

AB INITIO METHODS FOR FINITE NUCLEI: AN OVERVIEW

Pierre Arthuis



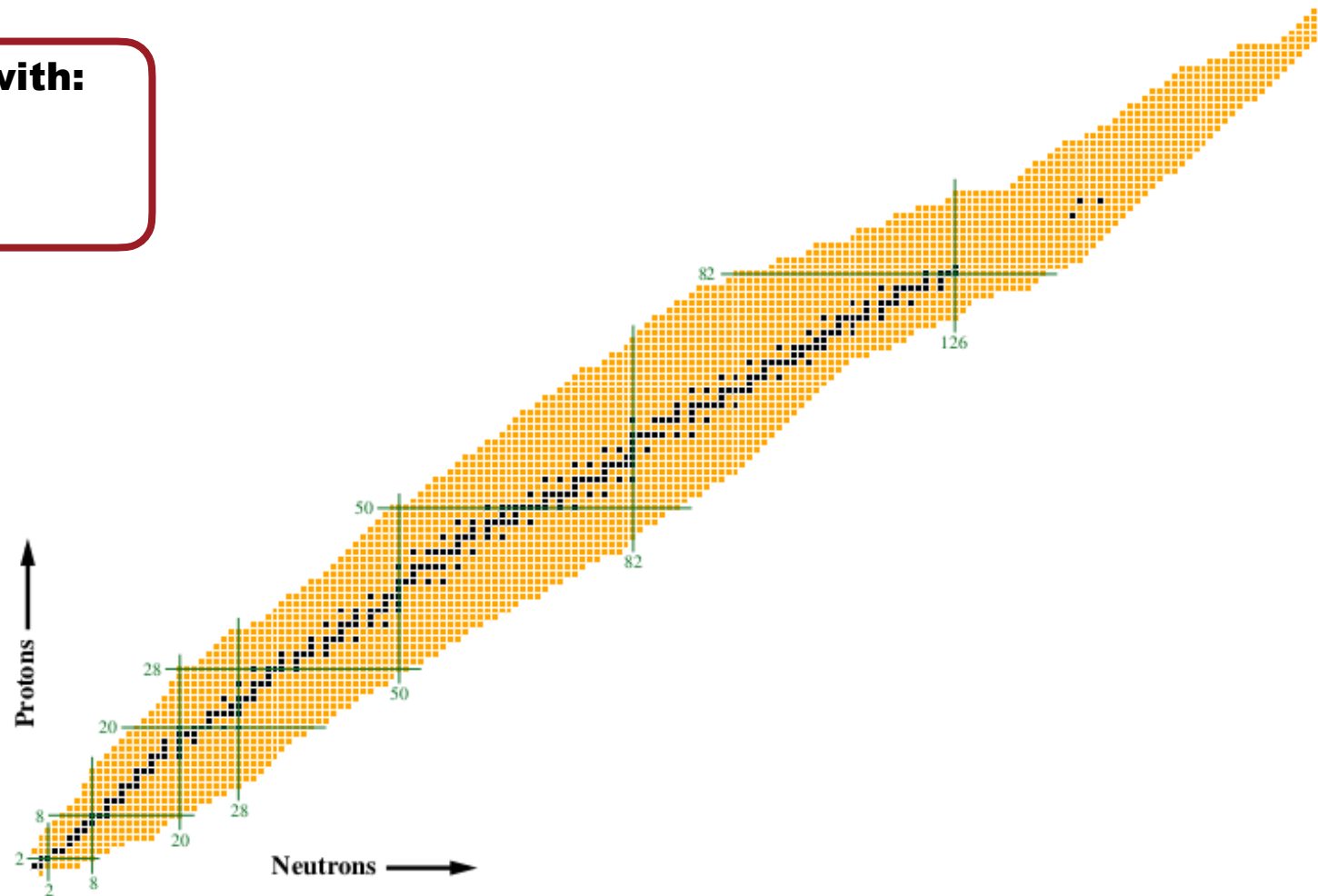
**Funded by
the European Union**



A-body system with:

Z protons

N neutrons





Low-energy ab initio nuclear theory

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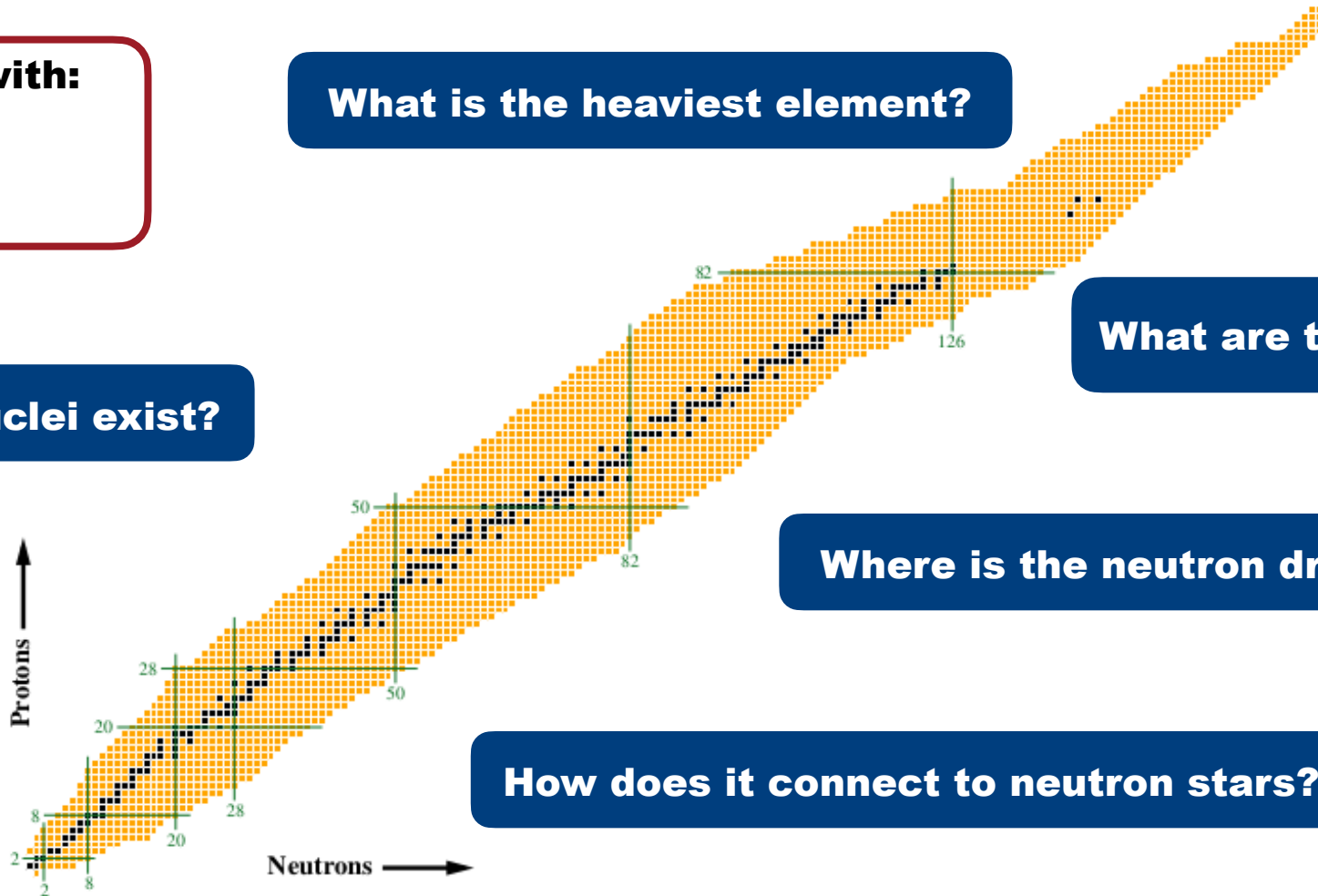
What is the heaviest element?

How many nuclei exist?

What are the magic numbers?

Where is the neutron dripline?

How does it connect to neutron stars?





Some nuclear physics peculiarities

Diversity of phenomena

- Ground-state properties (mass, radius...)
- Excited states properties (vibrational, rotational bands...)
- Decay modes (strong, electroweak...)
- Reaction properties (scattering, fusion...)

A complex interaction

- Emerging from QCD
- Non-perturbative character
- Three-, four-, ..., body forces to be included

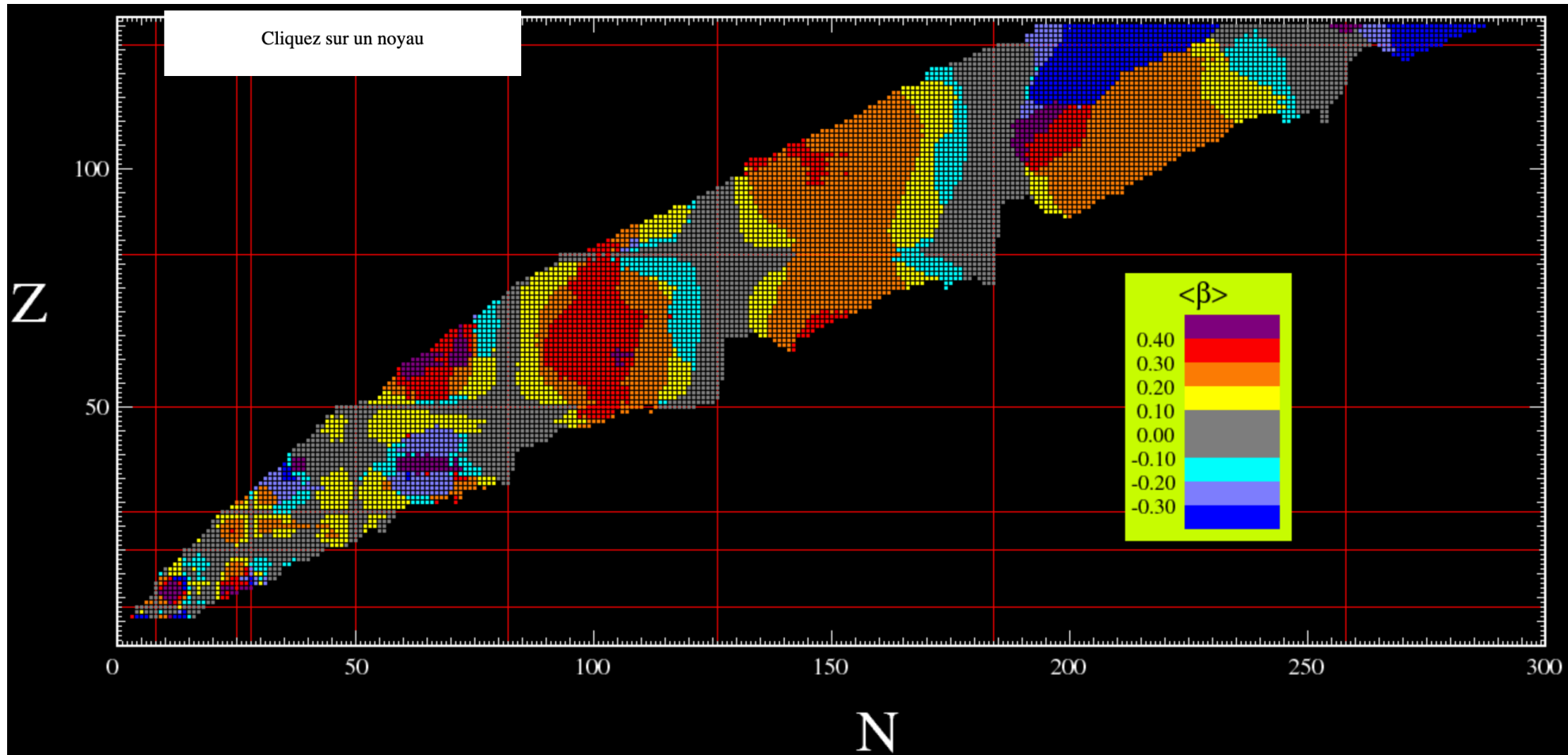
Complex many-body problem

- Mesoscopic system
- Importance of finite-size effects
- Various excitations modes at similar energies



A highly-correlated system: the example of deformation

See Jacek's talk!



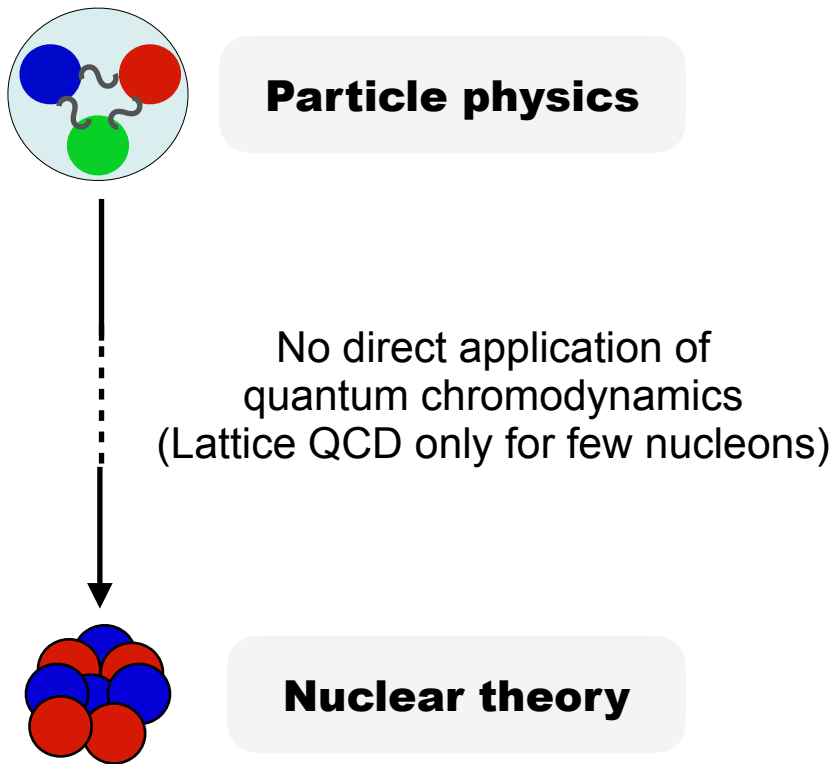
Deformation computed from Gogny density functionals: <https://tinyurl.com/GognyNuclearChart>

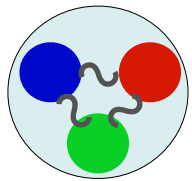


ON AB INITIO METHODS



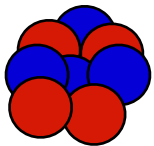
Ab initio many-body scheme





Particle physics

No direct application of
quantum chromodynamics
(Lattice QCD only for few nucleons)



Nuclear theory

Interactions anchored in / inspired from Effective Field Theory

A-body Schrödinger equation

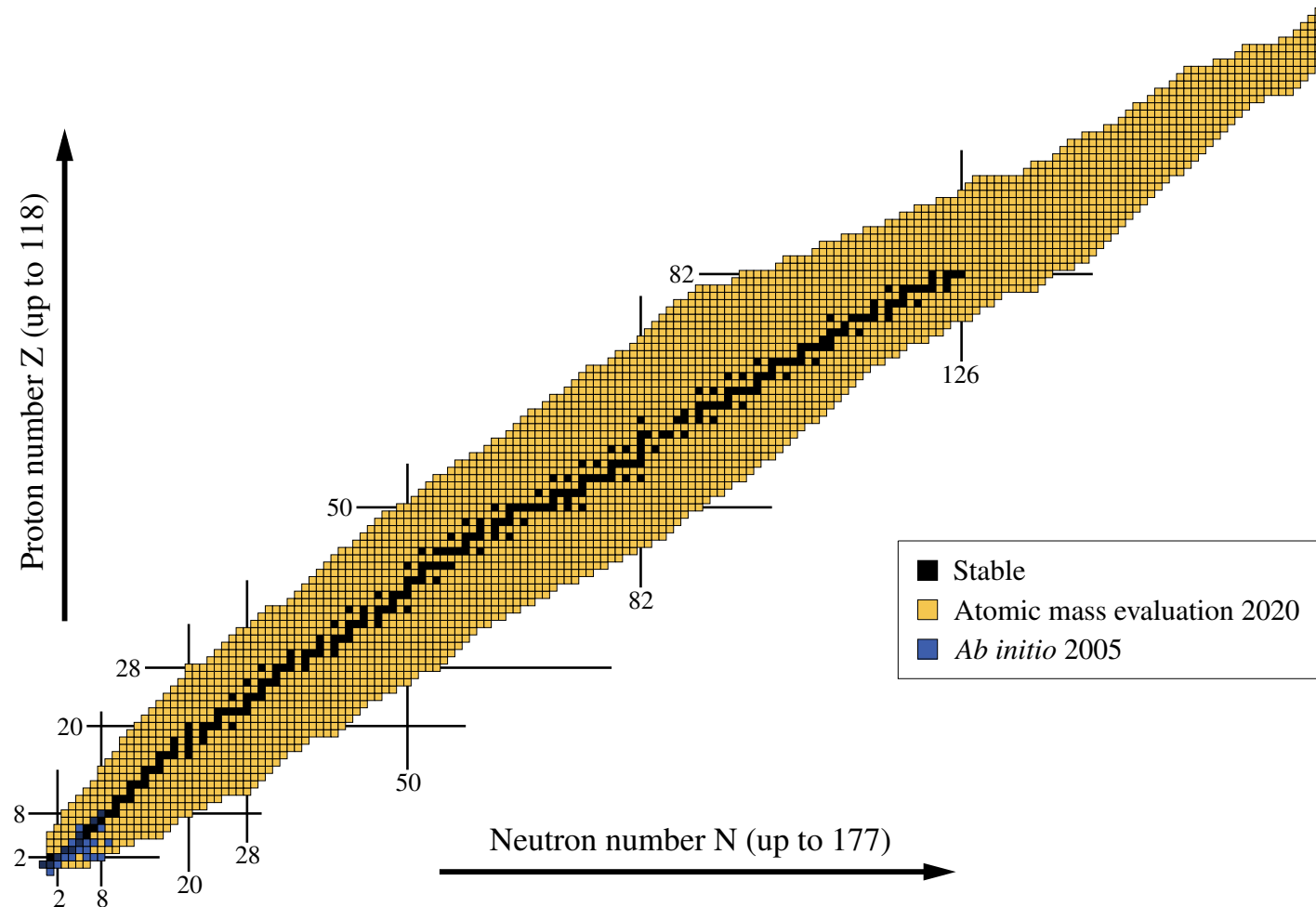
$$H|\Psi^A\rangle = E^A|\Psi^A\rangle$$

Obtain a description that is:

- Consistent
- Systematic
- Accurate enough
- From inter-nucleon interactions
- Rooted in quantum chromodynamics



