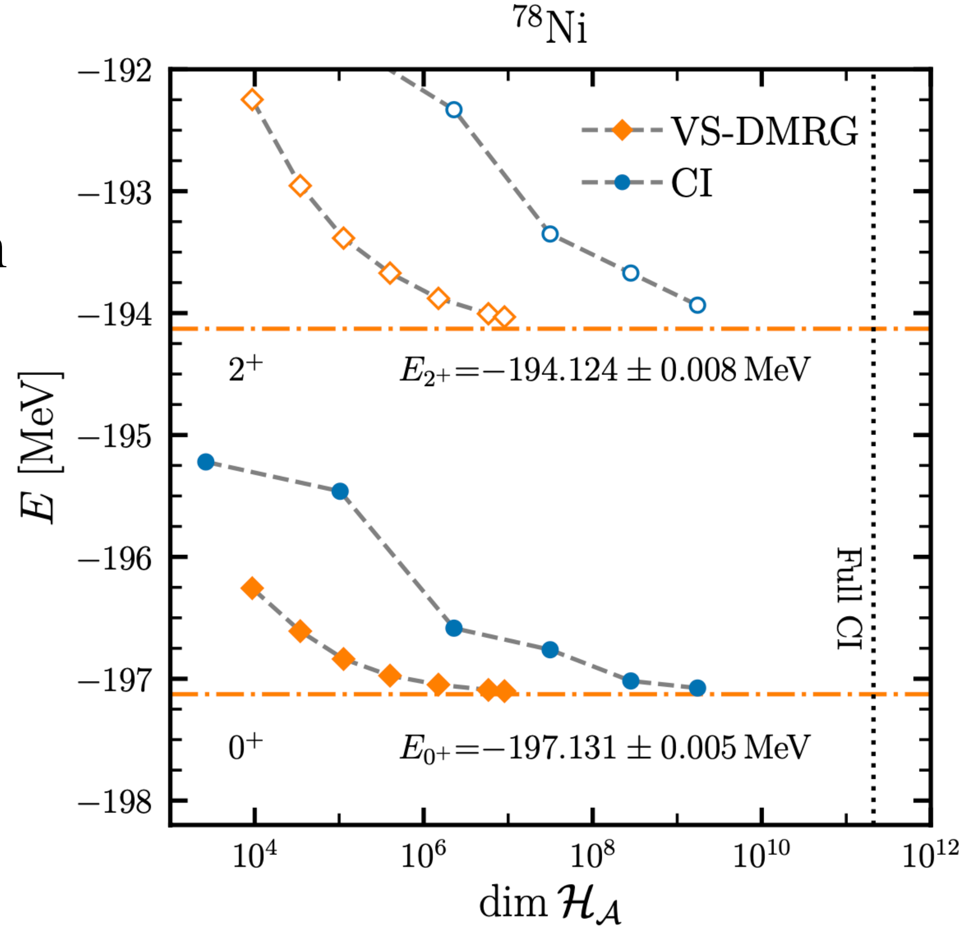
Tichai et al., arXiv:2207.01438

valence-space diagonalization for medium-heavy nuclei challenging due to rapidly increasing dimension

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

VS-DMRG efficiently samples correlations, good convergence with bond dimension, in ~100 smaller dimensions



