NLEFT in the Exascale era

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Outline

- Motivation
  - Introduction to NLEFT
  - Calculations near the Sn Dripline
- Summary

What is Nuclear Lattice Effective Field Theory?

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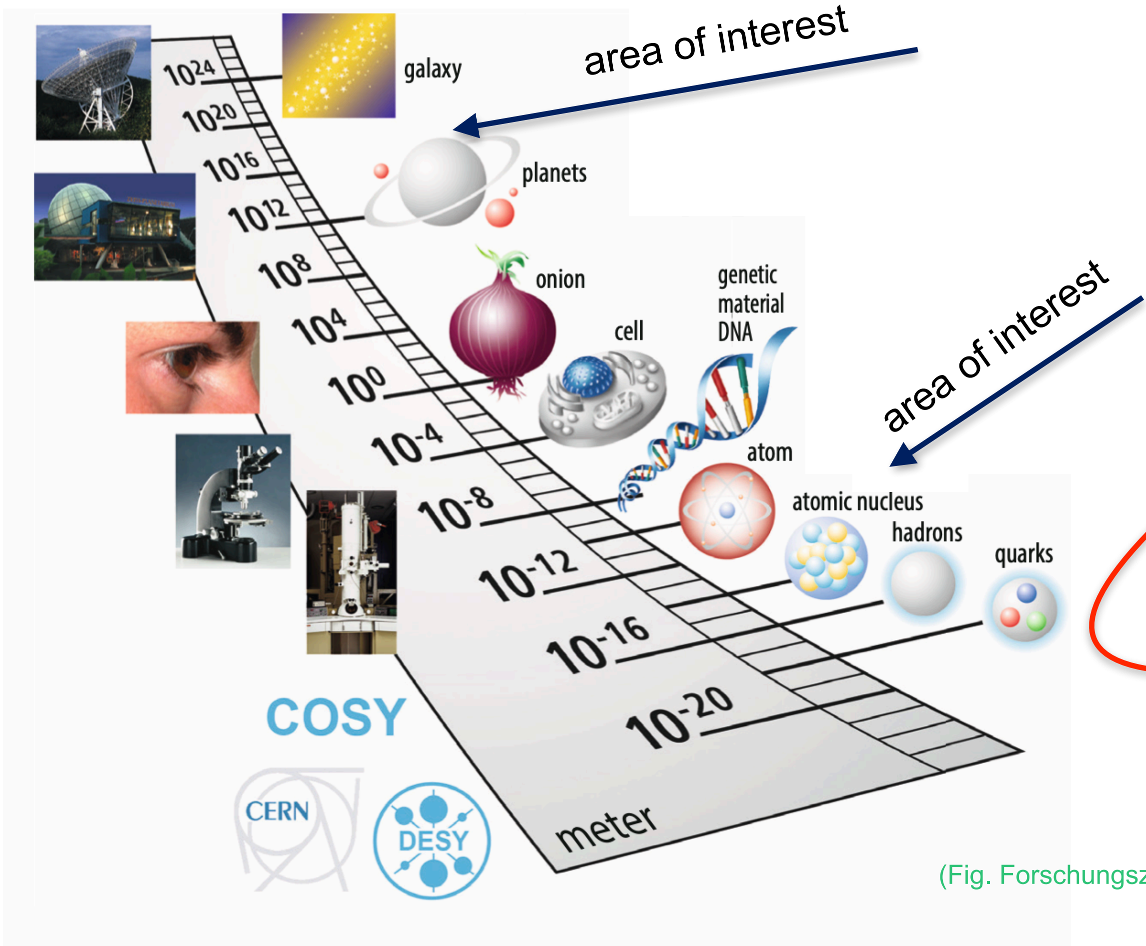
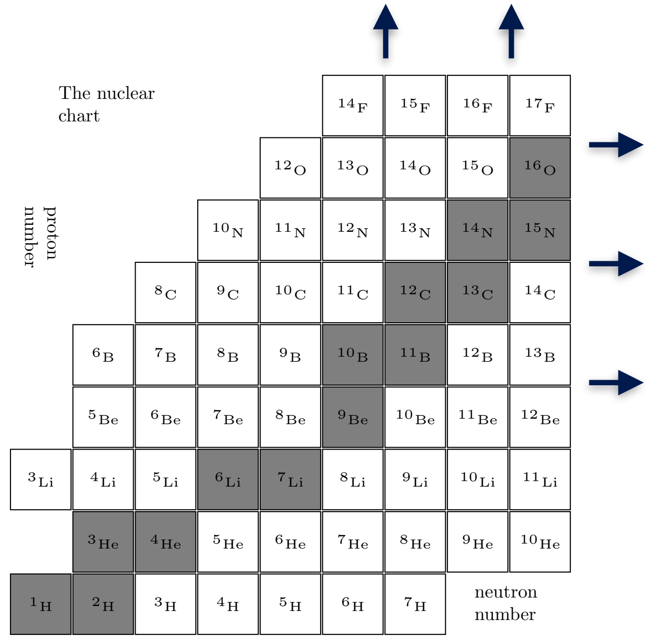
- Goal: understanding nuclear structure and reactions
  from small systems to stars