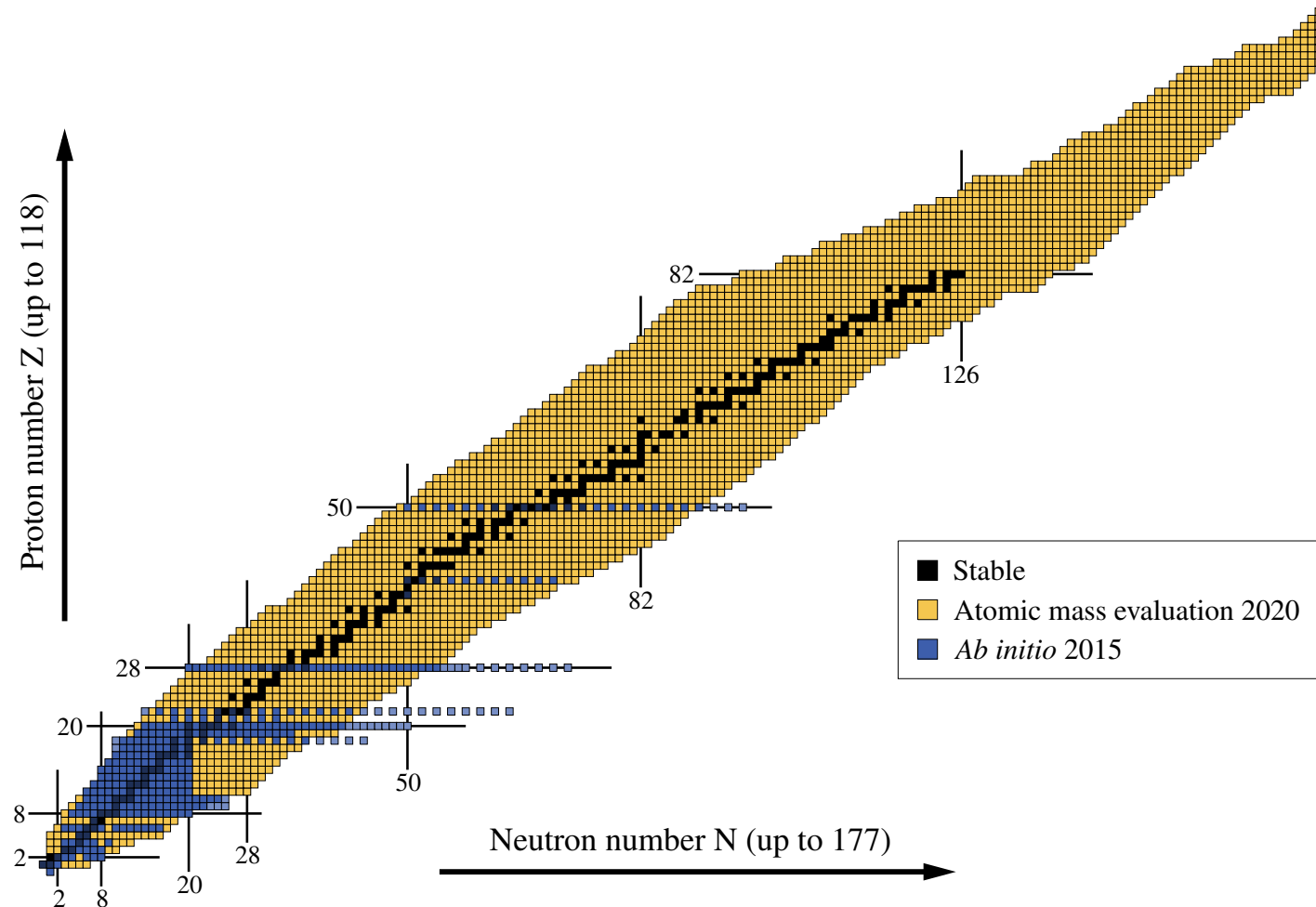
Ab initio many-body methods range



Adapted from B. Bally



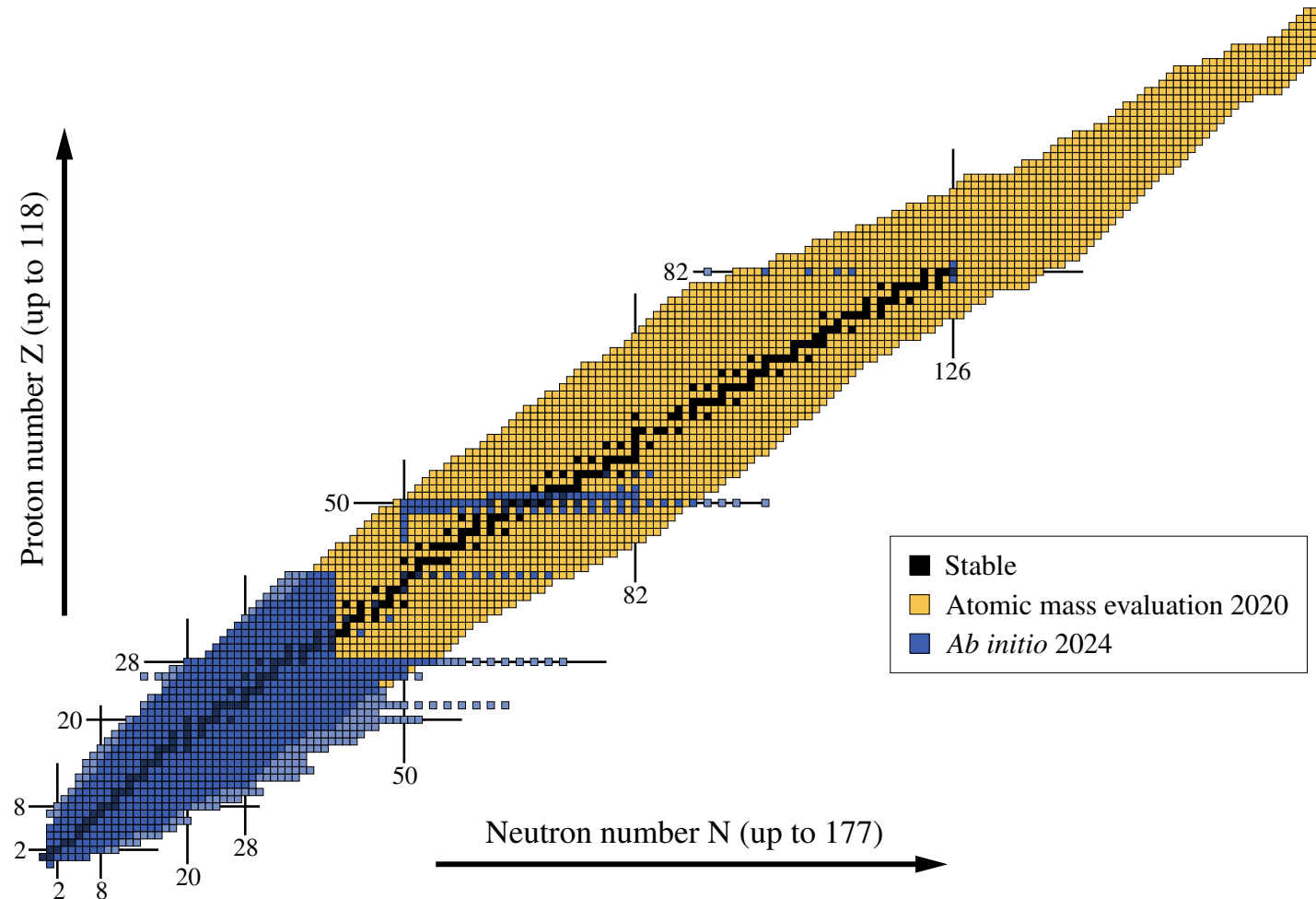
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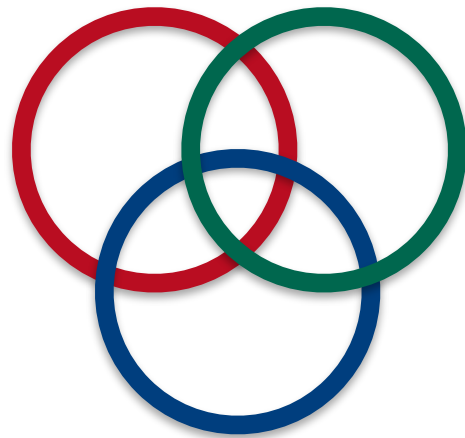
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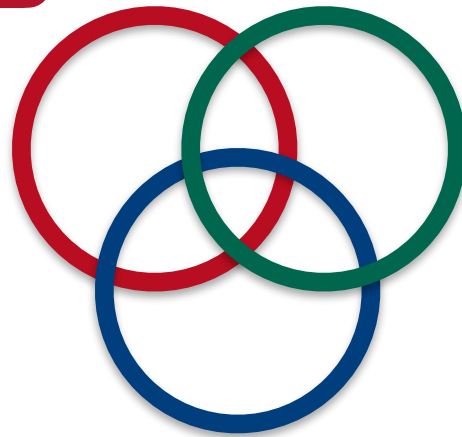
Determine an observable O for a system S with precision η





Determine an observable O for a system S with precision η

Nuclear interaction

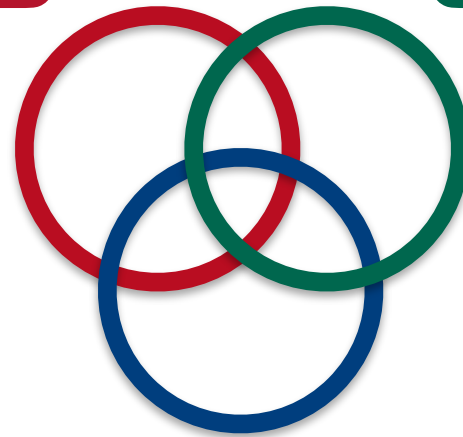




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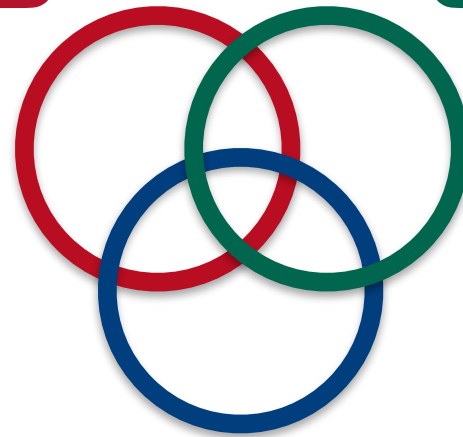


Nuclear physics challenge(s)

Determine an observable O for a system S with precision η

Nuclear interaction

Many-body method

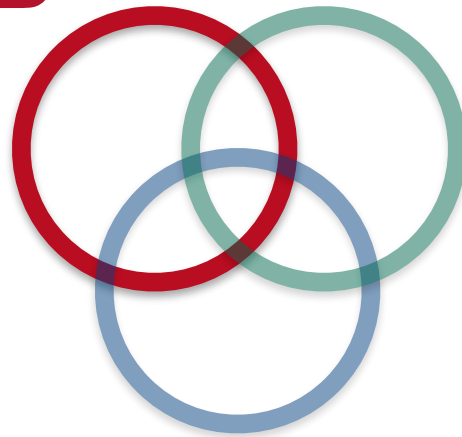


Numerical method



Determine an observable O for a system S with precision η

Nuclear interaction





A quick look at chiral interactions

Rationale

- Nucleons and pions as degrees of freedom
- Link to QCD through Hamiltonian symmetries
- Natural hierarchy of terms
- Systematically improvable

$$M_{\text{low}} \sim m_{\pi} \quad M_{\text{high}} \sim \Lambda_{\chi} \quad \Lambda = \{\Lambda_{\text{NN}}, \Lambda_{\text{3N}}, \dots\}$$

	Two-nucleon force	Three-nucleon force	Four-nucleon force
LO (Q^0)			
NLO (Q^2)			
N ² LO (Q^3)			
N ³ LO (Q^4)			
N ⁴ LO (Q^5)			

[Epelbaum, *PoS CD15* (2016)]

See Bira's and Vincenzo's talks!



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In practice

- NN terms up to N⁴LO (though mostly N³/N²)
- 3N terms up to N³LO (though mostly N²LO)

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Footnote: Similar expansion with Δ excitation

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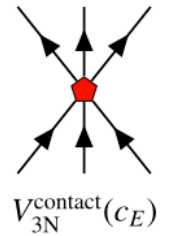
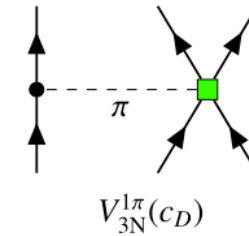
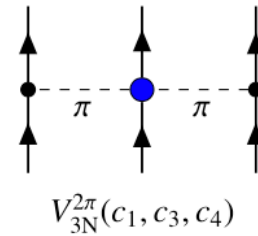
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The leading three-body force

N2LO contributions

- Two-pion exchange: LECs set in the NN sector
- Two new LECs: one-pion exchange and contact term
- c_D, c_E only new parameters in 3N sector



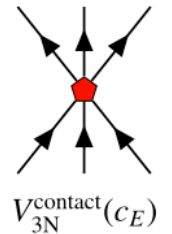
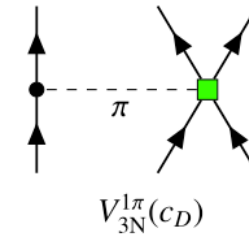
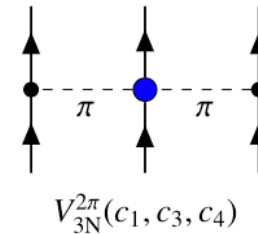
[Hebeler, *Phys. Rept.* 890 (2021)]



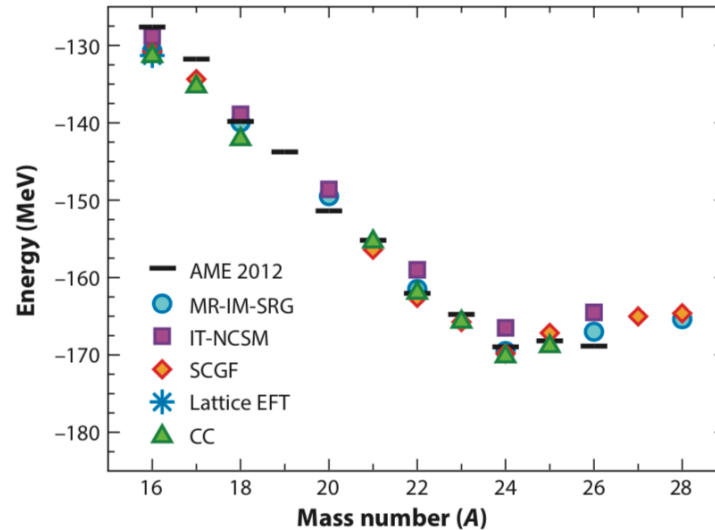
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[Hebeler *et al.*, *Annu. Rev. Nucl. Part. Sci.* 65 (2015)]

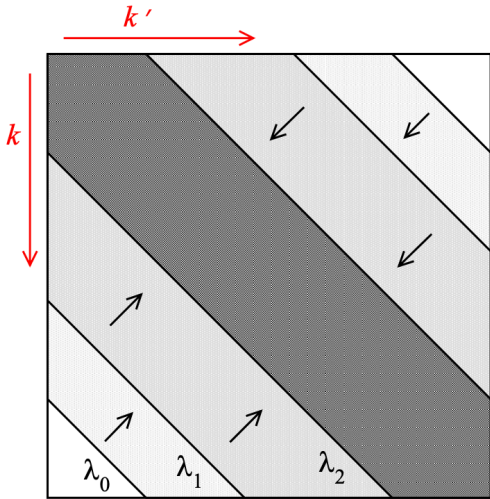
Practical aspects

- Most often fitted in the 3N sector
- Bring repulsion necessary for a good qualitative description



Similarity Renormalization Group (SRG)

All figures here : [Furnstahl, Hebeler, *RPP* 76 (2013)]

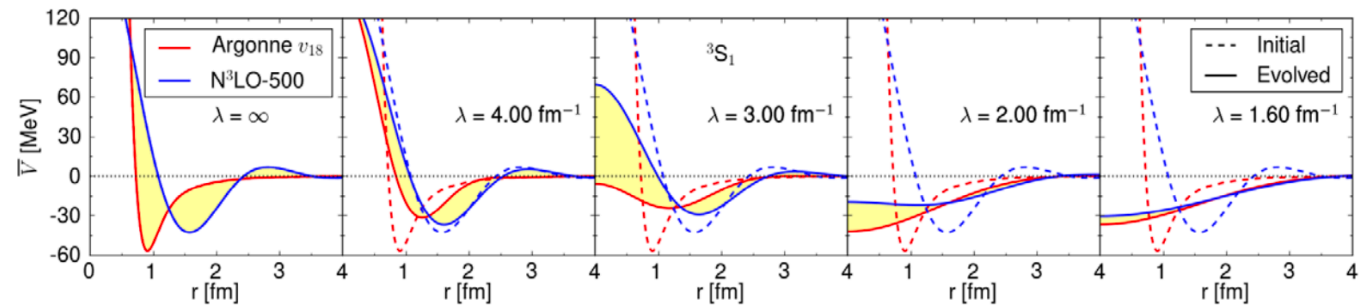
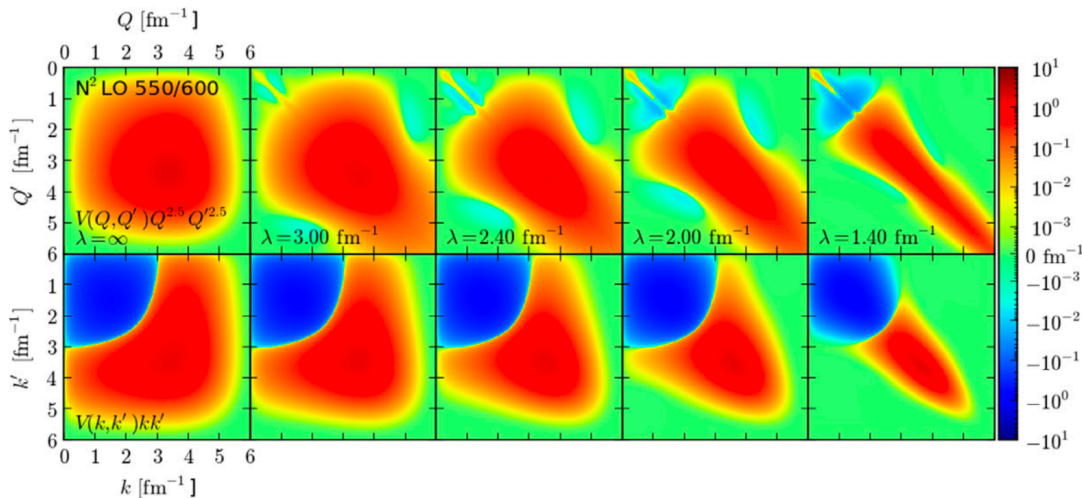
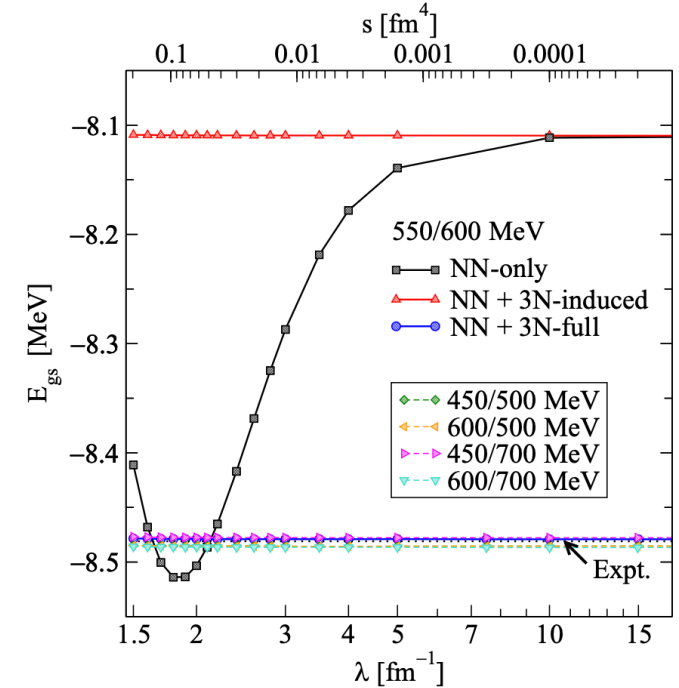


Pre-processing of the Hamiltonian

- Continuous, unitary transformation
- Deals with the hard-core / off-diagonal part of the interaction
- Keeps physics intact but generates higher-rank interaction
- Speeds up convergence w.r.t. model space

Flow equation

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





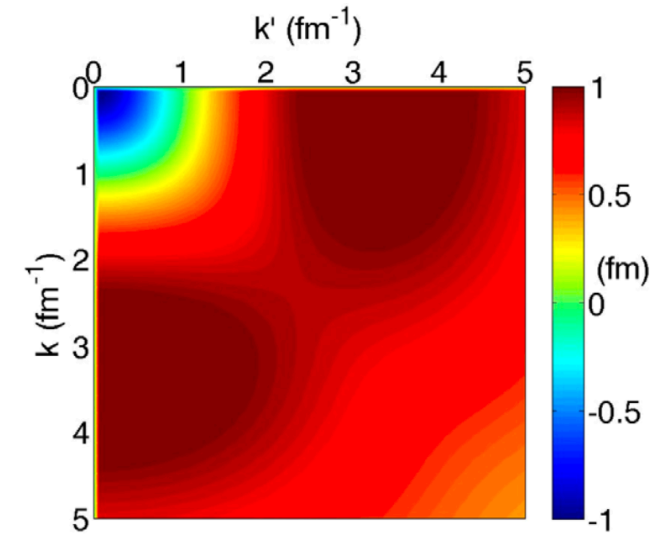
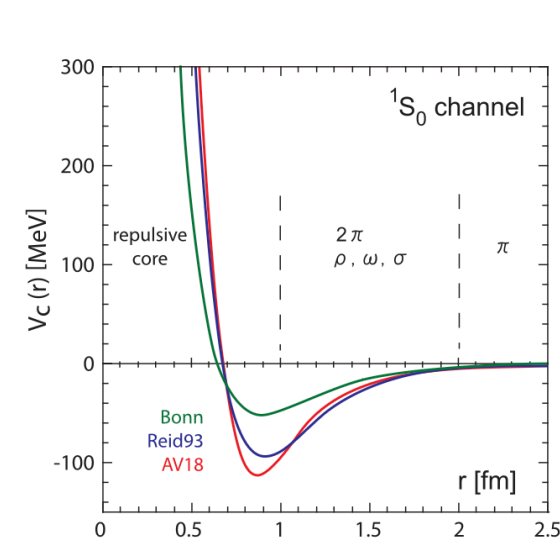
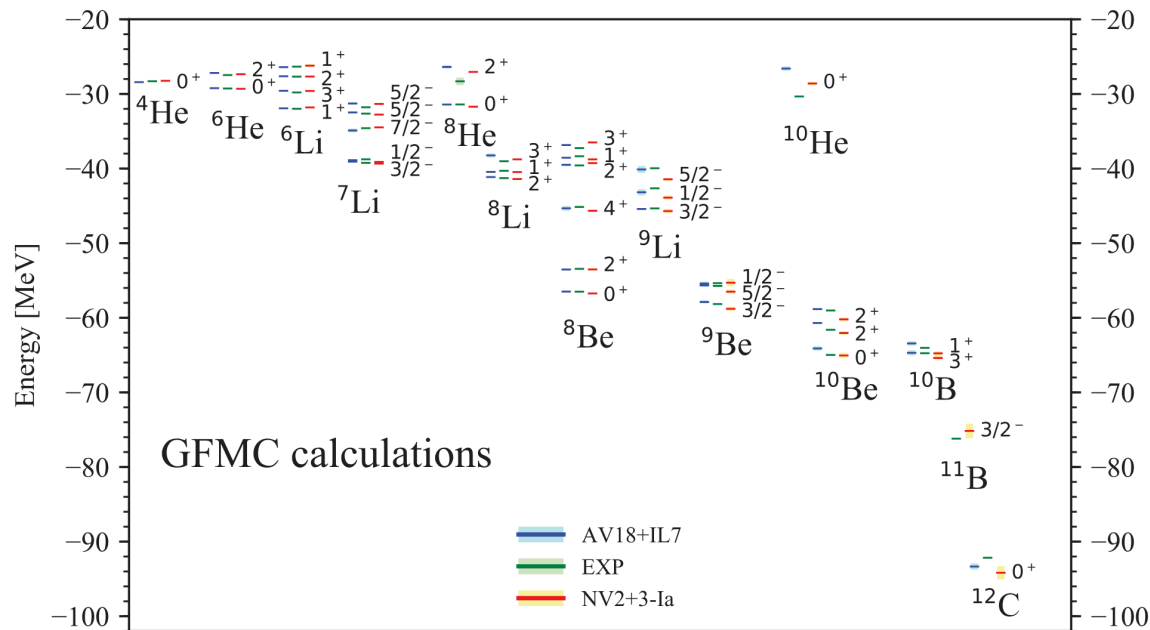
A BRIEF AND BIASED HISTORY OF CHIRAL INTERACTIONS



Before chiral interactions: AV18, CDBonn, ...