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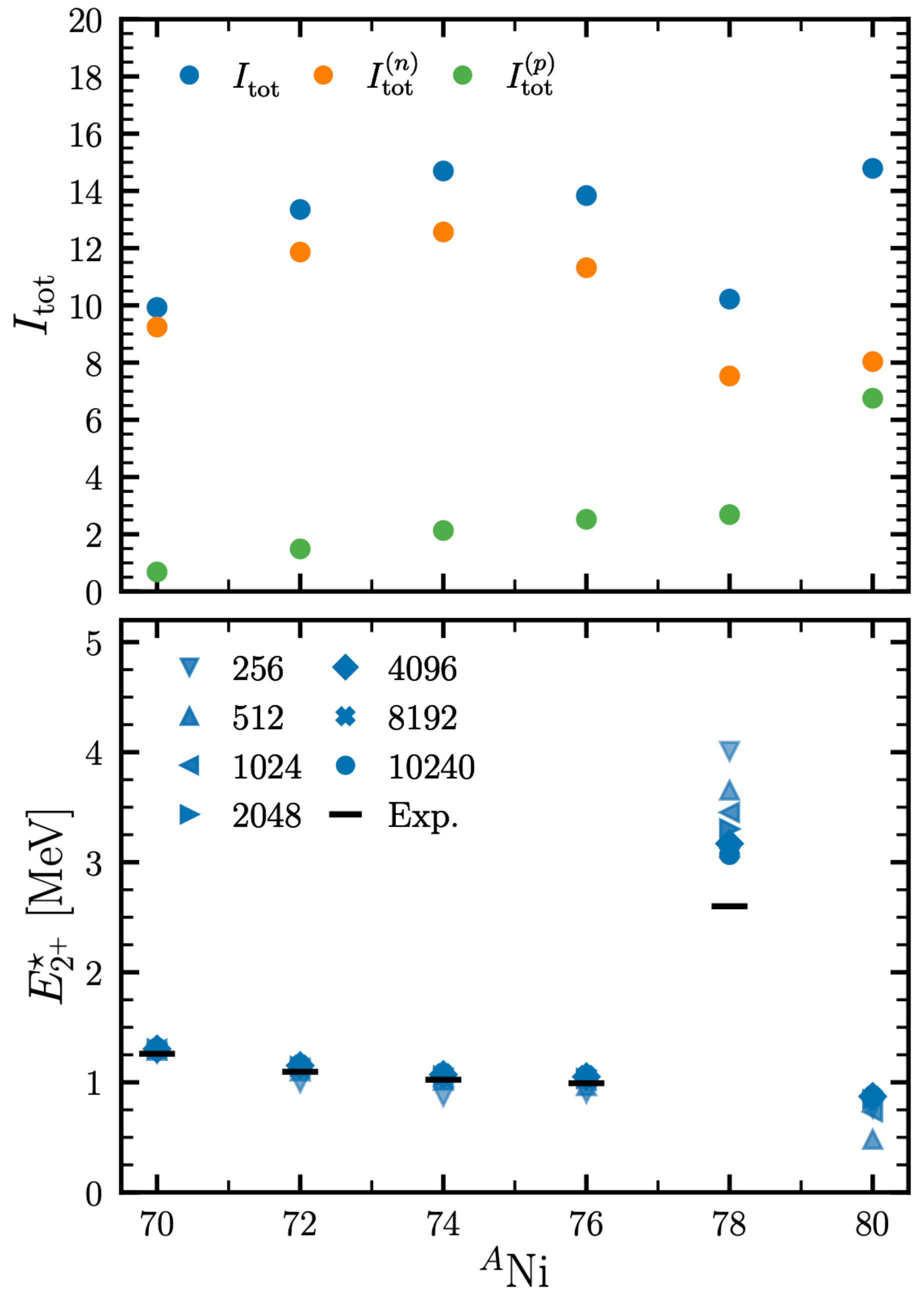
information entropy as measure of shell structure



Summary

Thanks to: Pierre Arthuis, Scott Bogner, Gaute Hagen, Kai Hebeler, **Matthias Heinz**, Jason Holt, **Jan Hoppe**, Ors Legeza, **Takayuki Miyagi**, Thomas Papenbrock, Johannes Simonis, Ragnar Stroberg, **Alexander Tichai**, Gergely Zarand

Ab initio calculations based on chiral EFT interactions, agree with many experiments for nuclei

In-medium similarity renormalization group powerful for all nuclei

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New development for open-shell nuclei: VS-DMRG