(Fig. Forschungszentrum Jülich)



Open questions:

- -Limits of stability
- -Three-body forces
- -Cluster structures
- -Neutron stars

- At different scales, there are different relevant degrees of freedom
- Resolution matters: exploit this separation of scales

Chiral Nuclear Effective Field Theory

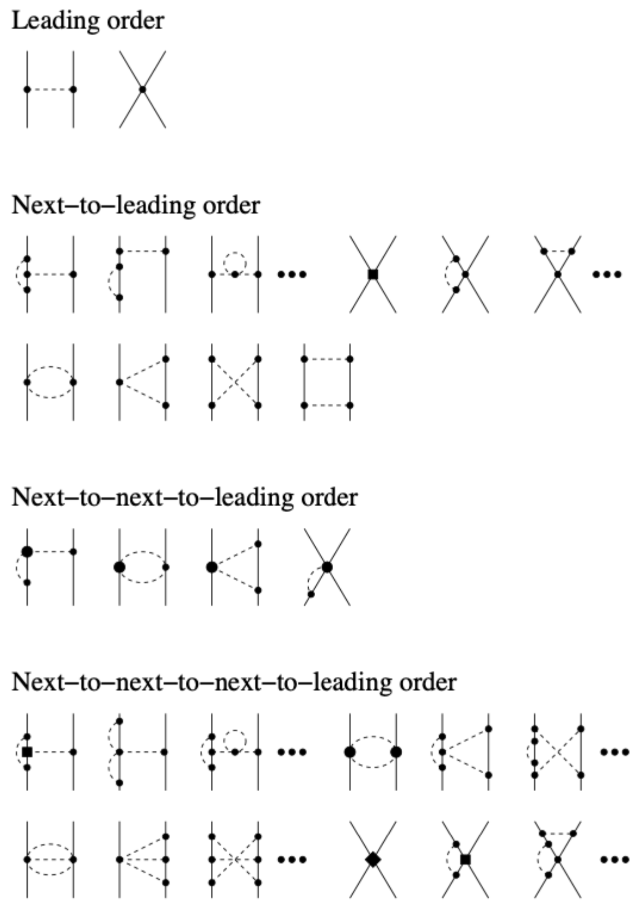
- Pick the correct scale : $\sim 10^{-15}\,\text{m} = 1$ fermi
- Pick the relevant degrees of freedom : protons and neutrons and pions

This is not Lattice QCD,
no quarks or gluons!

construct effective field theory

- Low energy chiral effective field theory of QCD
  - No model, systematic improvement is possible due to a hierarchy of forces
  - Systematic error analysis possible
  - Typical nuclear systems are far away from breakdown scale