Pioneering work

- High-precision reproduction of phaseshifts
- Pion- or meson-exchange terms
- Needed to be supplemented with a 3N force

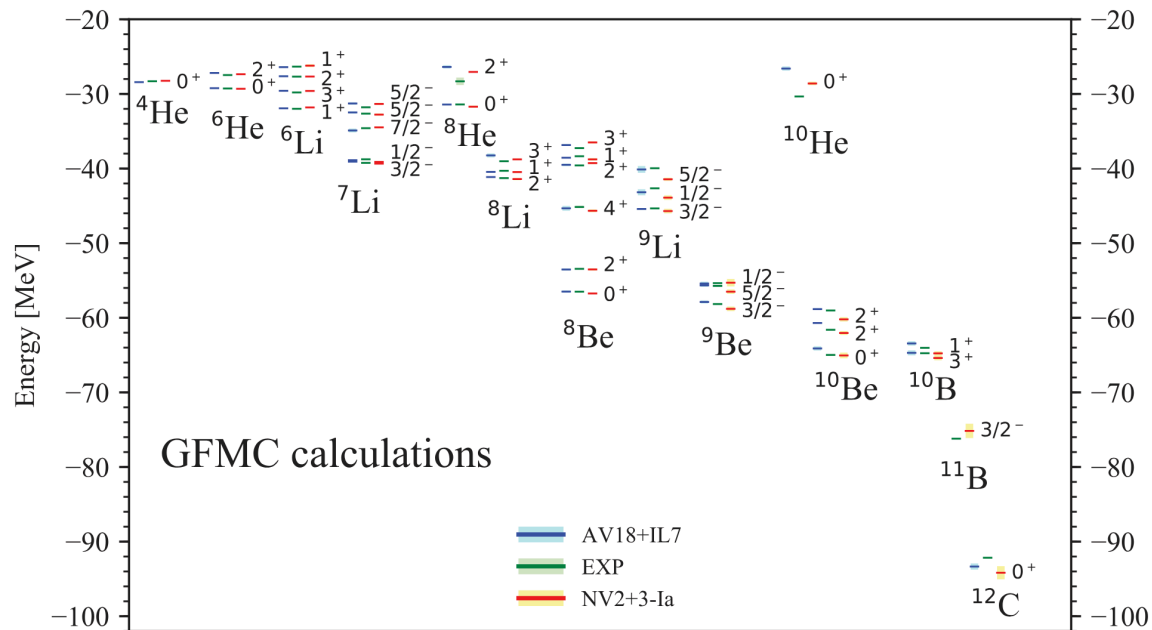




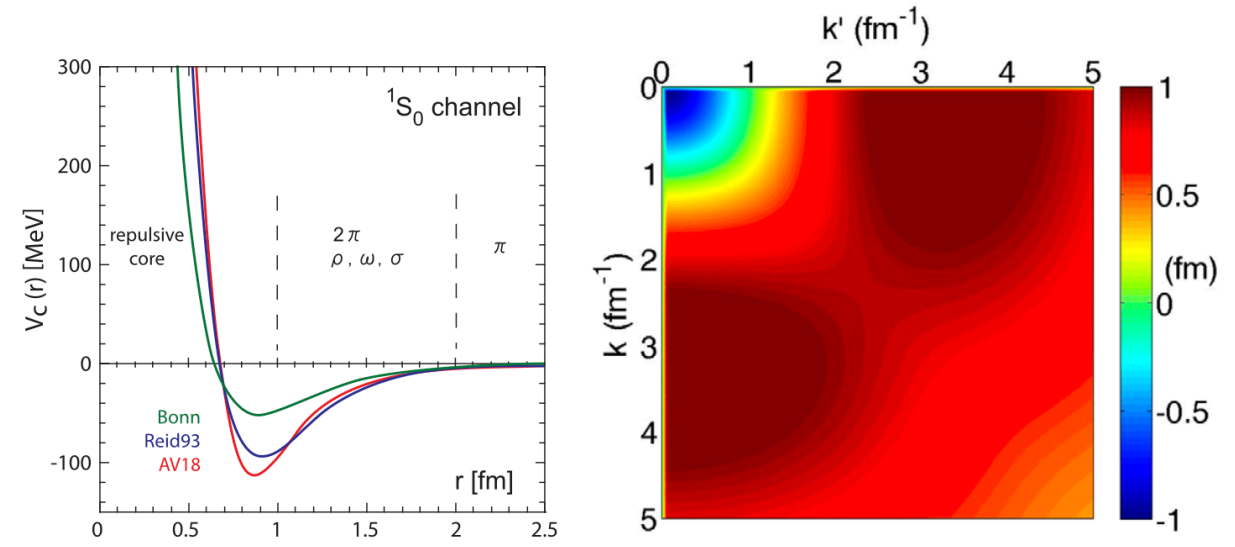
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[Piarulli, *et al.*, *PRL* 120 (2018)]



[Furnstahl, Hebeler, *RPP* 76 (2013)]

Legacy

- Excellent results with QMC
- Too “hard” for many-body perturbation theory
- No obvious way to improve things



Pioneering work

- Reproduce quality of phenomenological potentials
- Fitting by reproducing NN phaseshifts
- Had to be supplemented with a 3N force



Entem-Machleidt 500 (sometimes just 'N3LO')

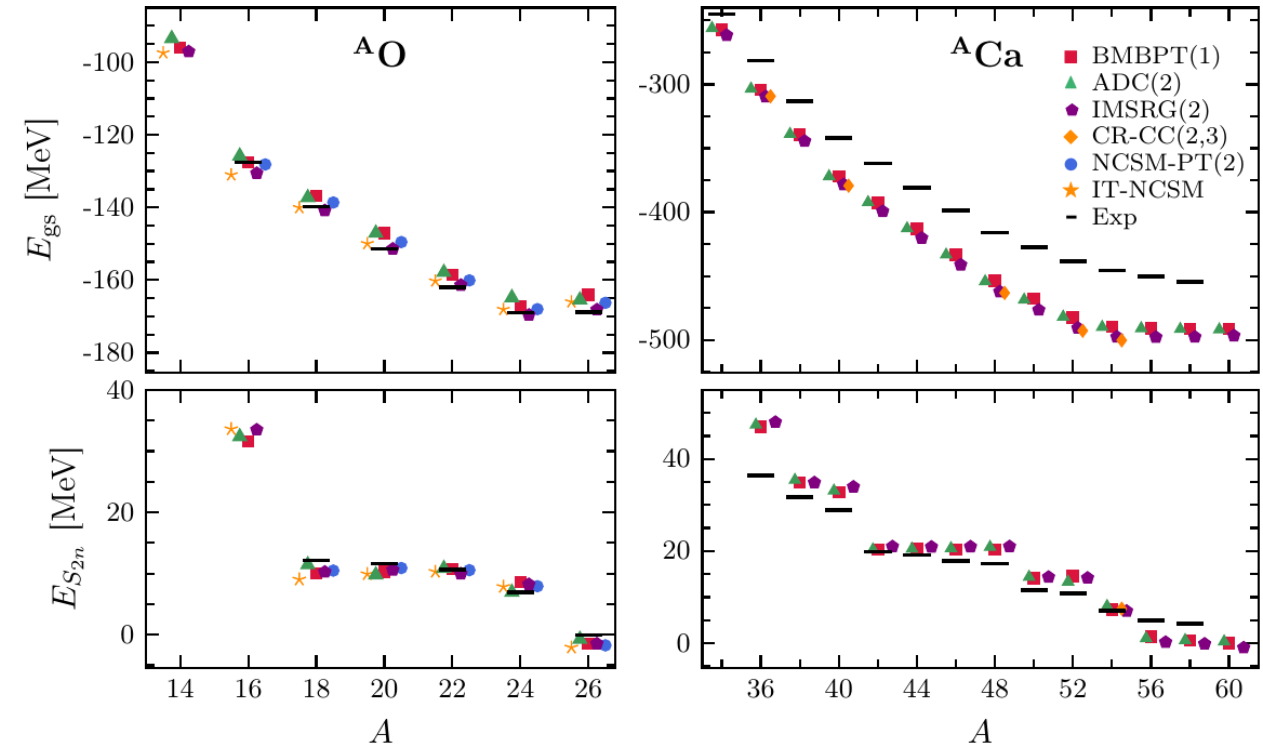
[Entem, Machleidt, *PRC* 68 (2003)]

Pioneering work

- Reproduce quality of phenomenological potentials
- Fitting by reproducing NN phaseshifts
- Had to be supplemented with a 3N force

Legacy

- Still one of the most used NN forces
- NN+3N combinations often fell short
- Hard interaction: require large model spaces



[Tichai, Arthuis *et al.*, *PLB* 786 (2018)]



The λ/Λ family and the 1.8/2.0 (EM)

[Hebeler, Bogner, Furnstahl, Nogga, Schwenk, *PRC* **83** (2011)]

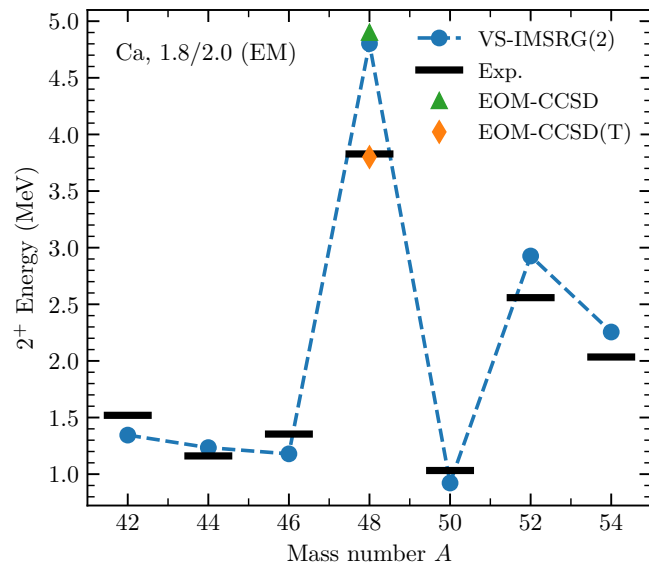
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- Build on the success of the EM500
- SRG-evolve the EM, add bare 3N on top
- Low- Λ re-fit of c_D, c_E for 3NF absorb missing physics



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- Vastly successful with energies
- Underpredicts radii
- Soft interaction, made for very broad use

IMSRG: [Simonis, Stroberg, *et al.*, *PRC* **96** (2017)]

CC: [Hagen, Jansen, Papenbrock, *PRL* **117** (2016)]

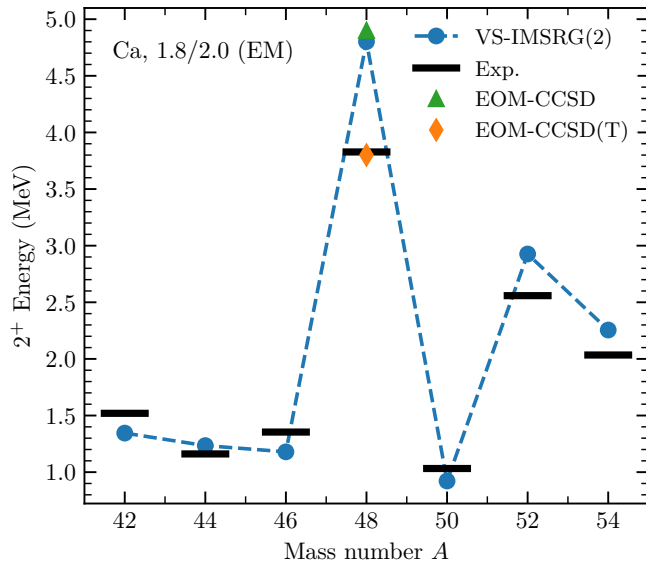


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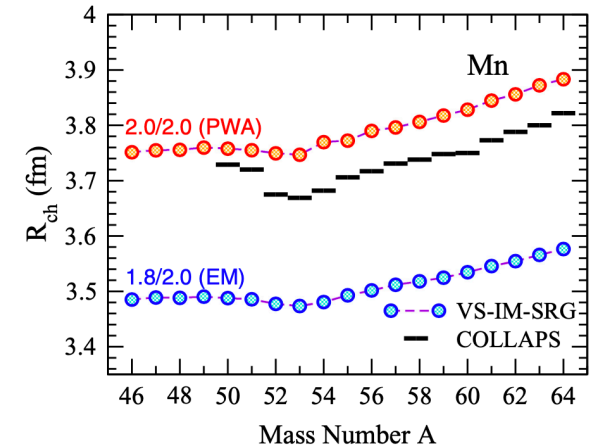
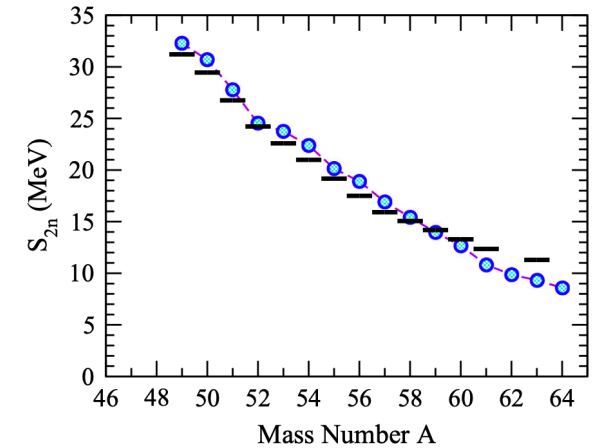
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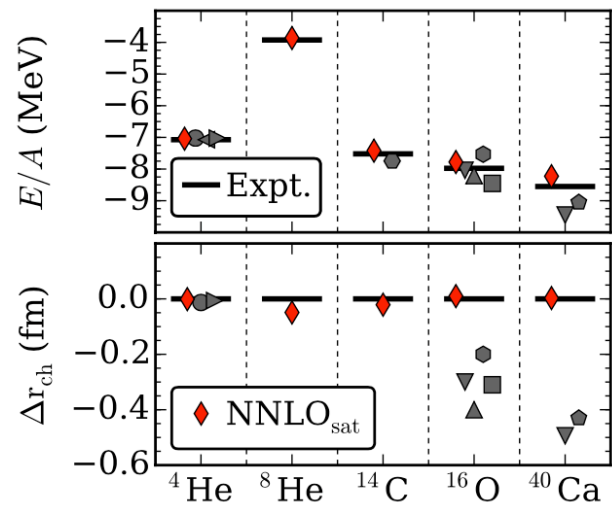
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- Interactions fitted on NN, 3N underpredict radii
- Incorporate *low-energy* many-body data in the fit
- Simultaneous fit of all LECs

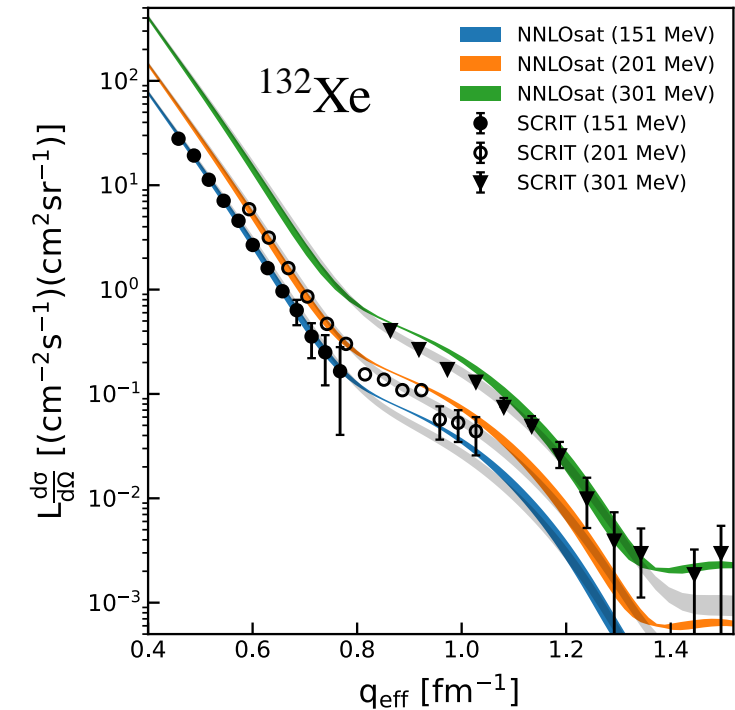


Incorporating many-body data: NNLOsat

[Ekström, Jansen, Wendt, Hagen, Papenbrock, Carlsson, *PRC* **91** (2015)]



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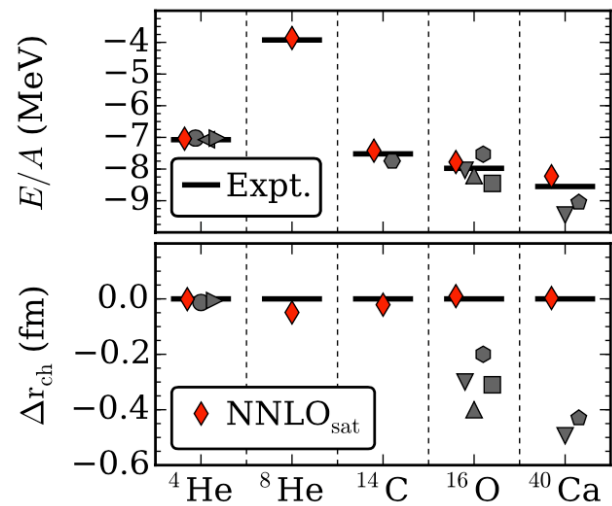
[Ekström, Jansen *et al.*, *PRC* **91** (2015)]

[Arthuis, Barbieri, *et al.*, *PRL* **125** (2020)]



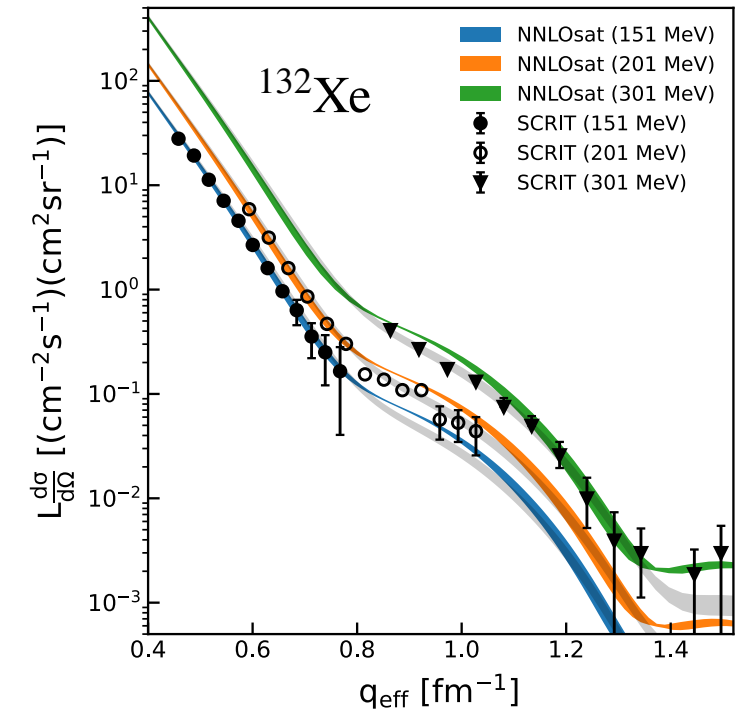
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- Legacy**
- Excellent radii and associated quantities
 - Underbinds in the heavy sector
 - Pioneered the use of many-body data



[Ekström, Jansen *et al.*, *PRC* **91** (2015)]

[Arthuis, Barbieri, *et al.*, *PRL* **125** (2020)]



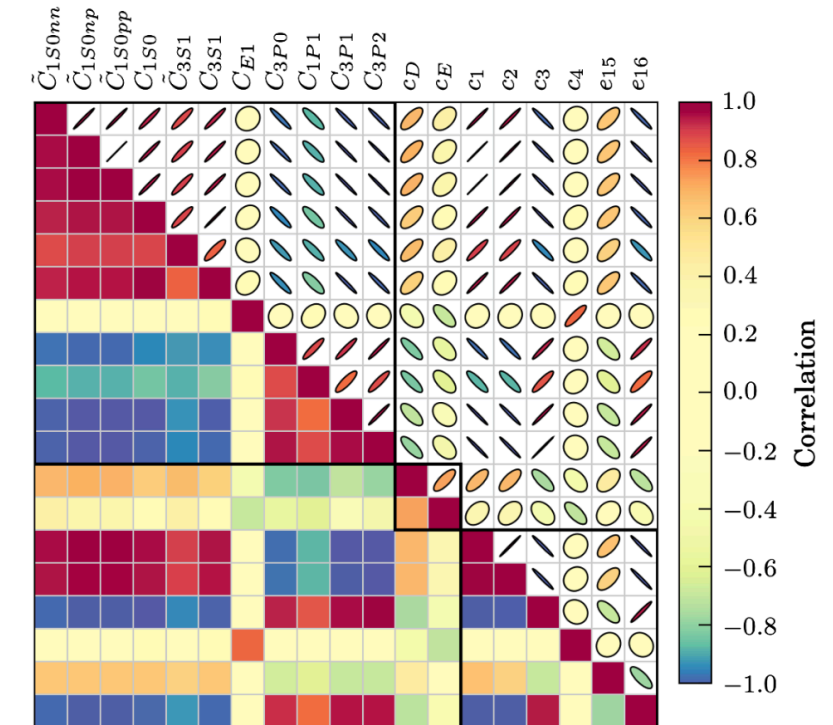
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- Study the importance of NN+3N fitting approach
- Order-by-order fits, various cutoffs
- NN+3N consistently from the very start



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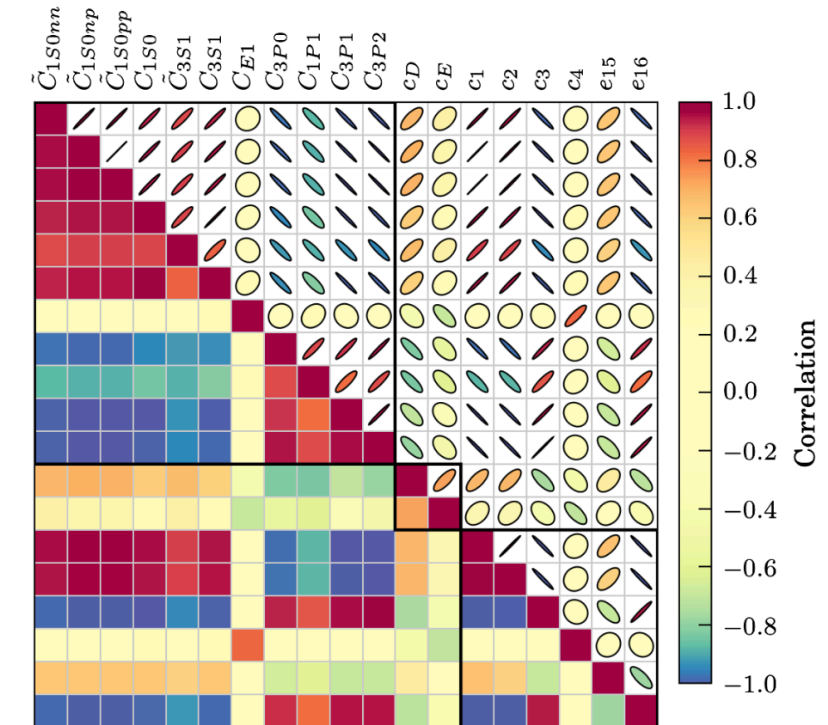


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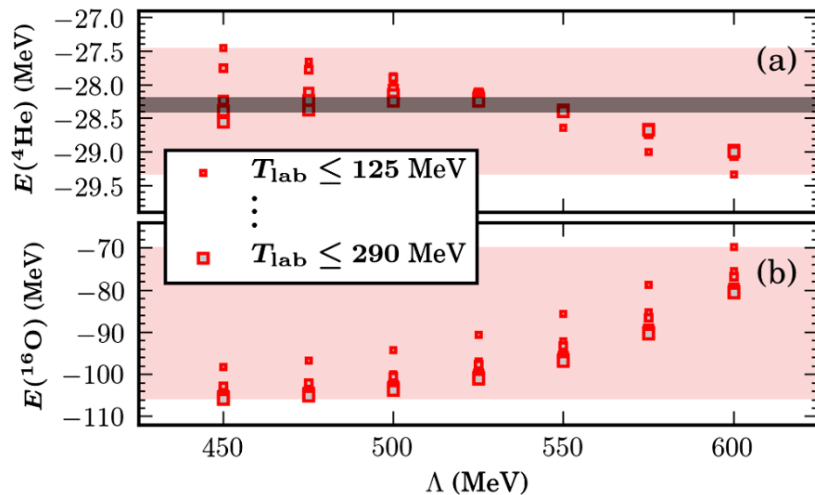
Legacy

- Introduced detailed correlation studies
- Barely ever used in practical applications

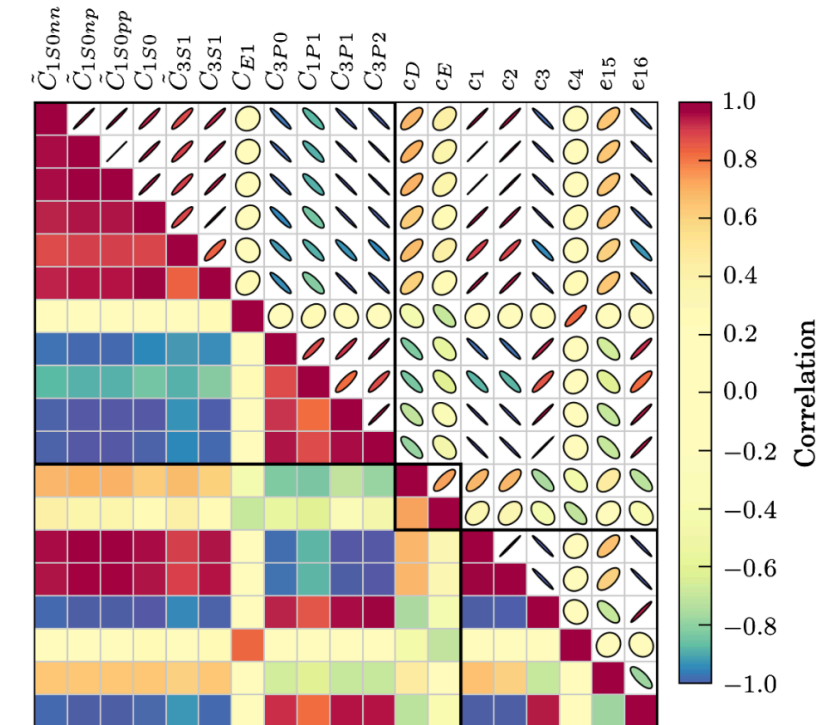


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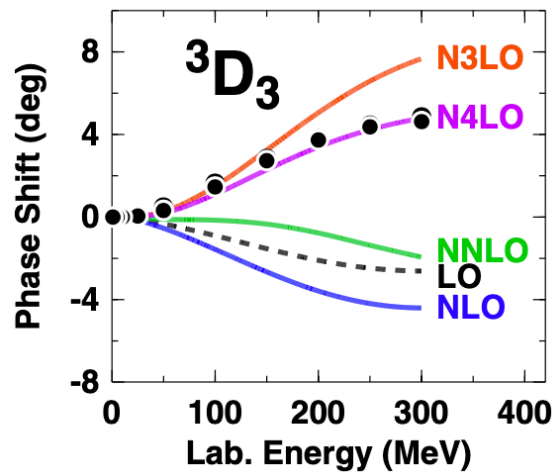
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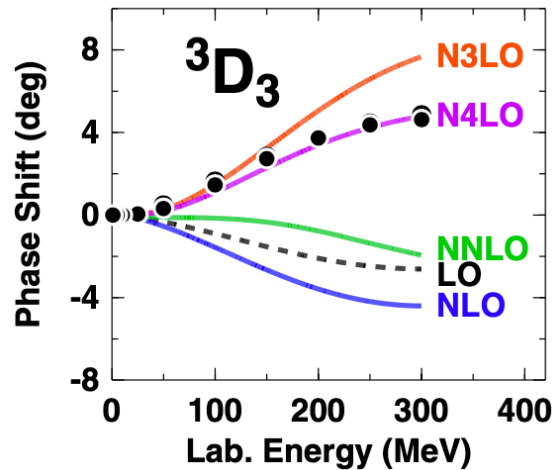


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- Use πN scattering analysis data for c_i 's
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- Still NN-only: needs to be supplemented



[Entem, Machleidt, Nosyk, *PRC* **96** (2017)]



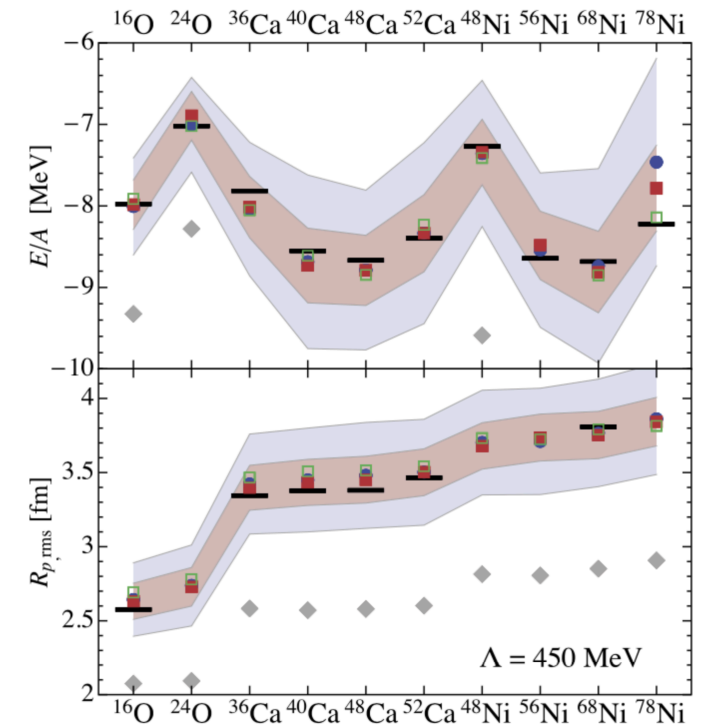
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- Helped systematised chiral order studies
- Extended in multiple ways to the 3N sector

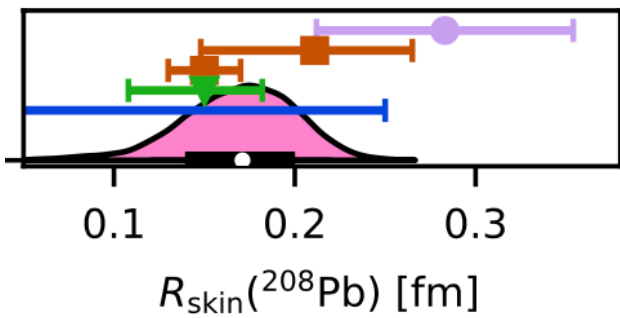


[Hüther, Vobig, *et al.*, *PLB* **808** (2020)]



Explicit Δ : $\Delta\text{NNLO}_{\text{GO}}$ & the non-implausibles

[Jiang, Ekström, Forssén, Hagen, Jansen, Papenbrock, *PRC* **102** (2020), ...]

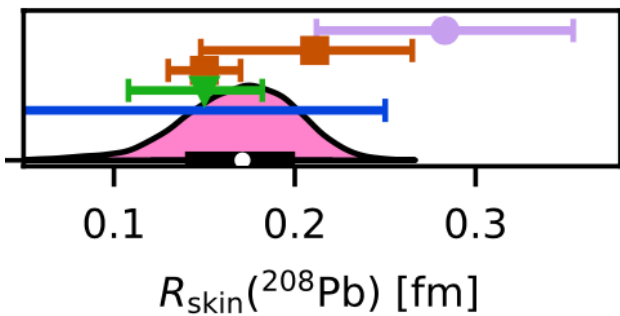


[Hu, Jiang *et al.*, *Nat. Phys.* **18** (2022)]



Explicit Δ : $\Delta\text{NNLO}_{\text{GO}}$ & the non-implausibles

[Jiang, Ekström, Forssén, Hagen, Jansen, Papenbrock, *PRC* **102** (2020), ...]



Rationale

- Δ excitation is relatively low in energy
- Study convergence of deltaful chiral EFT
- Use many-body data from the start
- NLO, NNLO interactions
- More exhaustive strategy: non-implausible int.

[Hu, Jiang *et al.*, *Nat. Phys.* **18** (2022)]

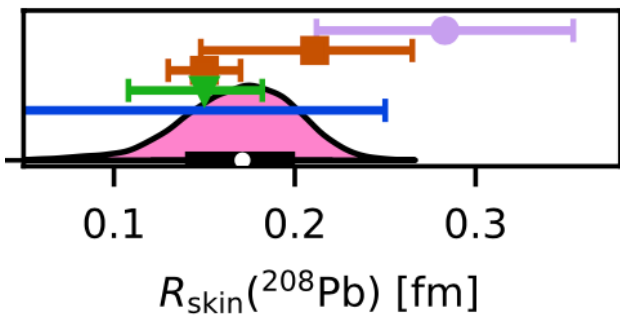


Explicit Δ : $\Delta\text{NNLO}_{\text{GO}}$ & the non-implausibles

[Jiang, Ekström, Forssén, Hagen, Jansen, Papenbrock, *PRC* **102** (2020), ...]

Rationale

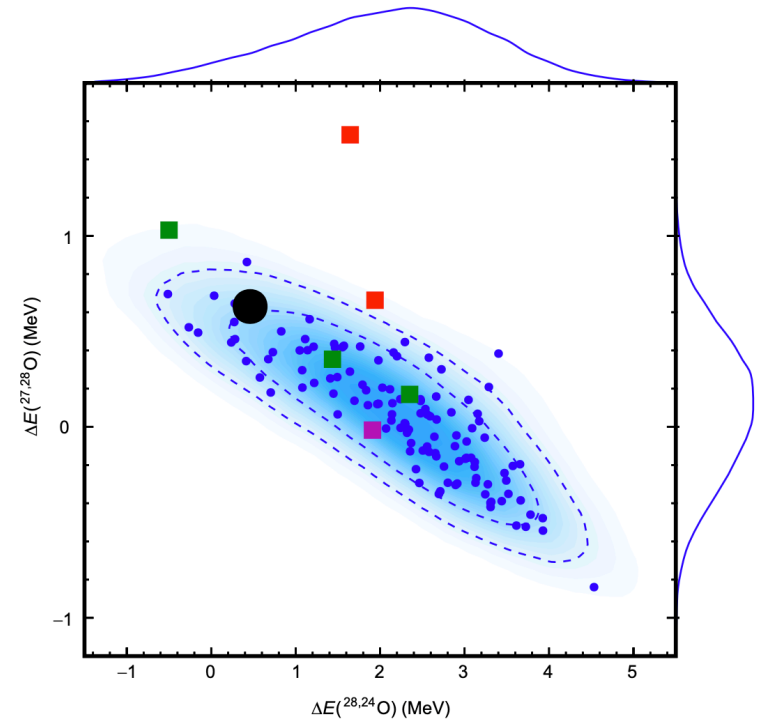
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- Use many-body data from the start
- NLO, NNLO interactions
- More exhaustive strategy: non-implausible int.



[Hu, Jiang *et al.*, *Nat. Phys.* **18** (2022)]

Legacy

- Good simultaneous reproduction of radii & ground-state energy
- Very encouraging order-by-order convergence



[Kondo *et al.* (SAMURAI 21), *Nature* **620** (2023)]



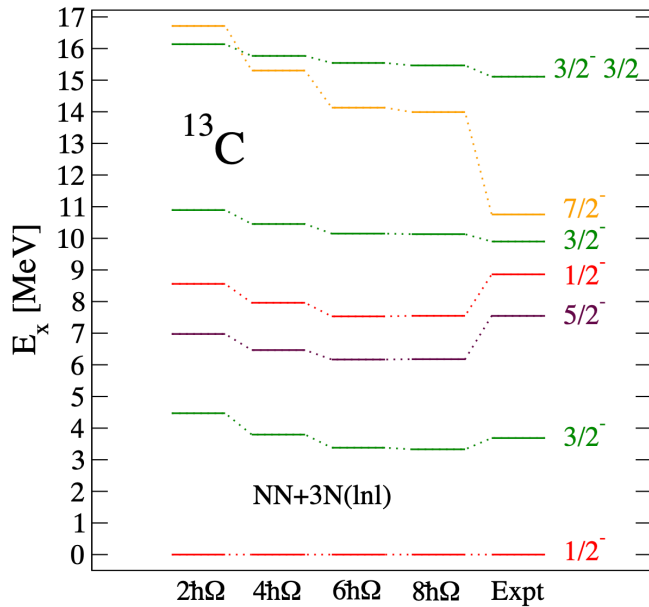
The Local-Non-Local

[Somà, Navrátil, Raimondi, Barbieri, Duguet, *PRC* **101** (2020)]



Rationale

- Combine qualities of local and non-local regulators
- Fit only in the few-body sector



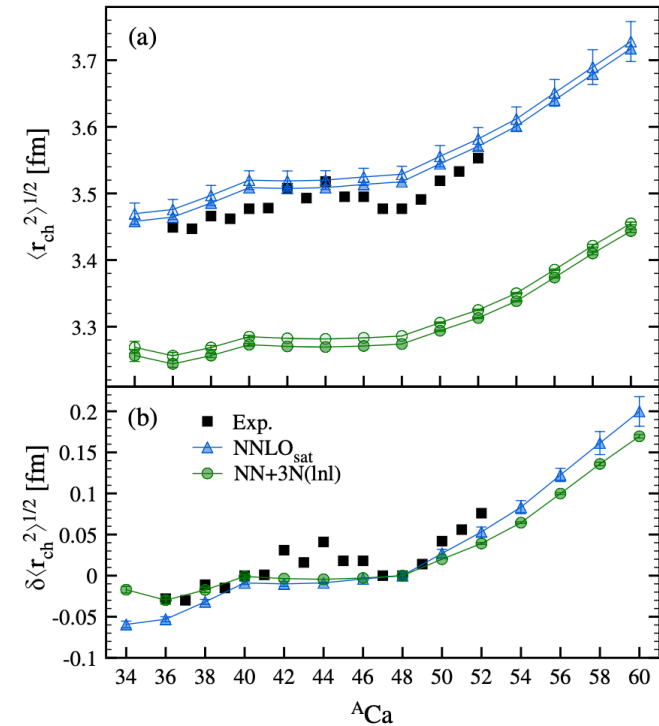
[Somà, Navrátil, *et al.*, *PRC* **101** (2020)]

Rationale

- Combine qualities of local and non-local regulators
- Fit only in the few-body sector

Legacy

- Very succesful for spectroscopy
- Underpredicts radii in the medium and heavy sectors



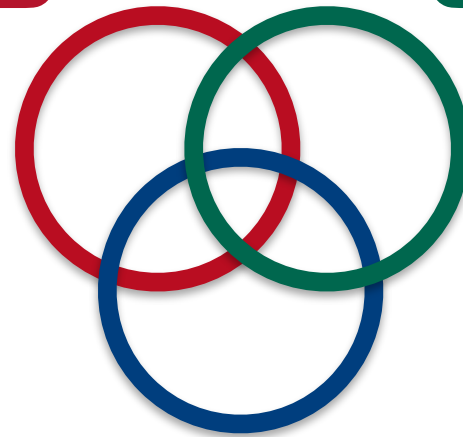
[Somà, Barbieri, *et al.*, *EPJA* **57** (2021)]



Determine an observable O for a system S with precision η

Nuclear interaction

Many-body method

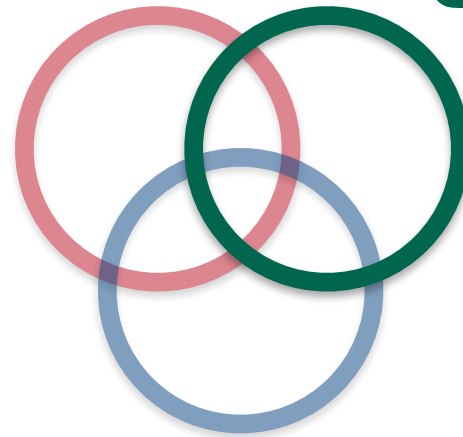


Numerical method



Determine an observable O for a system S with precision η

Many-body method

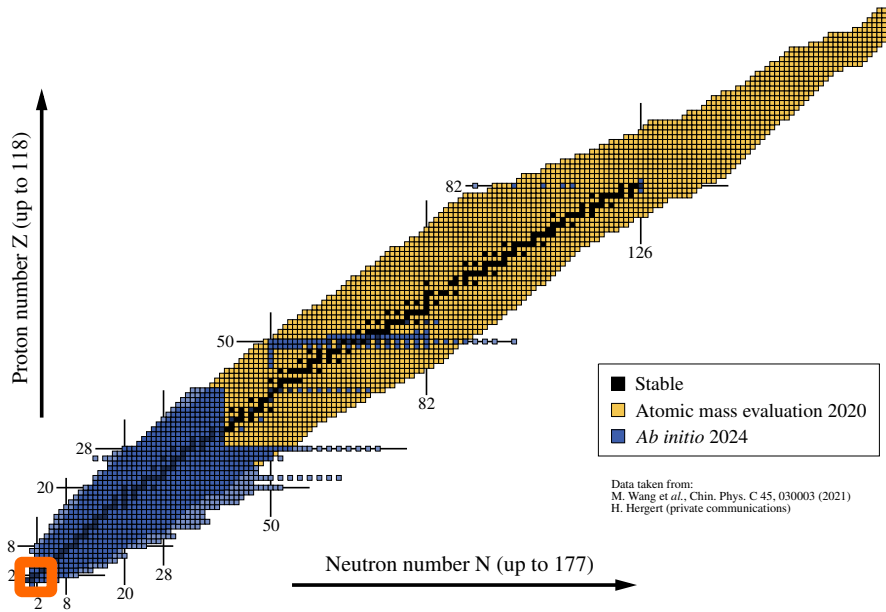




A WALK THROUGH AB INITIO METHODS



Few-body / exact methods

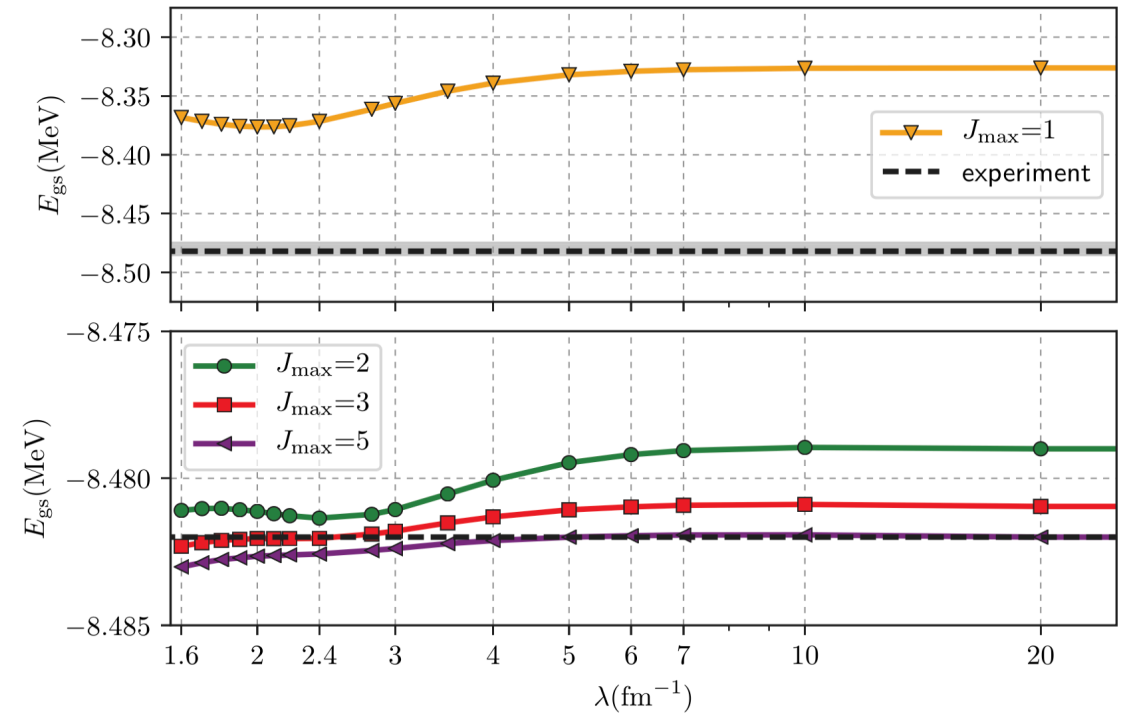


Present use

- Exact computation of light nuclei properties for interaction fits
- Exact benchmarks of new interactions
- Application to specific few-body problems

Faddeev-Yakubovski

Hyperspherical hamonics

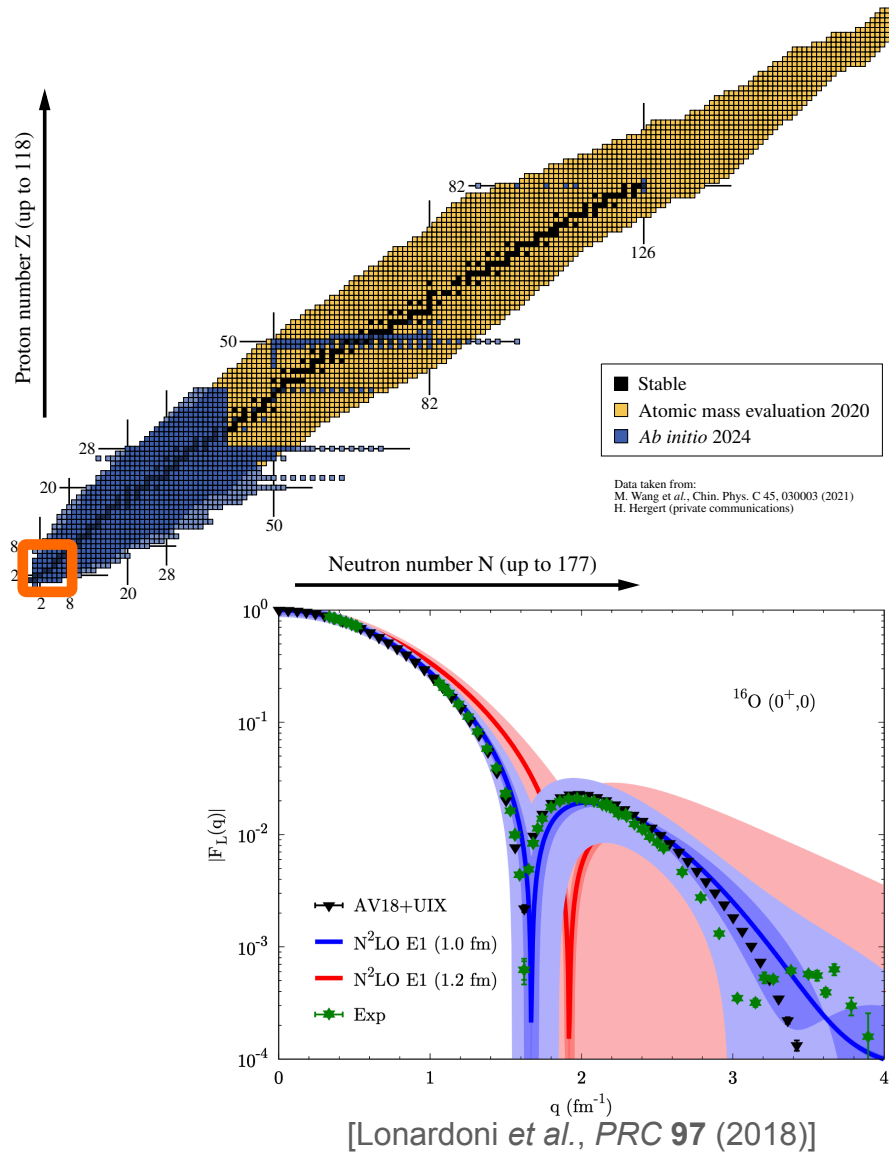


[Hebeler, *Phys. Rept.* **890** (2021)]



Quantum Monte Carlo (QMC) methods

A compact review: [Lynn *et al.*, *Annu. Rev. Nucl. Part. Sci.* **69** (2019)]



Key idea

Obtain exact (up to statistical errors) properties with Monte-Carlo sampling

Variational Monte Carlo (VMC)

- Compute an upper-bound on the g.s.e. from a trial wave-function
- Replace exact integrals with Monte-Carlo sampling

Green's Function Monte Carlo (GFMC)

- Imaginary-time evolution towards the exact g.s. wave function
- Replace path integrals with Monte Carlo walkers

Auxiliary Field Diffusion MC (AFDMC)

- Extend the sampling to spin/isospin states for better scaling

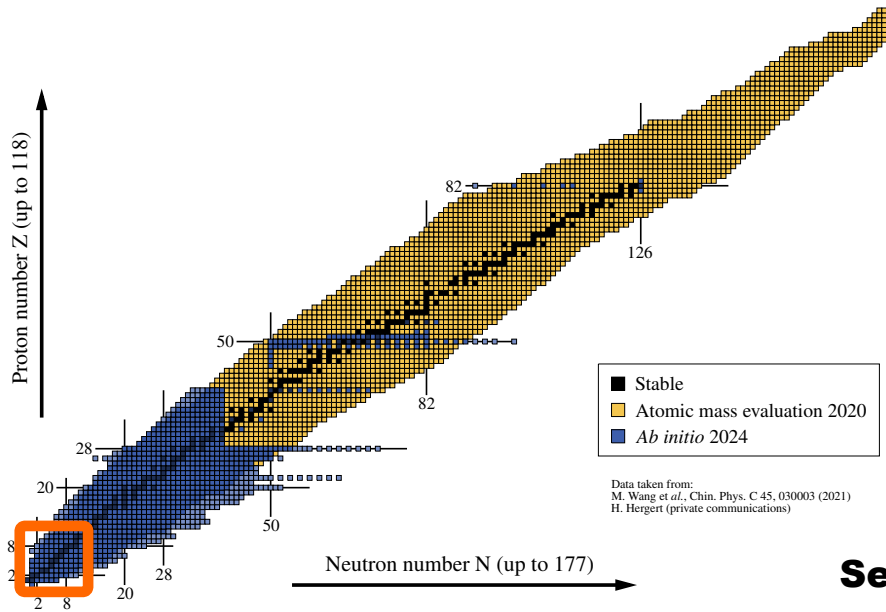


No-Core Shell Model (NCSM)

A structure and reactions review: [Navrátil et al., *Phys. Scr.* **91** (2016)]

Specific case of Configuration-Interaction method

$$|\Psi_n\rangle = \sum_i C_i^{(n)} |\Phi_i\rangle \leftarrow \text{Slater det. basis}$$

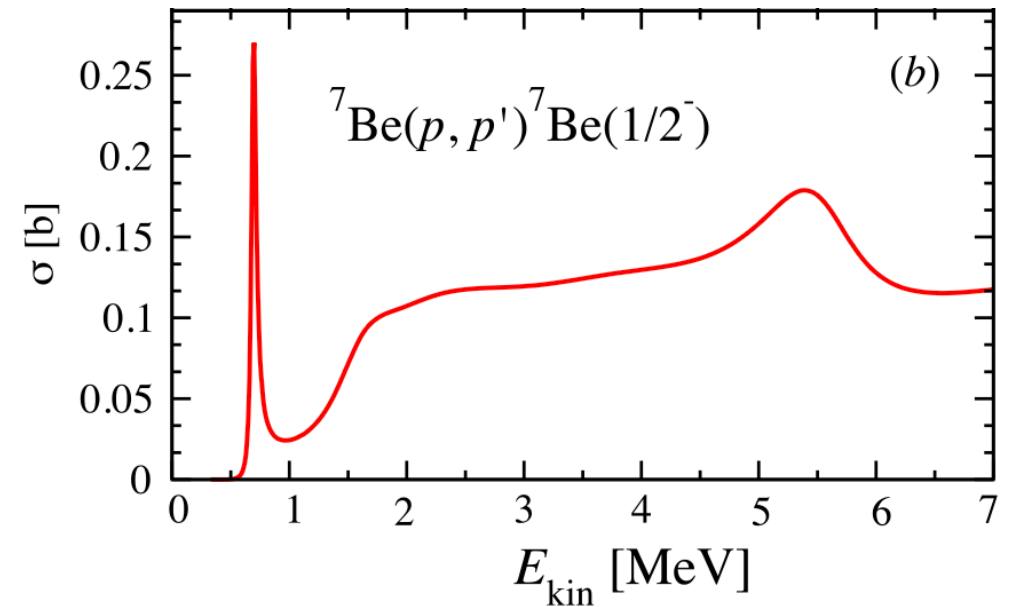


Data taken from:
M. Wang et al., *Chin. Phys. C* **45**, 030003 (2021)
H. Hergert (private communications)

See Lotta's talk!