combine with lattice methods



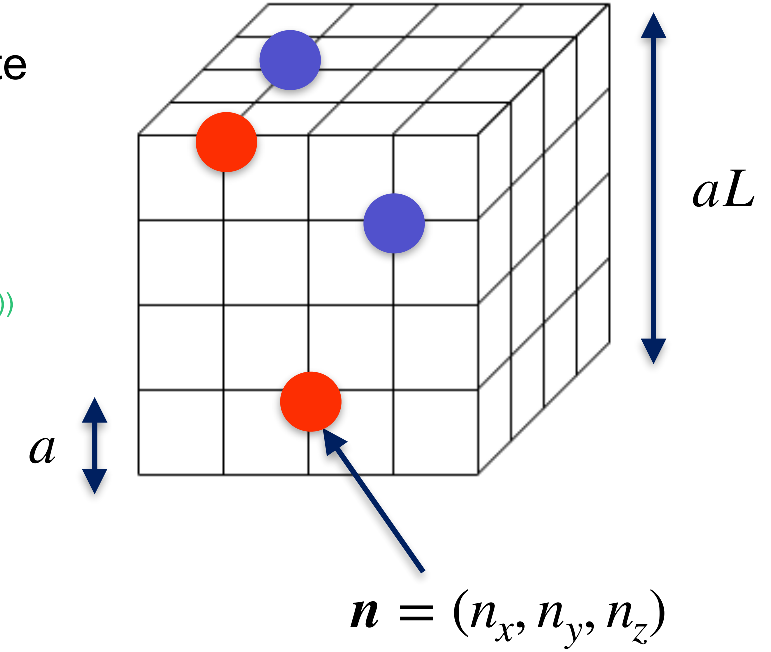
(Epelbaum et al. RevModPhys.81.1773 (2008))

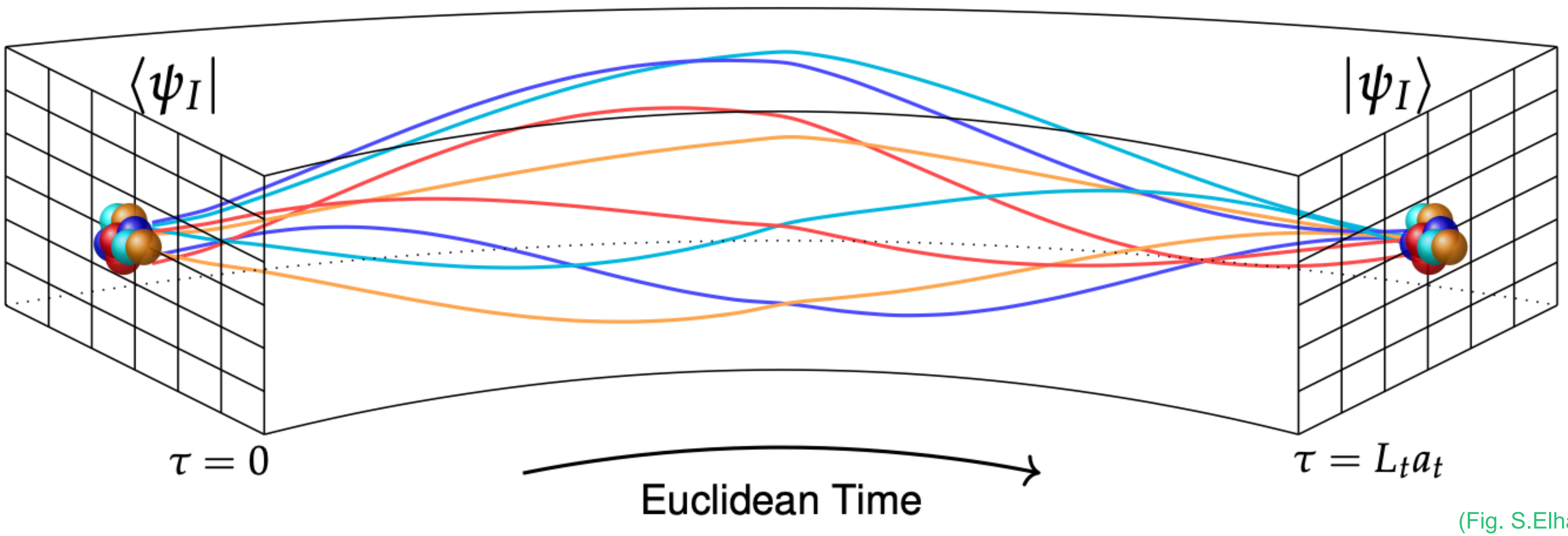
Method: Lattice Monte Carlo

- Lattice $\Rightarrow$ cubic volume of size $(La)^3$ with discrete lattice site

- Discretised chiral potentials, contact interactions one-pion exchange, Coulomb (Epelbaum et al. RevModPhys. 81.1773 (2008))