What does it do?

- Full Hamiltonian diagonalisation = matrix eigenvalue problem
- Access to a wide range of observables
- Very computationally costly so limited in range
- Extensions for connections to reactions, continuum
- Symmetry-adapted NCSM (SA-NCSM) for specific, heavier systems



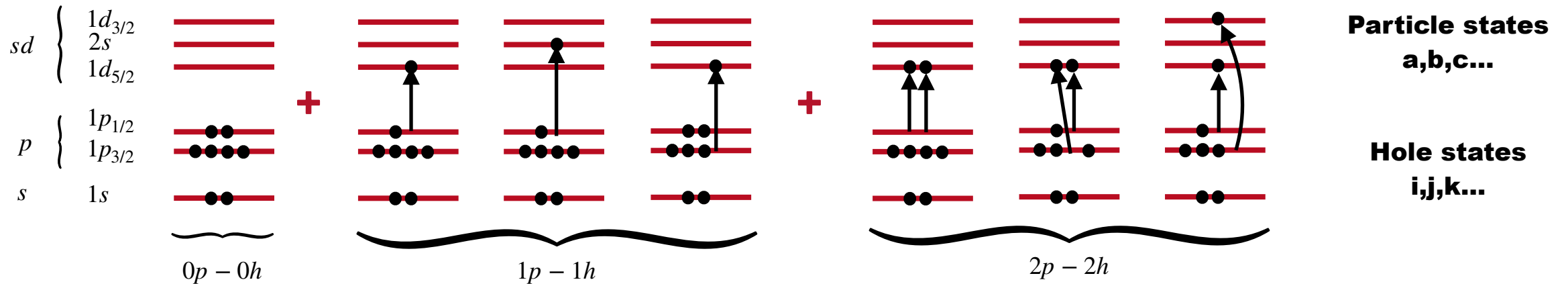
[Navrátil et al., *PLB* **704** (2011)]



The particle-hole representation

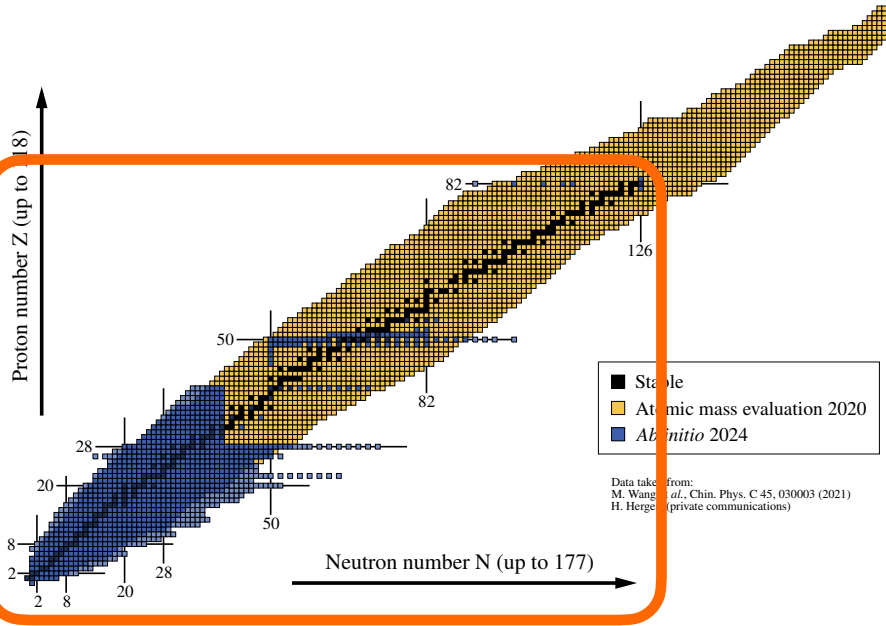
Why this paradigm?

- Intuitive representation starting from the independent shell model
- Emerges naturally from our second quant. representation
- NCSM resums all particle-hole configurations possible
- Other methods expressed in terms of those excitations





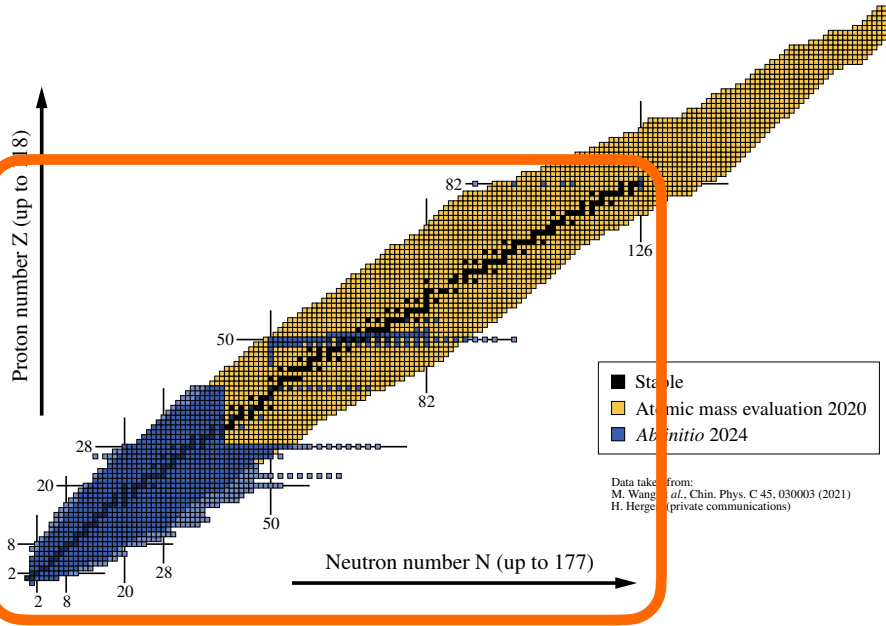
Expansion methods: *MBPT, *CC, *IMSRG, *SCGF...



Expansion methods

$$\begin{aligned} H|\Psi\rangle &= U(\infty)|\Phi\rangle \\ &= (U_1 + U_2 + U_3 + \dots)|\Phi\rangle \end{aligned}$$

Exact result not what we obtain any more!



Expansion methods

$$H|\Psi\rangle = U(\infty)|\Phi\rangle \\ = (U_1 + U_2 + U_3 + \dots)|\Phi\rangle$$

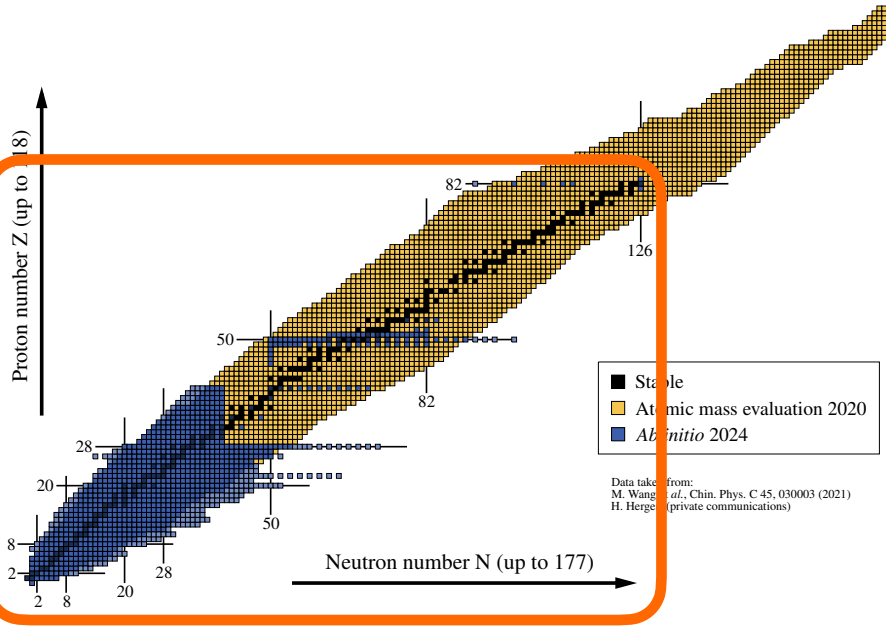
Exact result not what we obtain any more!

Reference state $|\Phi\rangle$

- Often obtained from Hartree-Fock(-Bogoliubov)
- Can be spherical/deformed...
- Should incorporate *collective* correlations

Horizontal correlations





Expansion methods

$$H|\Psi\rangle = U(\infty)|\Phi\rangle \\ = (U_1 + U_2 + U_3 + \dots)|\Phi\rangle$$

Exact result not what we obtain any more!

Vertical correlations

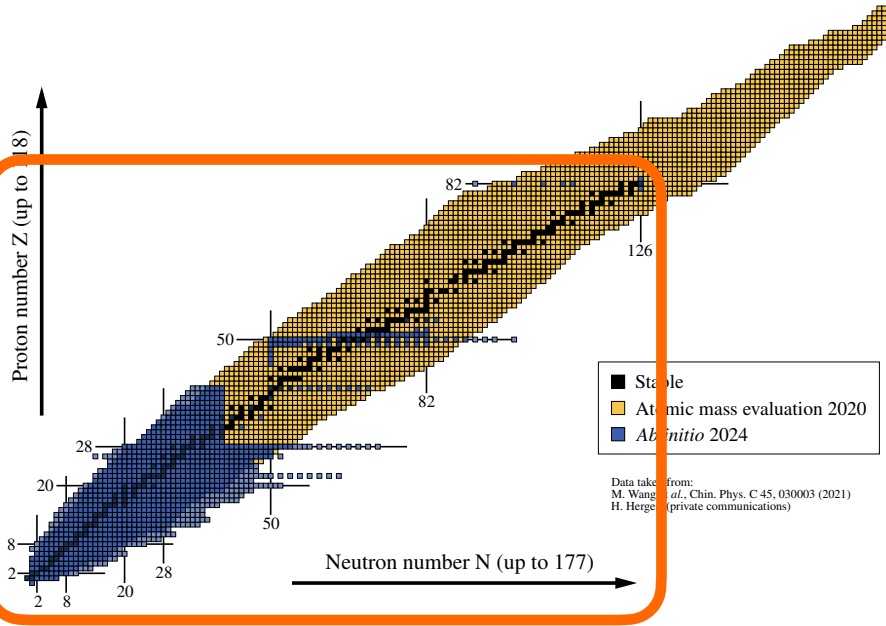
Horizontal correlations

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Expansion operator U

- Depends on the many-body method
- Expressed in terms of particle-hole excitations
- Should incorporate *particle-hole* correlations



Expansion methods

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Exact result not what we obtain any more!

Vertical correlations

Horizontal correlations

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- Can be spherical/deformed...
- Should incorporate *collective* correlations

Expansion operator U

- Depends on the many-body method
- Expressed in terms of particle-hole excitations
- Should incorporate *particle-hole* correlations

Taylor the combination depending on the system



Hamiltonian partition

$$H \equiv H_0 + H_1$$

Eigenstates for H_0

$$H_0 |\Phi_k\rangle = E_k^{(0)} |\Phi_k\rangle$$

Second-order expansion

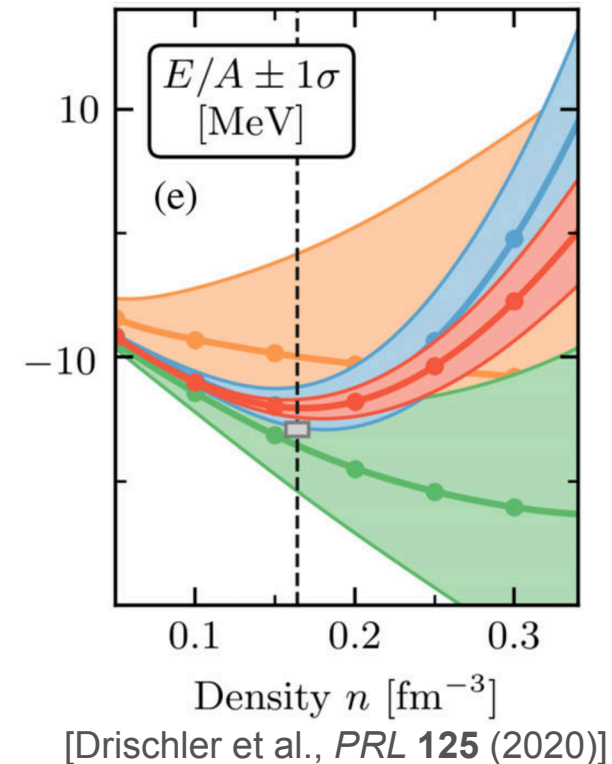
$$E^{(2)} = \sum_k \frac{\langle \Phi | H_1 | \Phi_k \rangle \langle \Phi_k | H_1 | \Phi \rangle}{E^0 - E_k^{(0)}}$$

In practice...

$$E^{(2)} = -\frac{1}{4} \sum_{abij} \frac{V_{abij} V_{ijab}}{E_a + E_b - E_i - E_j}$$

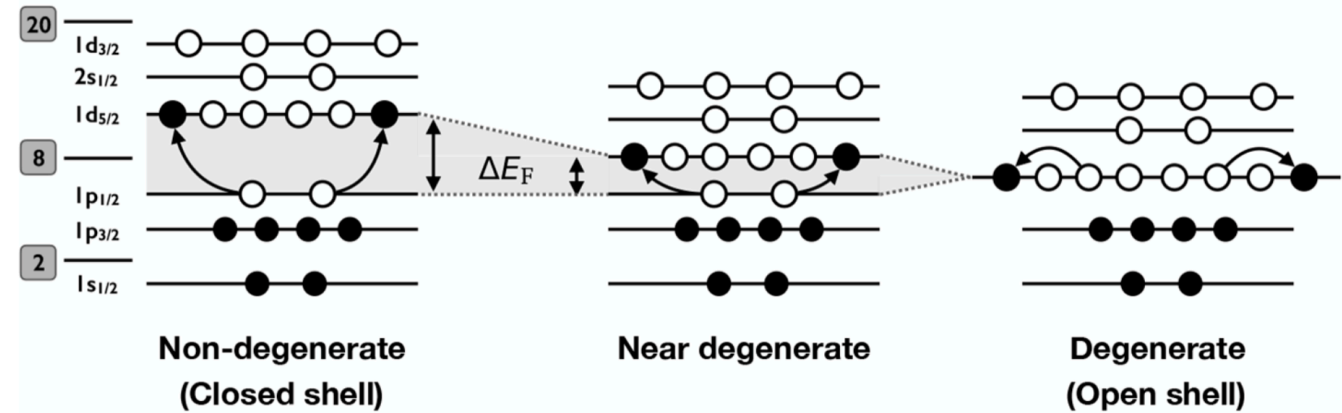
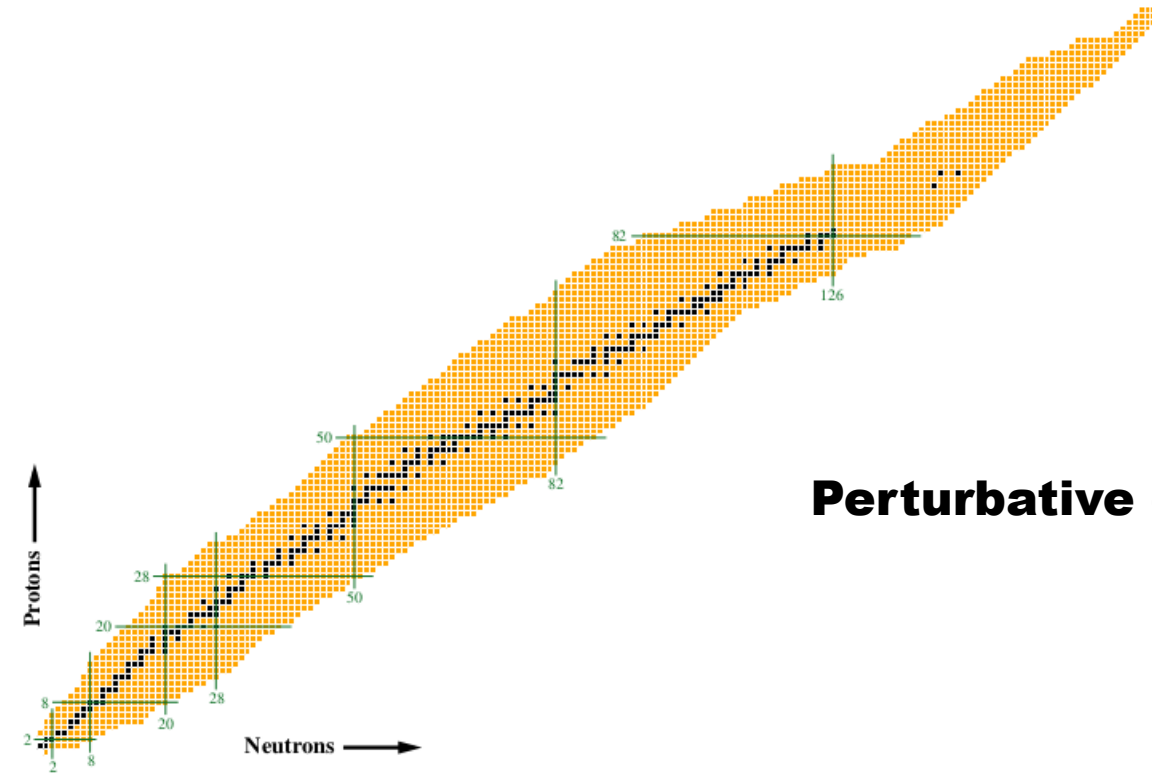
Areas of use

- Very popular for infinite matter (up to 6th order possible)
- Mainly used for emulation or uncertainty estimation in nuclei





Perturbative vs non-perturbative approaches

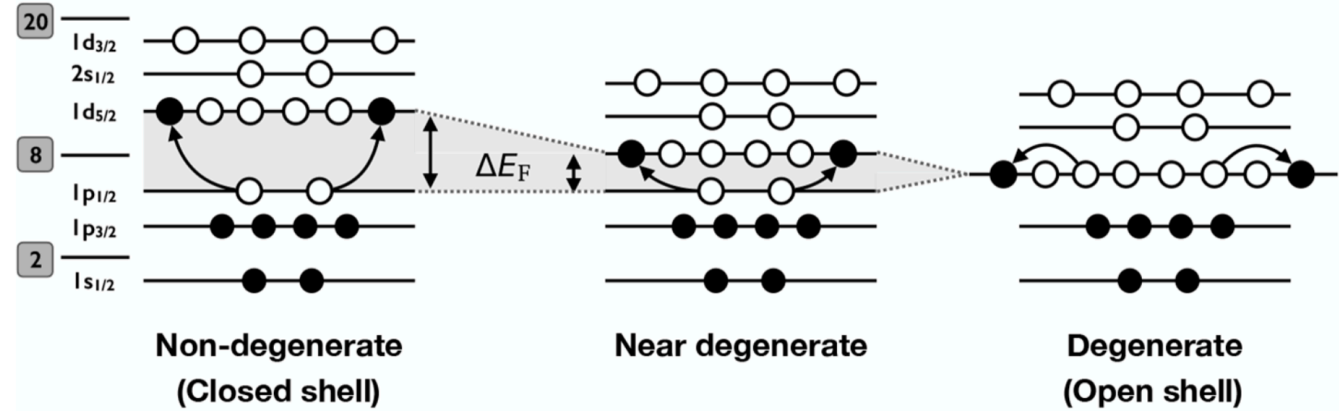
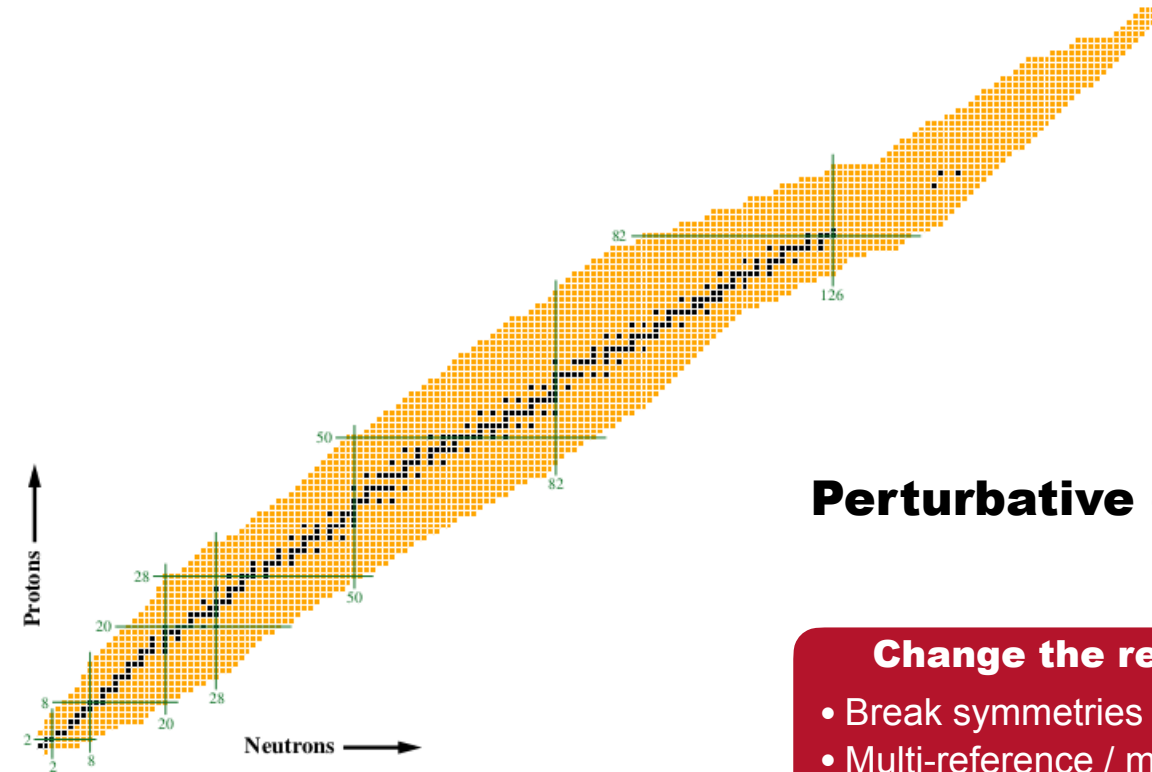


[Tichai, Duguet, Roth, *Front. Phys.* 8 (2020)]

Perturbative expansion breaks down for open-shell systems



Perturbative vs non-perturbative approaches



[Tichai, Duguet, Roth, *Front. Phys.* 8 (2020)]

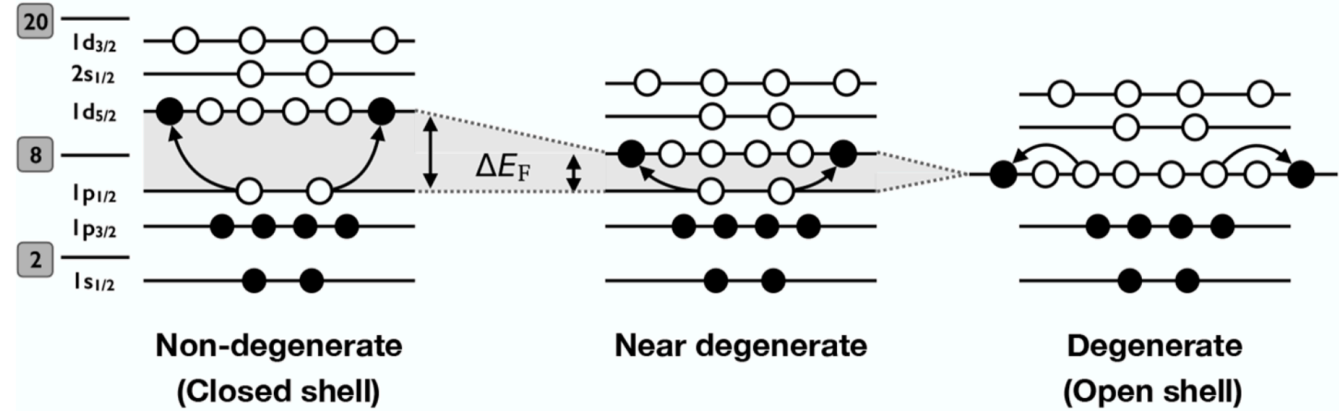
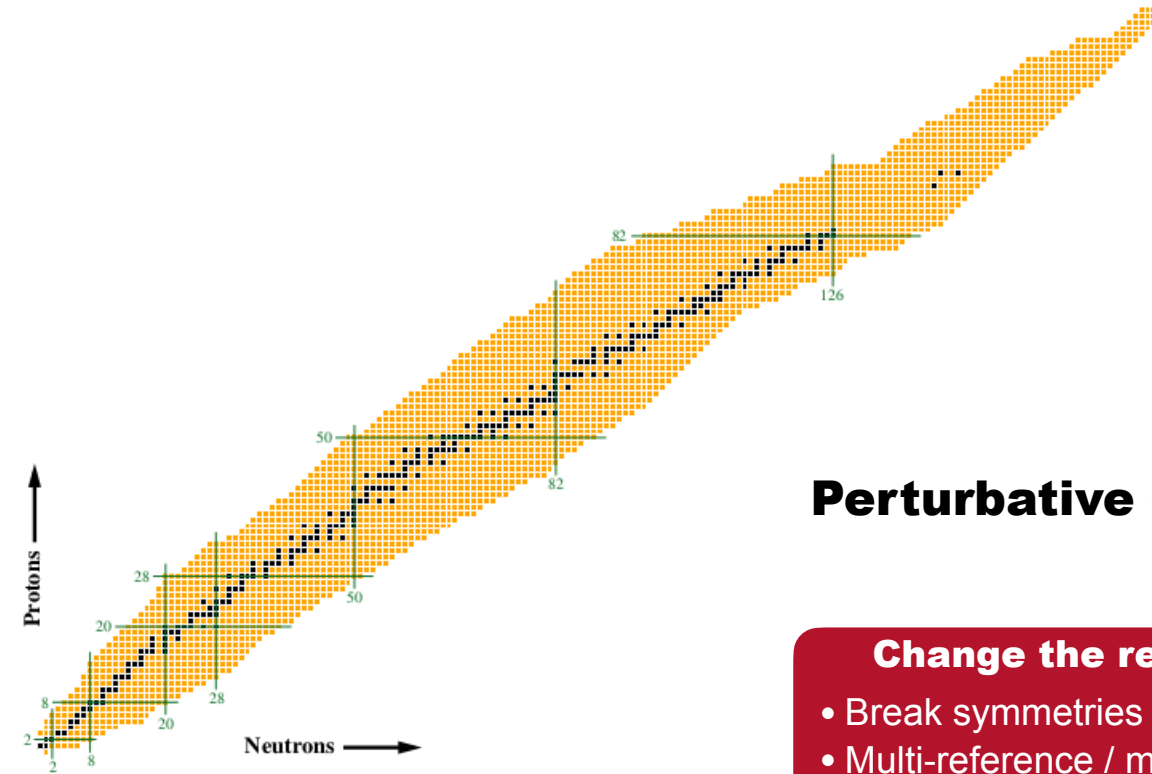
Perturbative expansion breaks down for open-shell systems

Change the reference state

- Break symmetries
- Multi-reference / multi-configuration



Perturbative vs non-perturbative approaches



[Tichai, Duguet, Roth, *Front. Phys.* 8 (2020)]

Perturbative expansion breaks down for open-shell systems

Change the reference state

- Break symmetries
- Multi-reference / multi-configuration

Change the expansion

- Non-perturbative methods
- Infinite resummation of MBPT contributions



Coupled-cluster ansatz

$$|\Psi\rangle = e^T |\Phi\rangle$$

Cluster operators

$$T_n = \frac{1}{(n!)^2} \sum_{i_1, \dots, i_n, a_1, \dots, a_n} t_{i_1 \dots i_n}^{a_1 \dots a_n} c_{a_1}^\dagger \dots c_{a_n}^\dagger c_{i_n} \dots c_{i_1}$$

Truncation scheme

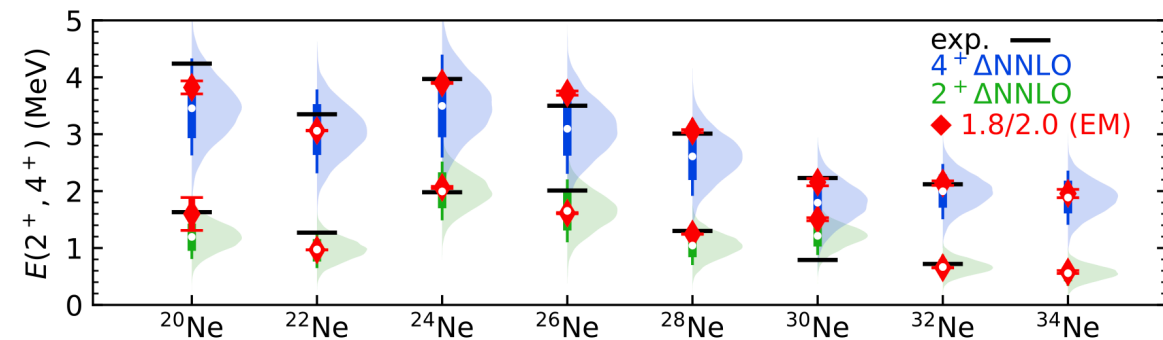
- Expressed in ph excitation multiplicity: singles (S), doubles (D), triples (T)...
- Start with CCD, then CCSD, CCSDT... (no singles in MBPT(2))
- Current workhorse CCSD, partial inclusion of T for high-precision studies

Coupled-cluster equation

$$0 = \langle \Phi_{i_1 \dots i_n}^{a_1 \dots a_n} | e^{-T} H_N e^T | \Phi \rangle$$

with

$$H_N = H - \langle \Phi | H | \Phi \rangle$$



[Ekström et al., arXiv:2305.06955]

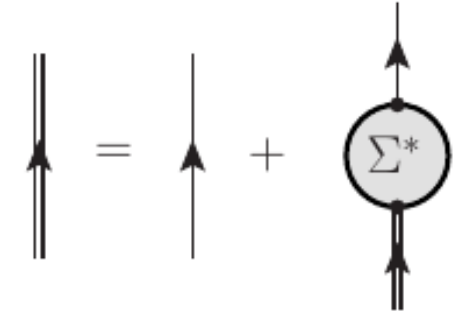


Self-Consistent Green's Functions (SCGF)

A finite nuclei review: [Somà, *Front. Phys.* 8 (2020)]

Key idea

Recast the solution of the Schrödinger equation as a set of one- to A-body Green's functions



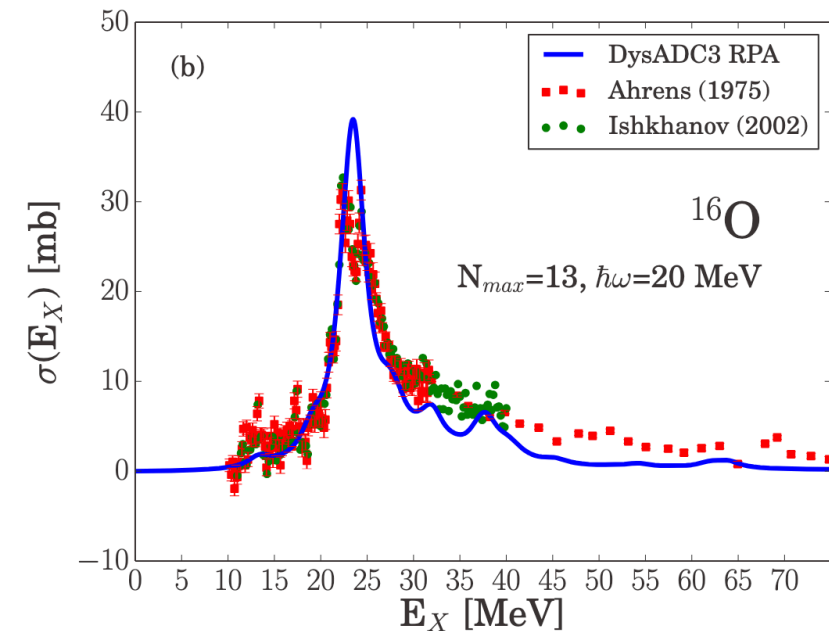
$$g_{\alpha\beta}(\omega) = g_{\alpha\beta}^{(0)}(\omega) + \sum_{\gamma\delta} g_{\alpha\gamma}^{(0)} \Sigma_{\gamma\delta}^*(\omega) g_{\delta\beta}(\omega)$$

Through the one-body Green's function:

- Ground-state energy
- One-body observables (radii, densities...)
- Spectroscopy of the $A \pm 1$ -body systems
- Elastic nucleon-nucleus scattering

Algebraic Diagrammatic Construct at order (n) [ADC(n)]

- MBPT(n) + necessary diagrams to maintain spectral properties
- ADC(∞) gives exact results
- In practice numerically: ADC(3) for Dyson, ADC(2) for Gorkov



[Raimondi, Barbieri, *PRC* 99 (2019)]



In-Medium Similarity Renormalization Group (IMSRG)

An exhaustive review: [Hergert et al., *Phys. Rep.* **621** (2016)]

Decouple the reference state from excitations

- Correlations absorbed in the evolved reference state
- Other operators (radii, etc.) evolved jointly

Continuous operator evolution

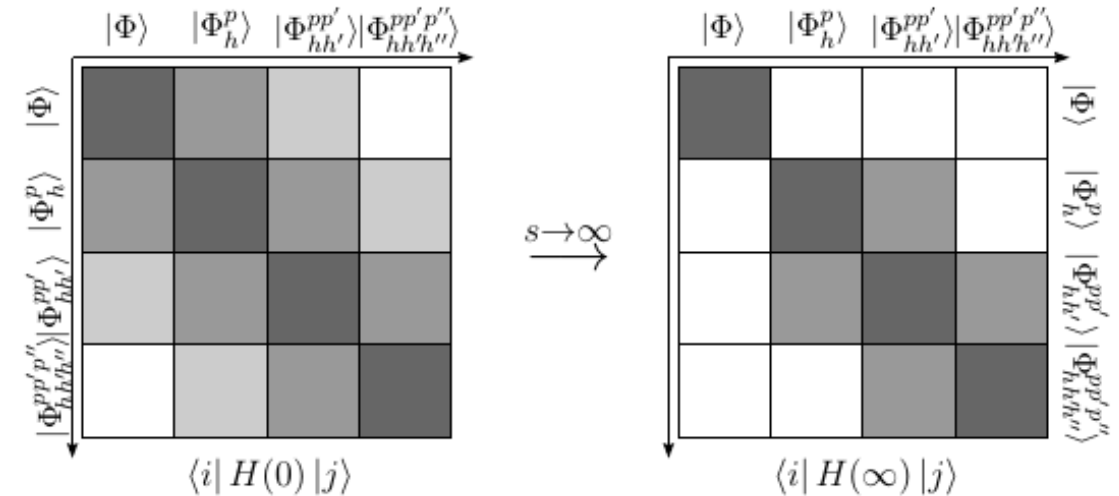
IMSRG flow equation

$$H(s) = U(s)H(0)U^\dagger(s) \quad \frac{dH(s)}{ds} = [\eta(s), H(s)]$$

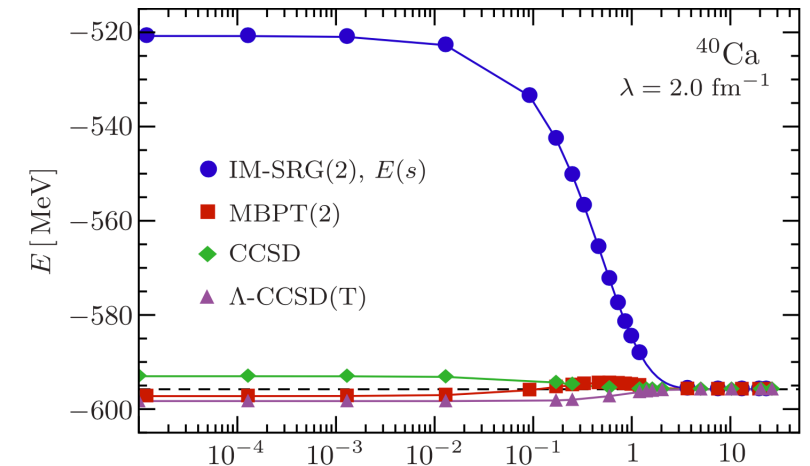
Truncation scheme

- Expressed in rank N of the operators treated in the evolution
- Current workhorse IMSRG(2), IMSRG(3) only in limited model-space

See Matthias' talk!



[Hergert et al., *J.Phys.Conf.Ser.* **1041** (2018)]



[Hergert et al., *Phys. Rep.* **621** (2016)]



Valence-space approaches (VS-IMSRG, CCEI)

A detailed intro: [Stroberg *et al.*, *Ann. Rev. Nucl. Part. Sci.* **69** (2019)]

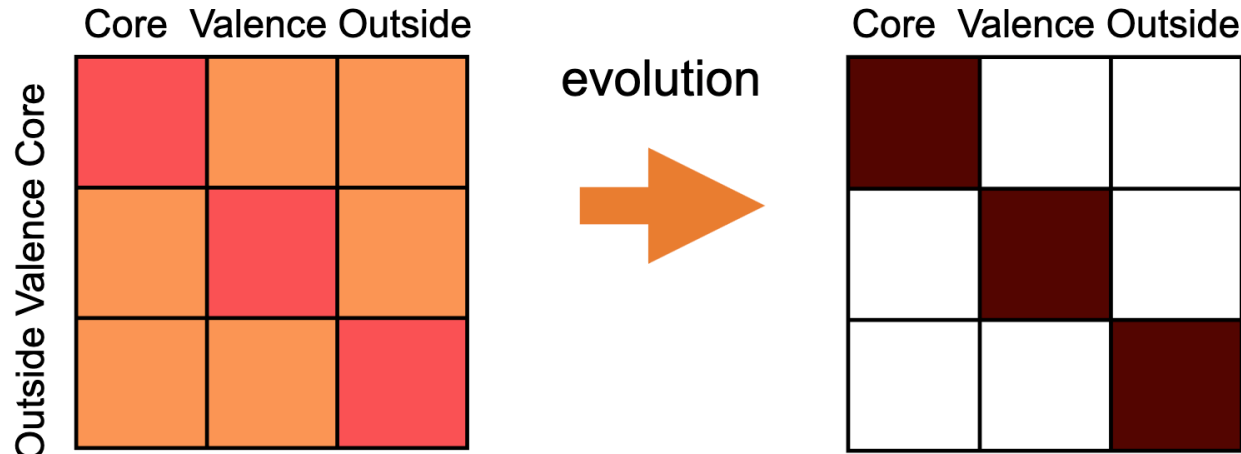
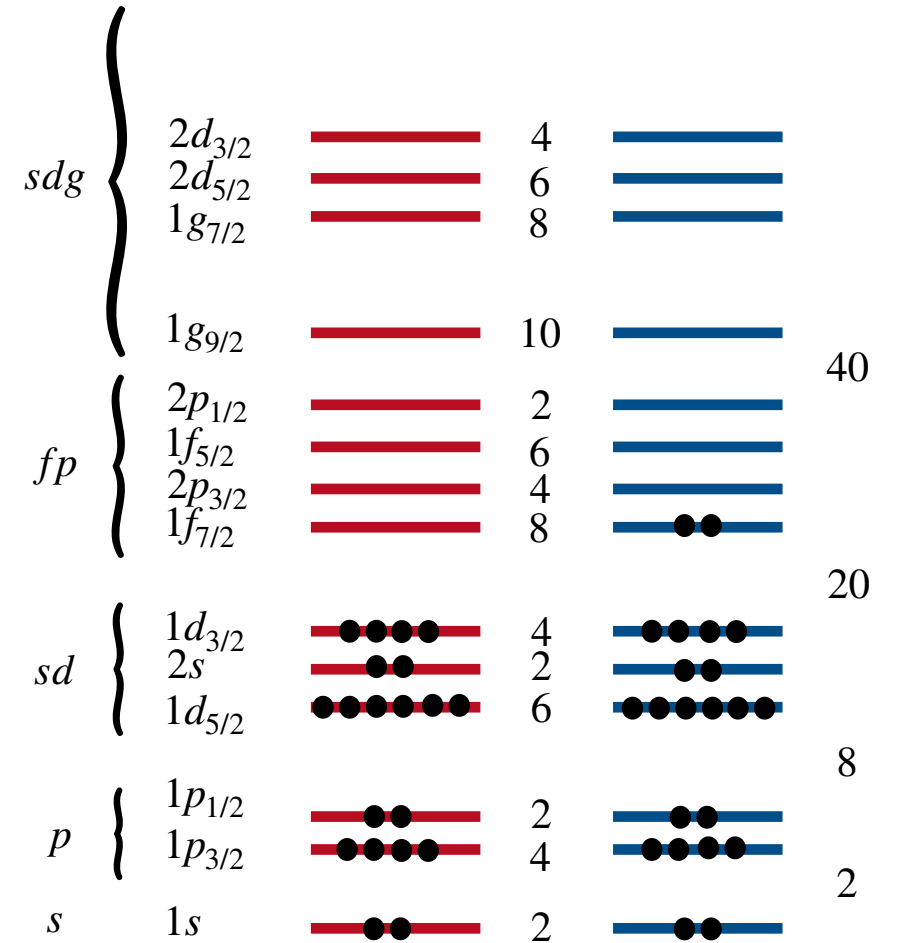


Figure courtesy of T. Miyagi

Decouple core, valence and outside space

- Use IMSRG/CC to generate an effective valence space Hamiltonian
- Use shell model codes to solve in the valence space
- Allows access to open-shell nuclei, excited states...
- Make for full use of the shell-model machinery and expertise





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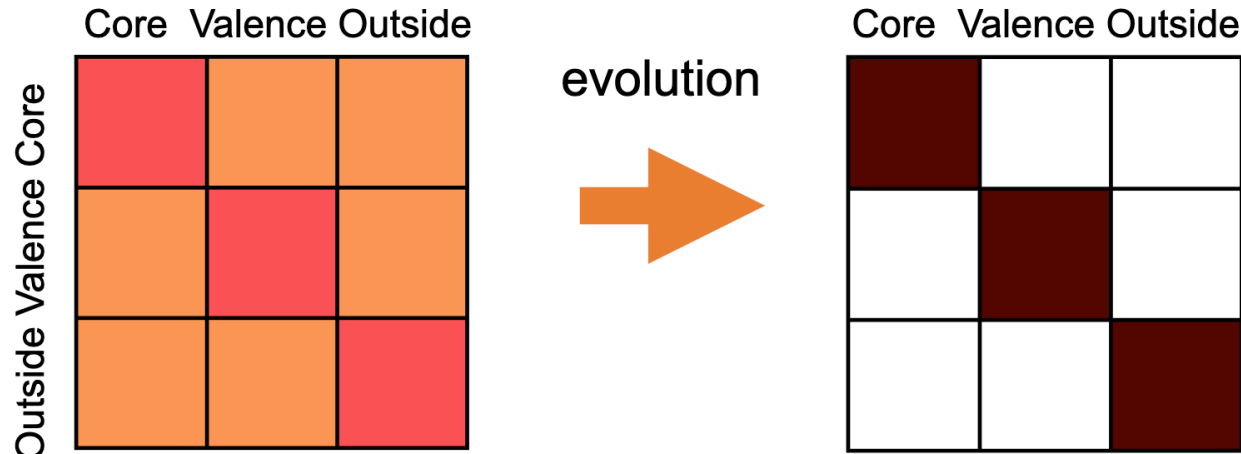
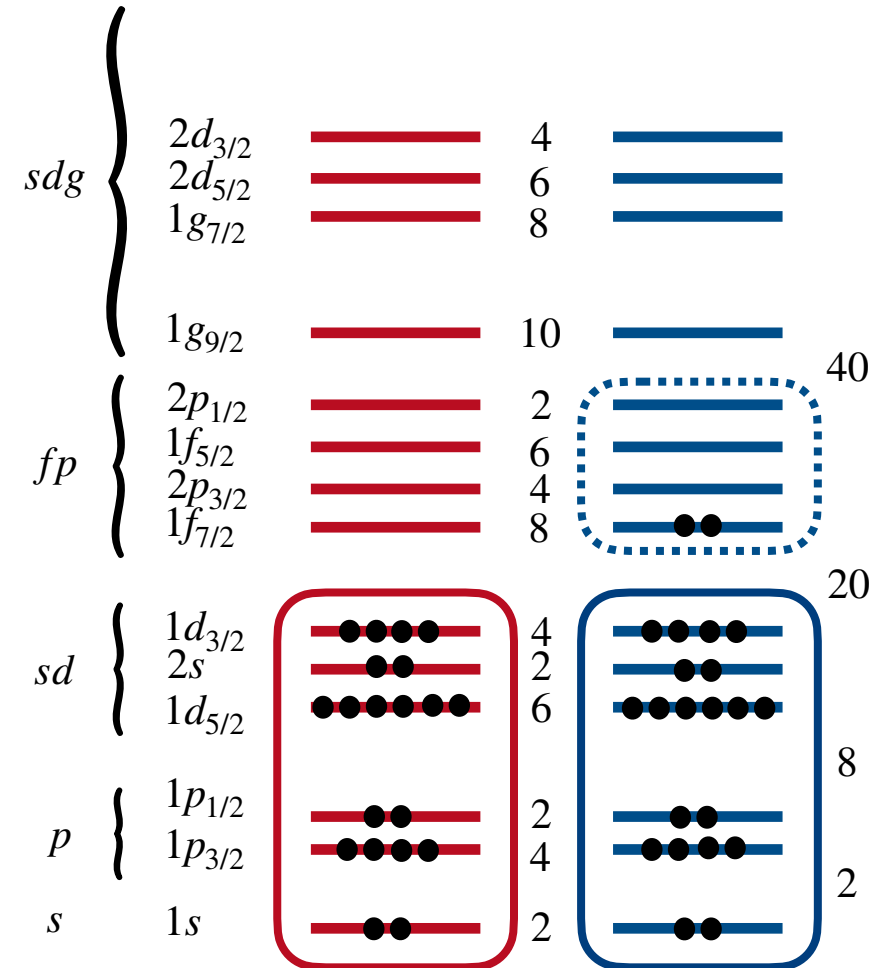