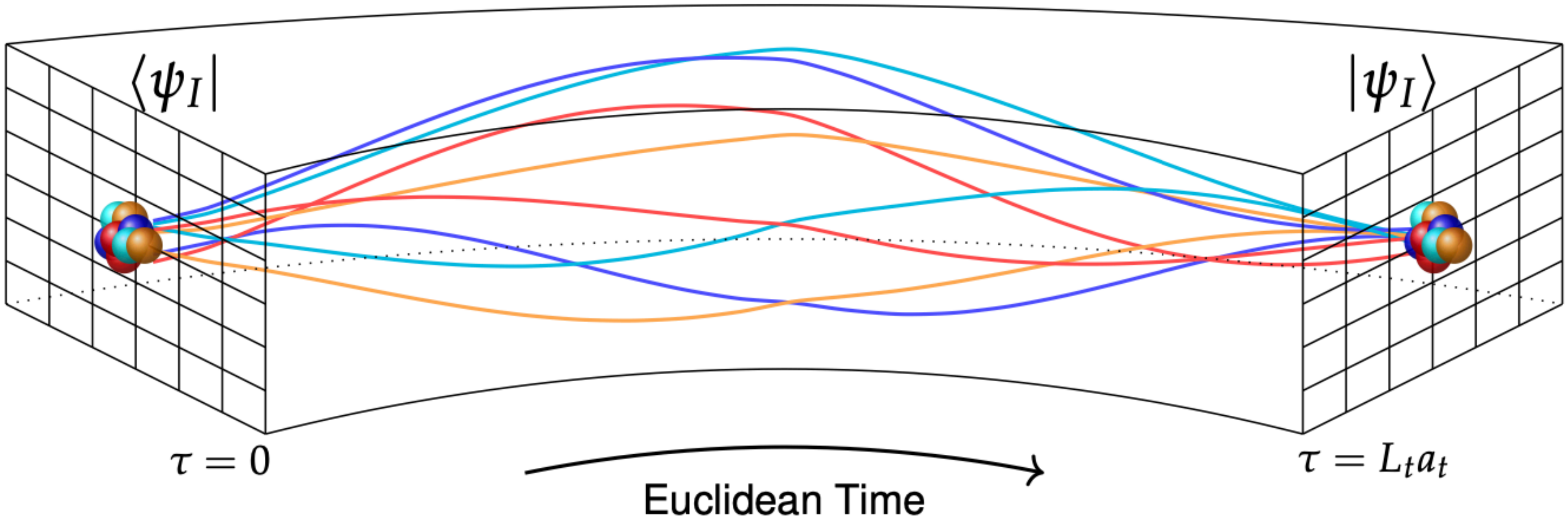
- Do Euclidean time evolution and extract i.e. energies as transient energy $E = -\frac{d}{d\tau} \ln(Z(\tau))$





(Fig. S.Elhatisari)

Method: Lattice Monte Carlo II



(Fig. S.Elhatisari)

- Auxiliary fields to handle many particles efficiently:
- Idea: replace interactions between nucleons with interaction of a nucleon with an auxiliary field

$$\exp(-\frac{C}{2}(N^\dagger N)^2) = \sqrt{\frac{1}{2}}\int \mathrm{d}A \exp\left[-\frac{A^2}{2} + \sqrt{C}A(N^\dagger N)\right]$$

Since nucleons only interact with an auxiliary field⇒ perfect for parallel computing

The Challenge : Sign Problem

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- Sign problem in a nutshell : makes life hard!

fermonic wave functions change sign when two fermions are interchanged. The systems are strongly interacting → highly oscillatory function, huge cancellation effects

no reasonable computation at higher orders possible

- First way out: utilize approximate SU(4) Wigner symmetry

(E. Wigner Phys.Rev 51(1937))

treats protons and neutrons on equal footing → same particle with different quantum number isospin

↓

create SU(4) invariant interactions, calculations are almost sign free

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some aspects of nuclear structure are well described

(S. Shen et al. Nature Commun.14 (2023))