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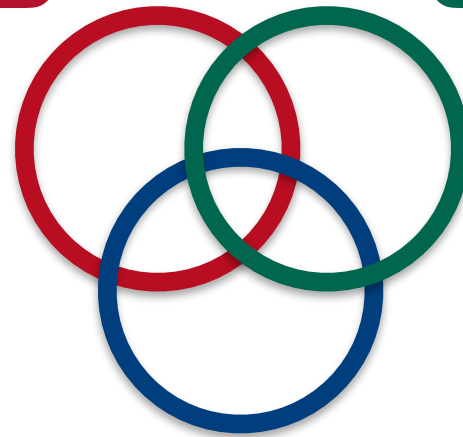




Determine an observable O for a system S with precision η

Nuclear interaction

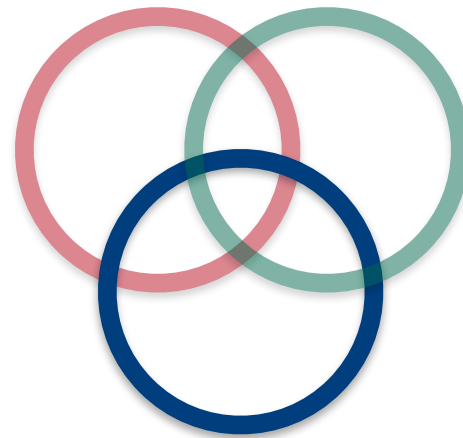
Many-body method



Numerical method



Determine an observable O for a system S with precision η



Numerical method



SOME COMPUTATIONAL JARGON



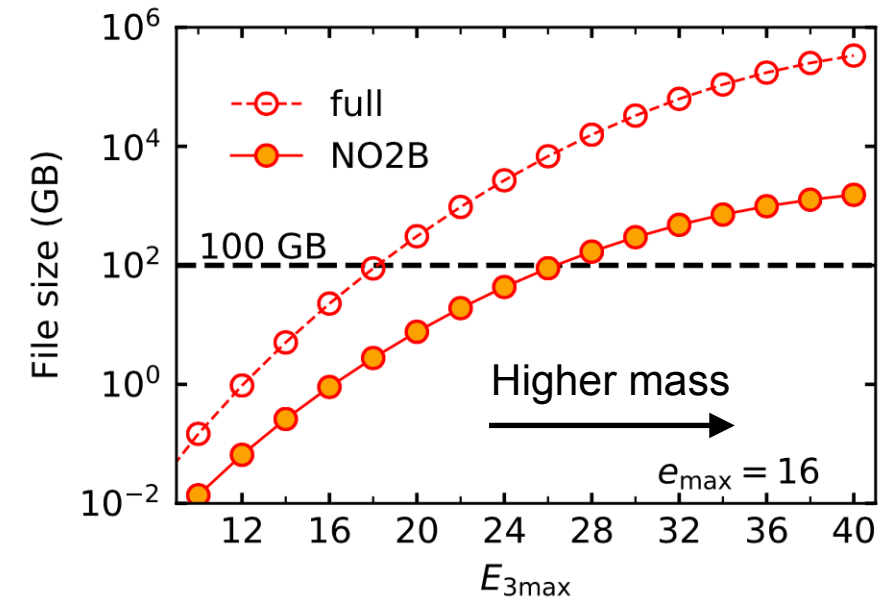
Computational jargon

Basis

- Usually start from (spherical) Harmonic Oscillator basis: frequency $\hbar\omega$
 - Then often switch to HF(B) for expansion
 - Truncation usually in $e_{\max} \equiv \max(2n + l)$ (standard: 12-14)
 - Three-body force truncated in $E3_{\max} \equiv \sum_1^3 E_{ind}$
- Ideal: $3 \cdot e_{\max}$. Standard: 16-24 (28 with half-precision)

A tale of memory

- Expansion methods mostly not limited by CPU time but memory
- Hamiltonian itself requires ~ 100 GB for state-of-the-art md. sp.
- Iterative methods need multiples copies of operators: prohibitive if three-body!
- Alternative storage schemes being explored (tensor contractions)



[Miyagi, Stroberg, *et al.*, *PRC* **105** (2022)]



Need for a clever storage scheme

- 3NF makes on-the-fly ME computation impossible
- Need to account for all possible configurations among millions...
- Strategy: Exploit nuclear interaction symmetries

Sociological peculiarities

- Many-body practitioners usually do not produce their MEs themselves
- Some QMC methods work in coordinate space and do not need this

Relative momentum/HO basis

SRG transformation

Relative momentum/HO basis

Talmi-Moshinski

Single-particle basis



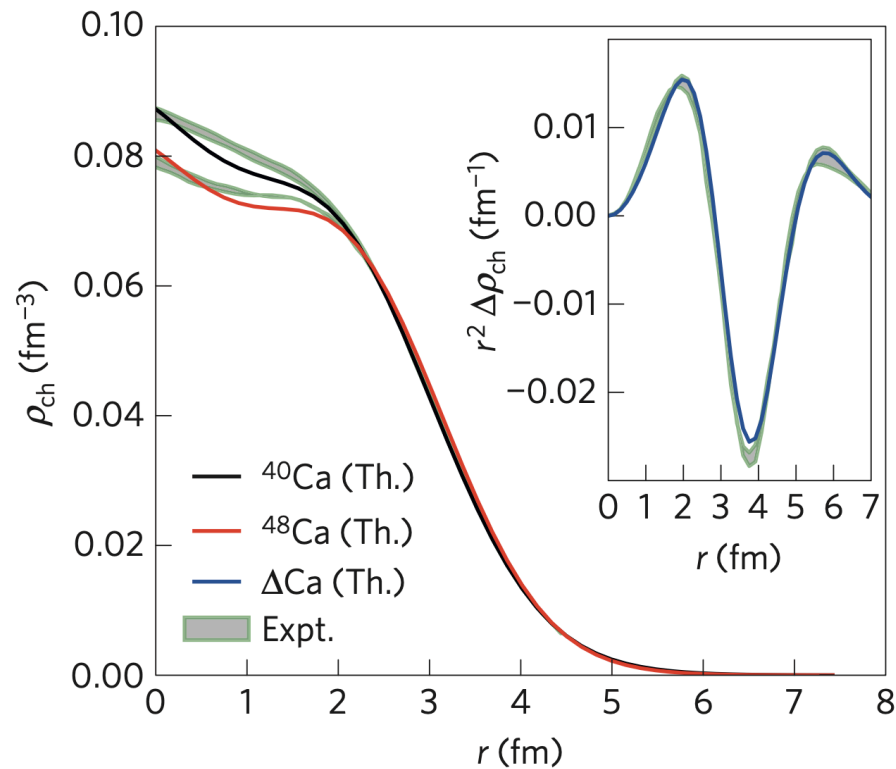
A SHORT SELECTION OF AB INITIO DENSITIES



Some early ab initio densities with NNLOsat

Charge densities of ^{40}Ca and ^{48}Ca

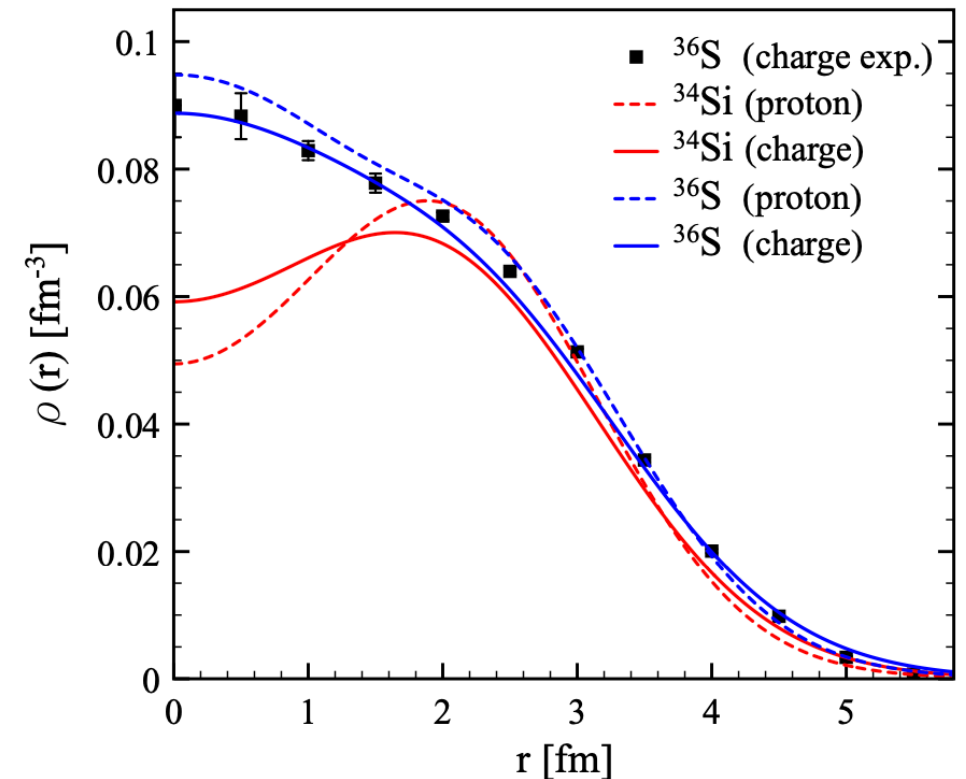
- First established NNLOsat as accurate interaction for ρ
- Connection to weak charge radius, R_{skin} and α_D



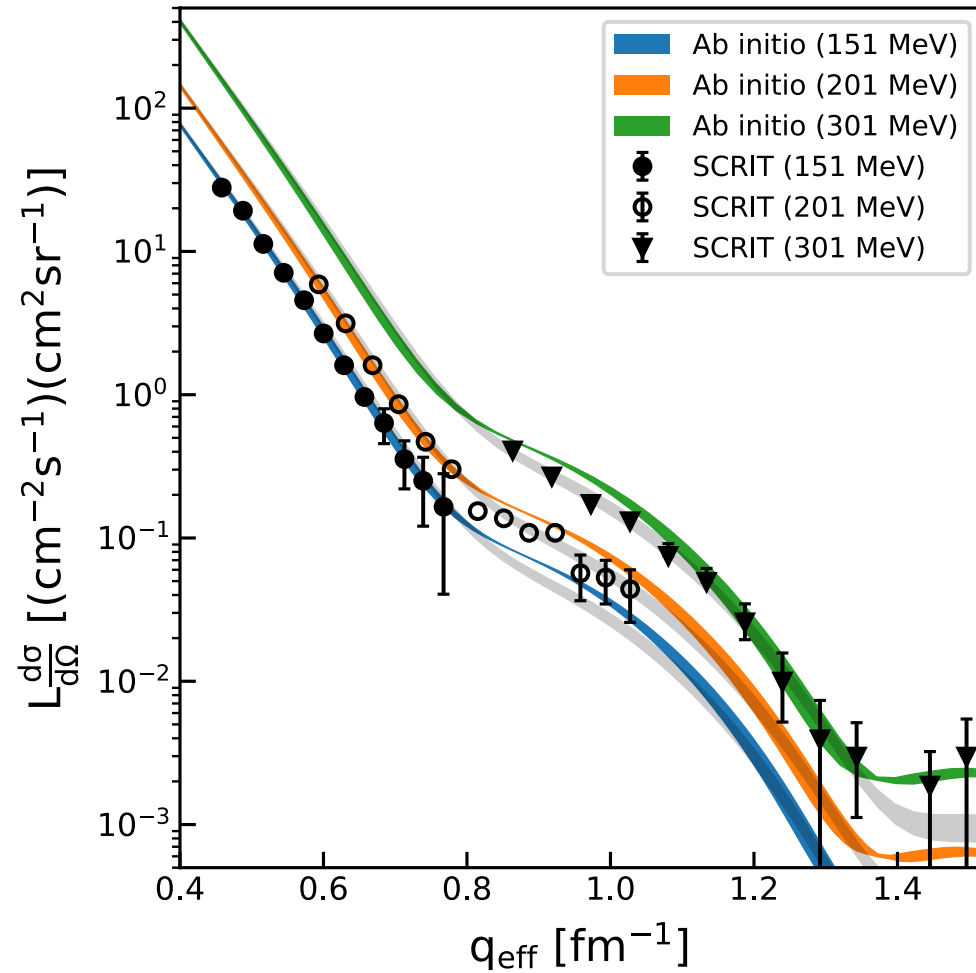
[Hagen *et al.*, *Nat. Phys.* **12** (2015)]

Study of candidate bubble nucleus ^{34}Si

- Investigation of the central depletion in ^{34}Si
- Link to details of the interaction and s.p. structure

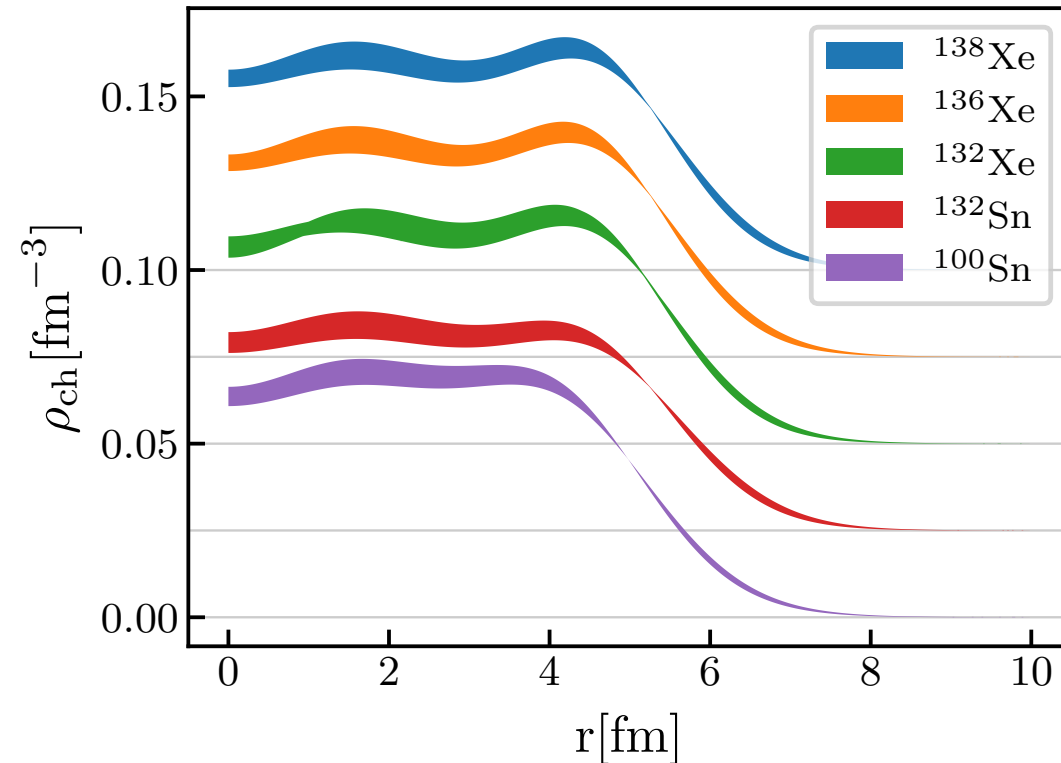


[Duguet *et al.*, *PRC* **95** (2017)]



First *ab initio* calculation past the Sn isotopic line

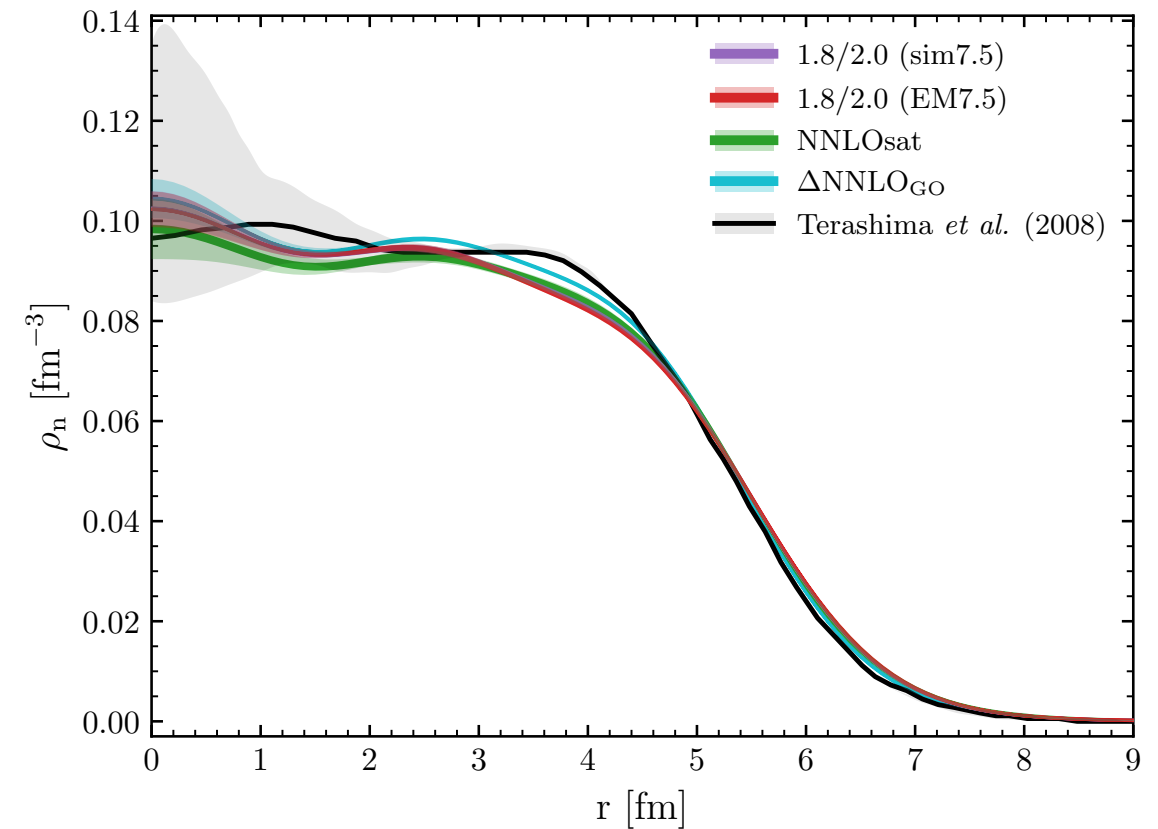
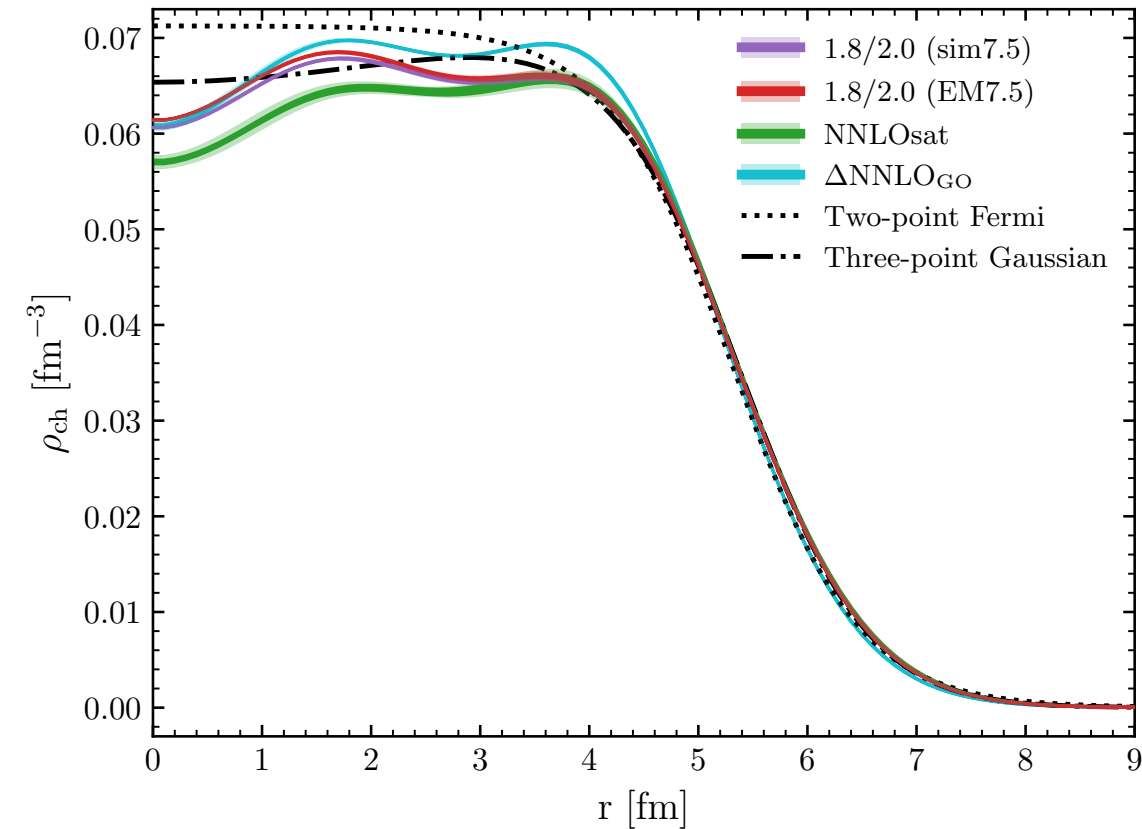
- Reproduce experimental electron scattering results
- Results meaningful for exp. despite moderate convergence





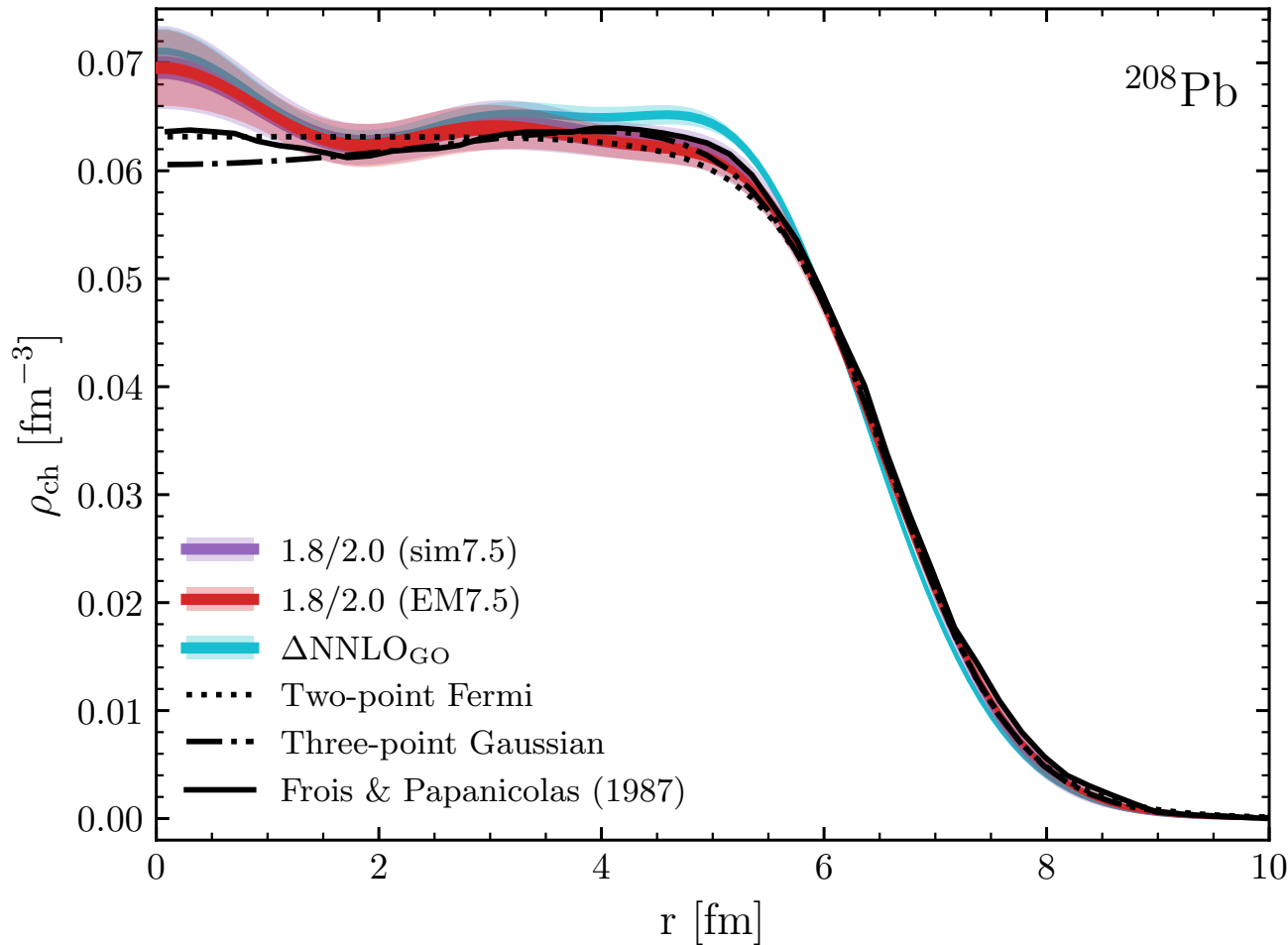
Ab initio densities for heavy systems: ^{120}Sn

[Arthuis, Hebeler, Schwenk, arxiv:2401.06675]



Excellent reproduction of ^{120}Sn densities

- Consistent picture over the different interactions
- Very moderate uncertainties



Charge density for ^{208}Pb

- Consistent picture over the different interactions
- 1.8/2.0s give excellent surface profile
- Inner density not fully converged yet

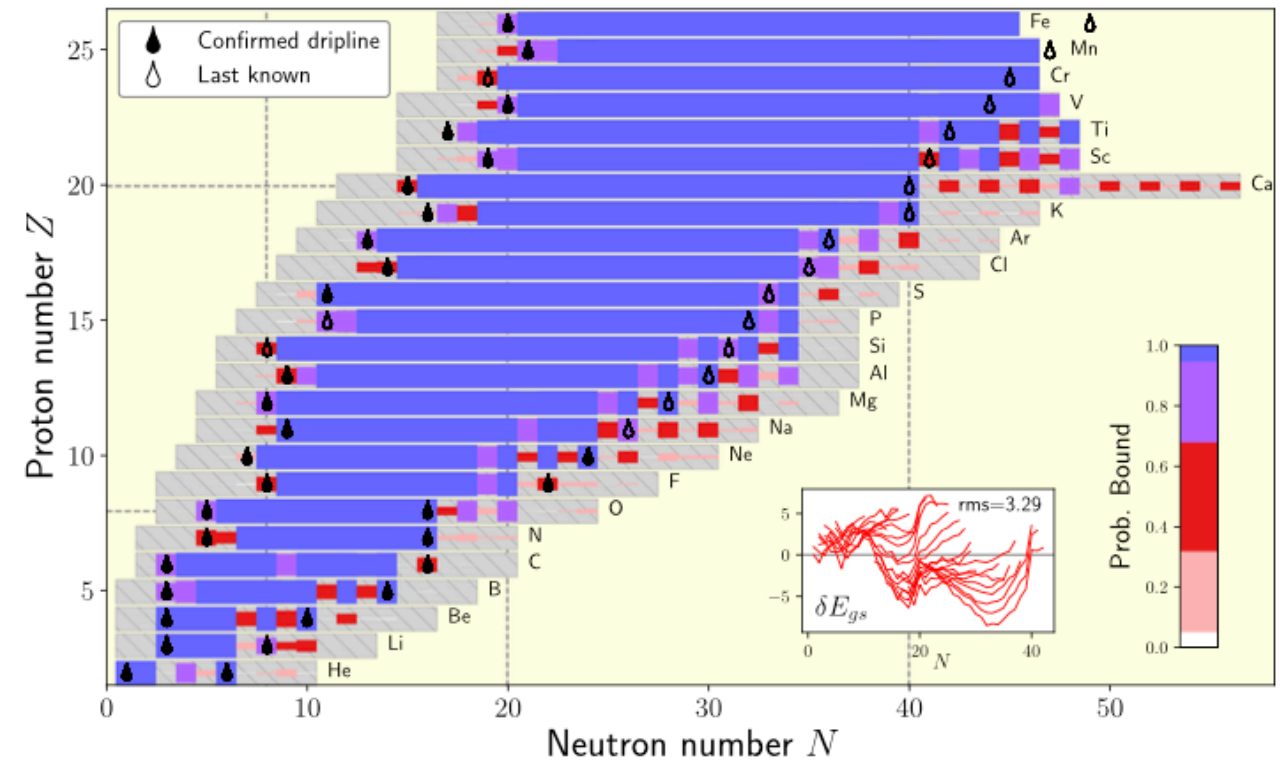


A BRIEF AND BIASED SELECTION OF RECENT AB INITIO RESULTS



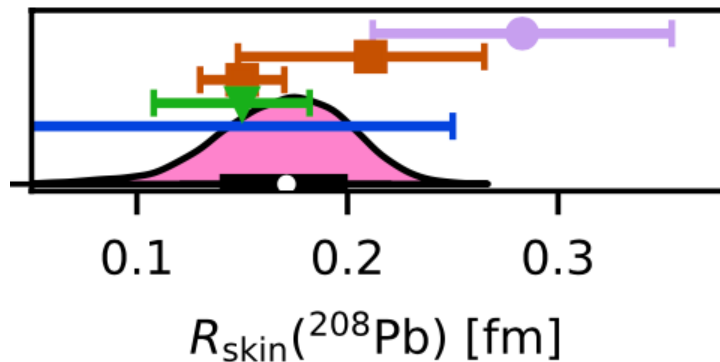
Lower nuclear chart fully computed

- Computation of ~700 isotopes in the lower chart
- Coupling to Bayesian statistics
- Estimation of a probability of being bound
- Reproduction of known experimental driplines
- Prediction of new driplines

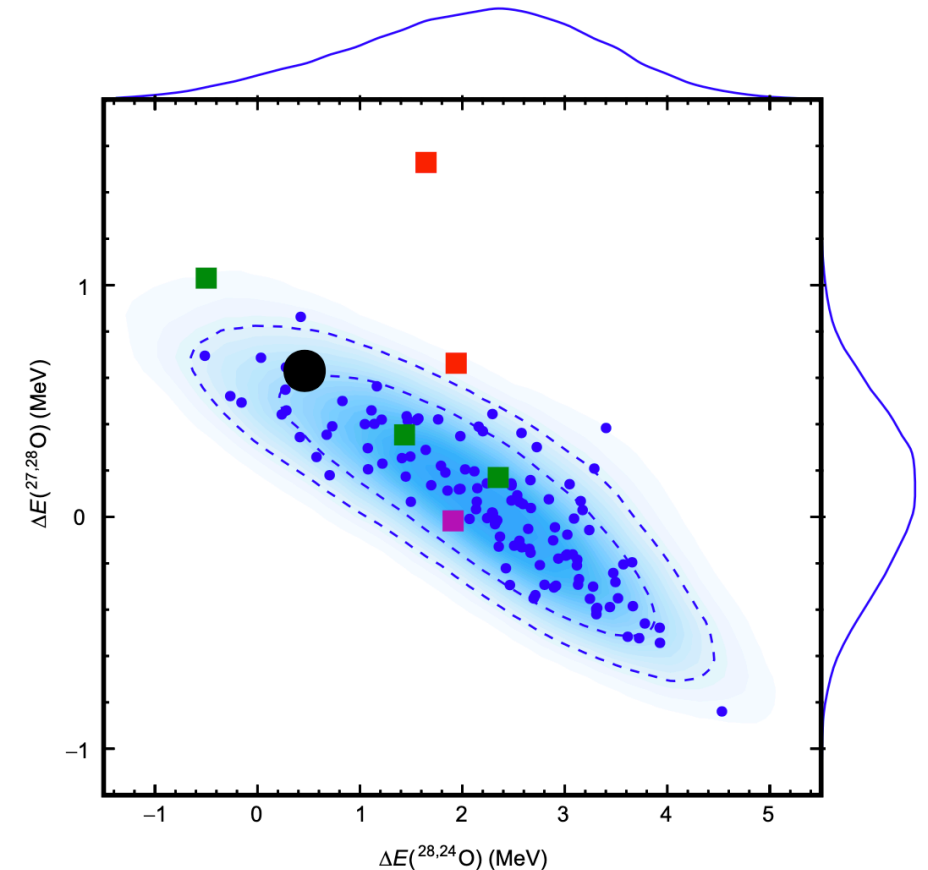


Rationale

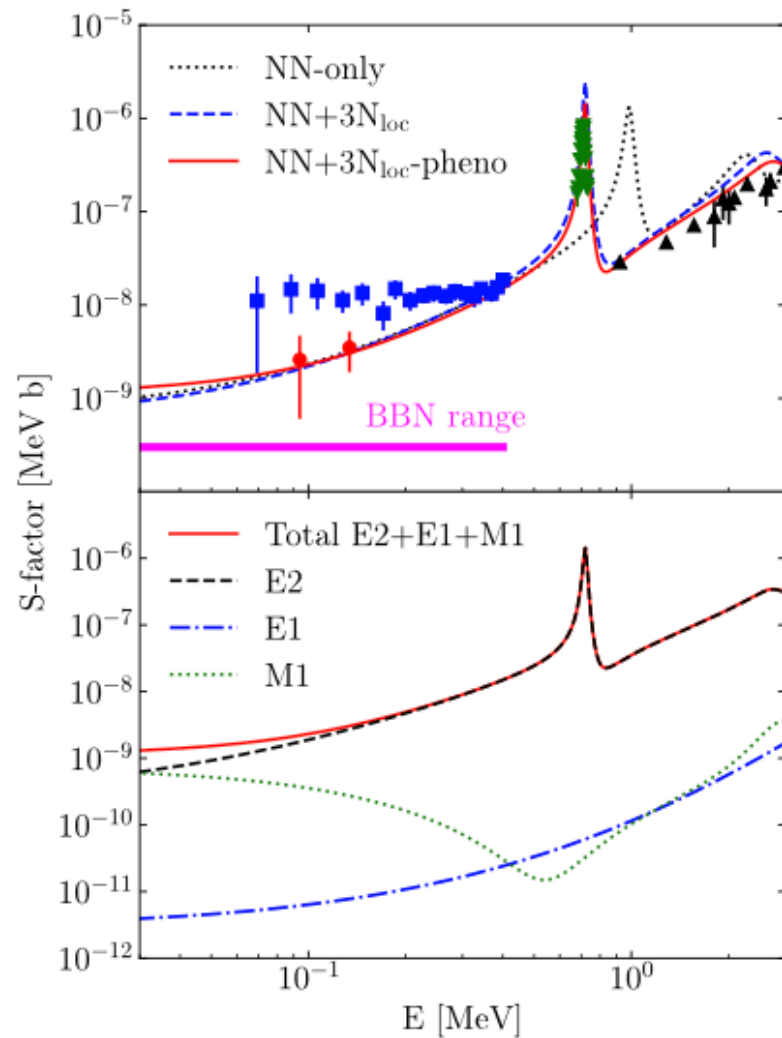
- Import of 'history matching techniques' to nuclear physics
- Determination of a set of 'non-implausible' interactions
- Agnostic approach to interaction determination
- Coupling with Bayesian method for full UQ
- Estimation of ^{208}Pb neutron skin
- Confirmation of ^{28}O as unbound



[Hu, Jiang *et al.*, *Nat. Phys.* **18** (2022)]

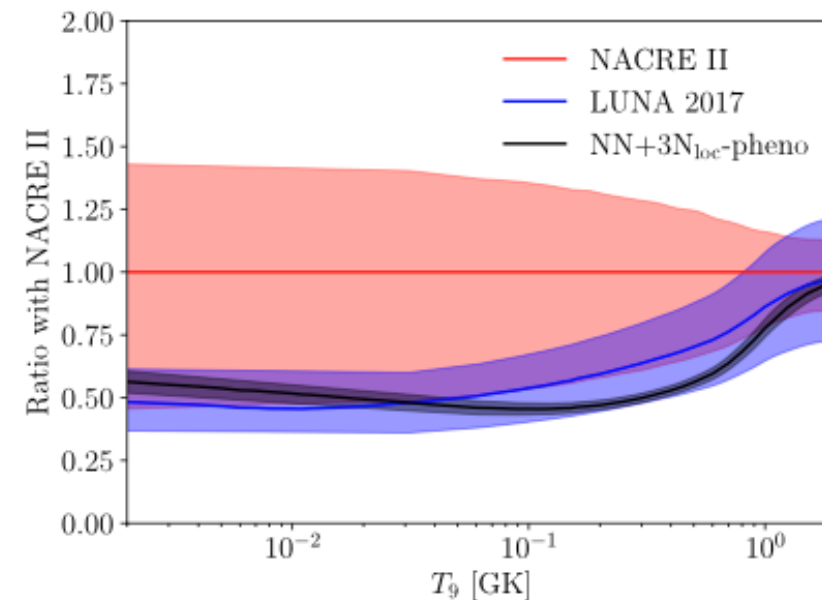


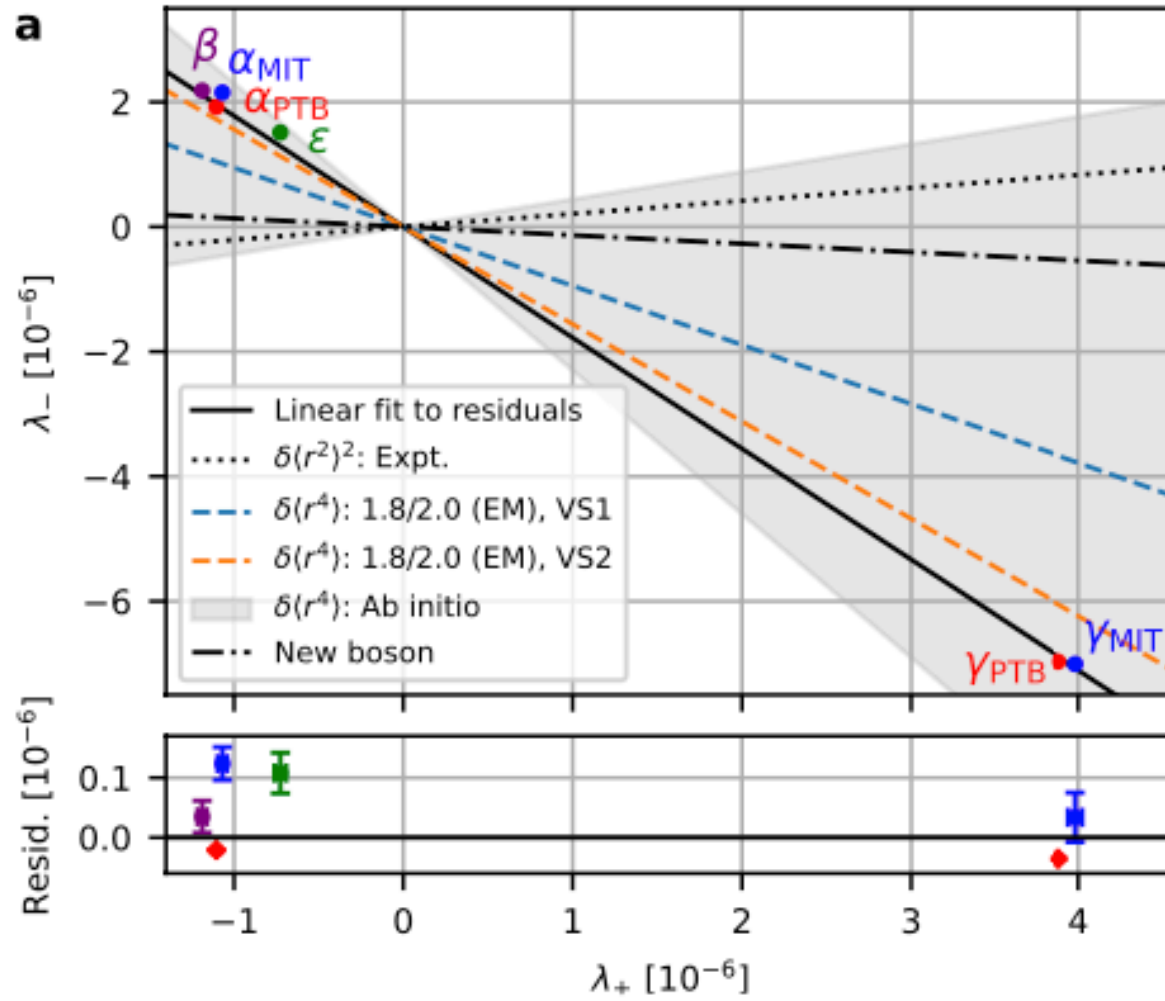
[Kondo *et al.* (SAMURAI 21), *Nature* **620** (2023)]



S-factor for astrophysical reaction

- Discrepancy between BB predictions and observations
- Radiative capture ${}^4\text{He}(d, \gamma){}^6\text{Li}$ key reaction
- Ab initio prediction highlight M1 transition role
- Uncertainties reduced by x7 w.r.t. NACRE





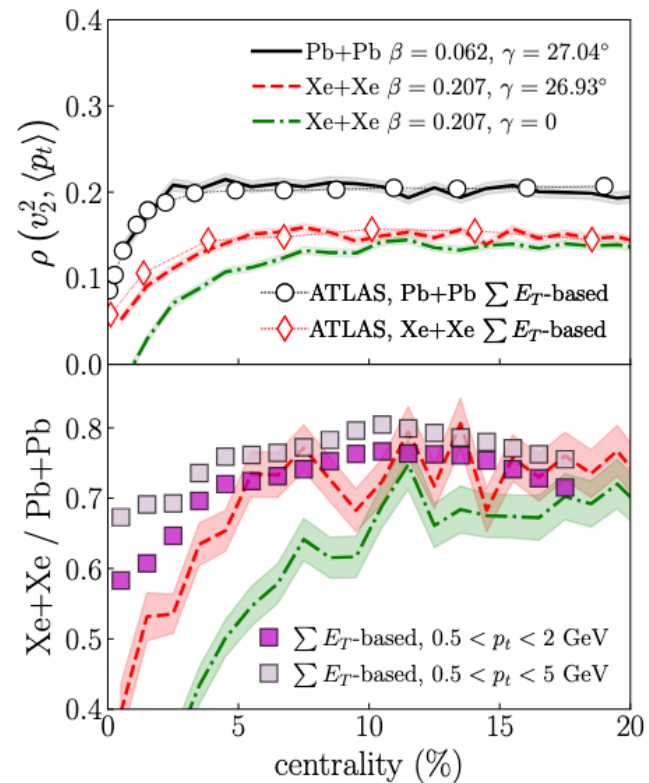
Isotope shifts in the $^{170-176}\text{Yb}$ chain

- Analysis of $\delta < r^4 >$ along the chain
- Possible trace of a new boson?
- Ab initio in excellent agreement with experiment
- New boson seems unlikely

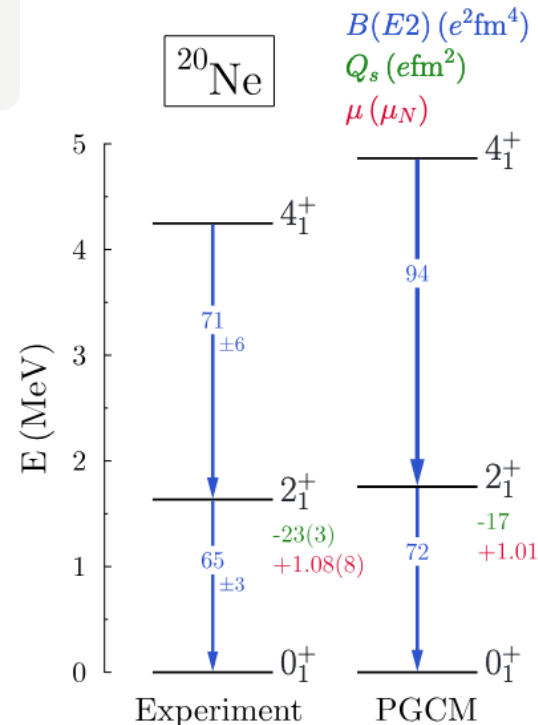


Nuclear deformation for HIC

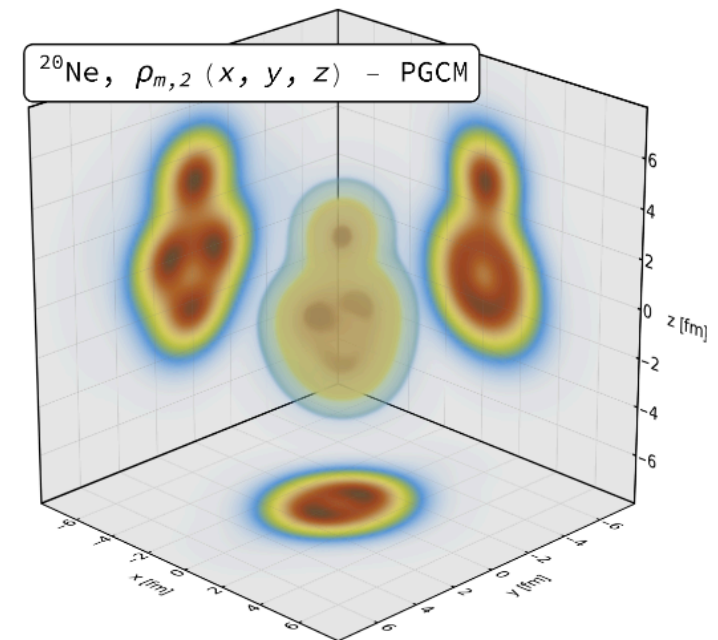
- Deformation more important than expected
- Pioneered with EDF
- Now ab initio for future LHC runs



[Bally, Giacalone, Bender, Somà, PRL 128 (2022)]



[Giacalone, Bally, Nijs, *et al.*, arXiv:2402.05995]





Ab initio methods now a staple of nuclear physics

- Offer a systematic approach to nuclear structure and reactions
- Tremendously improved reach in mass and observables
- Very active field of research, connected to other communities

Diverse set of approaches

- Complementary many-body methods
- Wide range of target systems and observables
- Continuous progress in interaction accuracy



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