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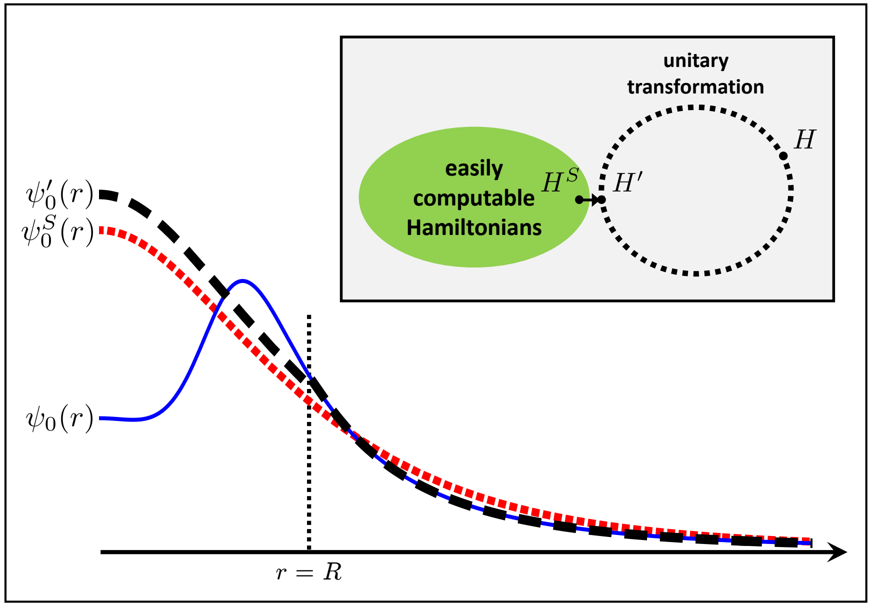
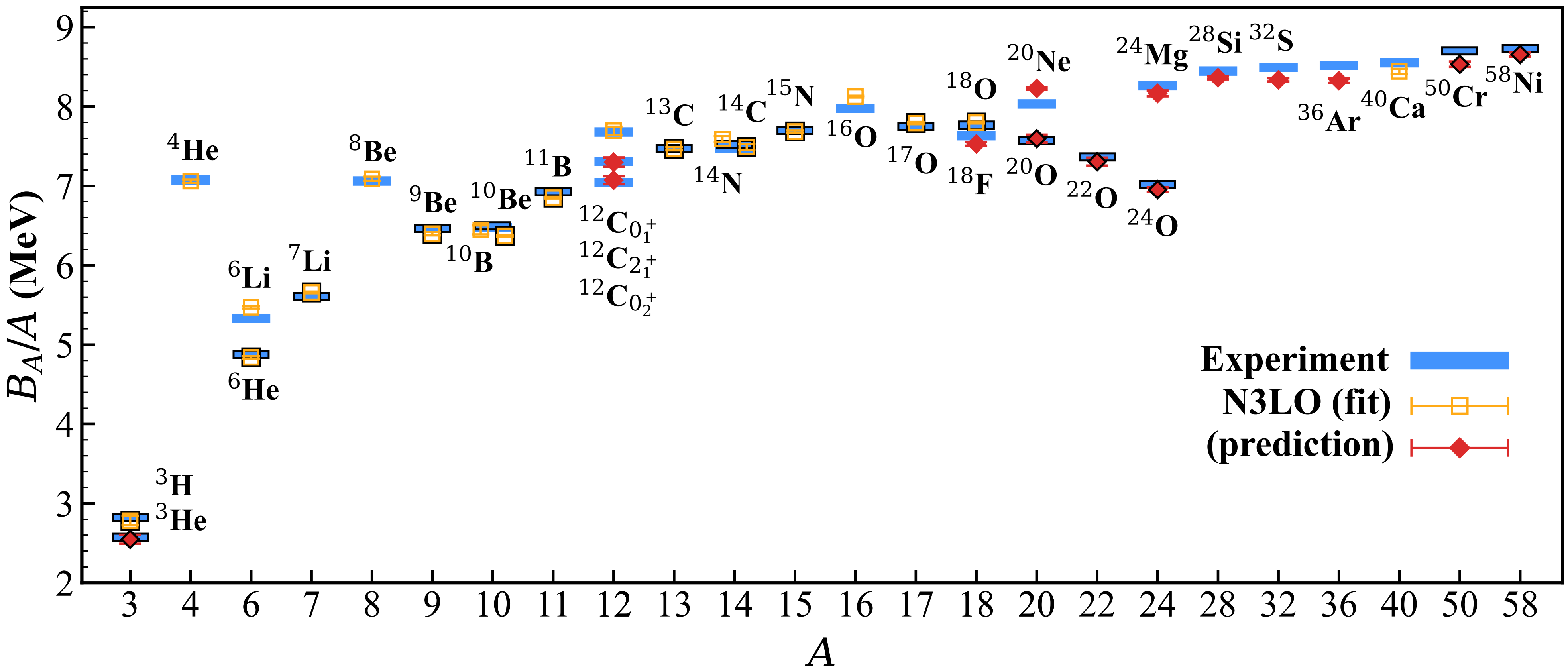
Solution: Wavefunction Matching

(S.Elhatisari,…,FH, et al. Nature 630(2024))



Binding Energy up to Medium Mass Nuclei

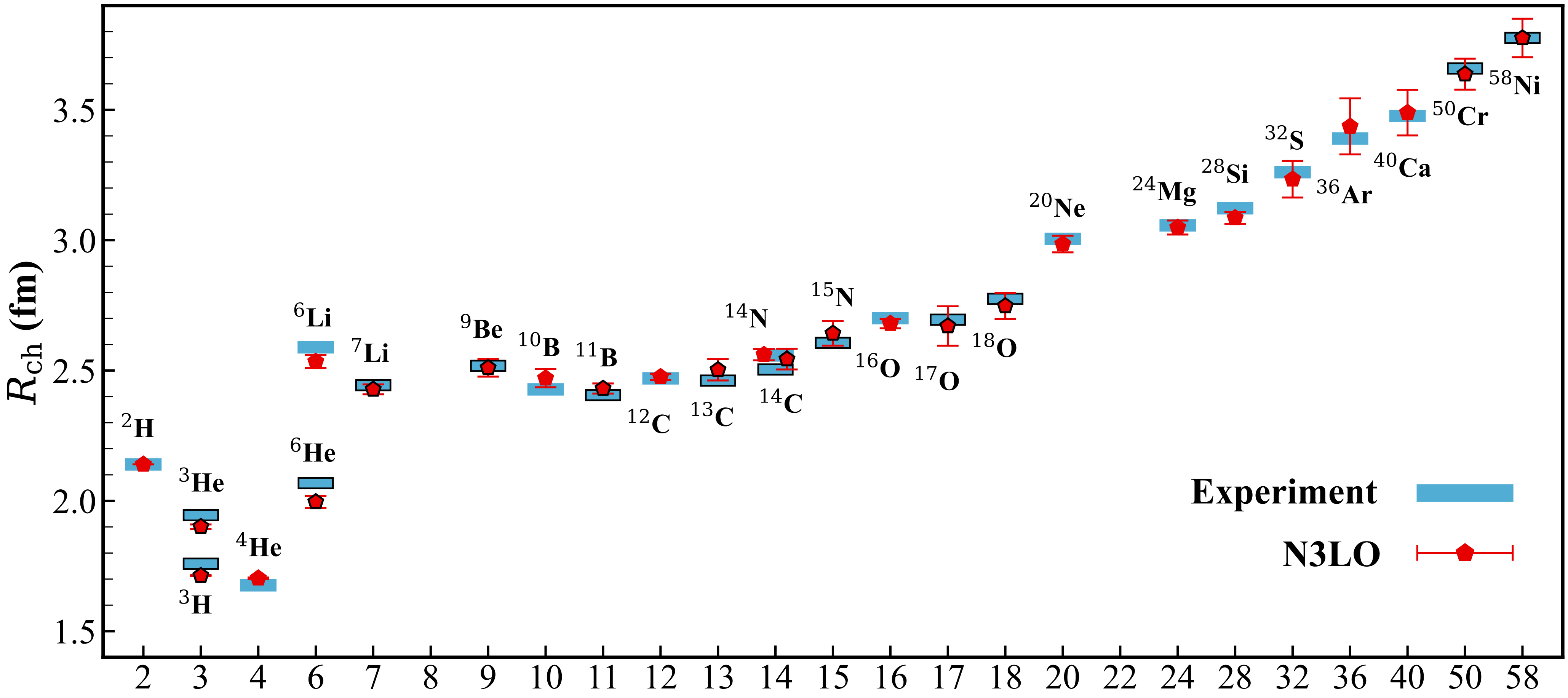
- Fix 3NF forces using history matching, systematic errors accessible
- Ground and exited states are well reproduced over a large excerpt of the nuclear chart
- $a = 1.32$ fm



(S.Elhatisari,…,FH, et al. Nature 630(2024))

Predictions for Charge Radii

- Charge radii are spot on!
- No fitting to charge radii, everything is a prediction!
- $a = 1.32$ fm, statistical errors can be reduced



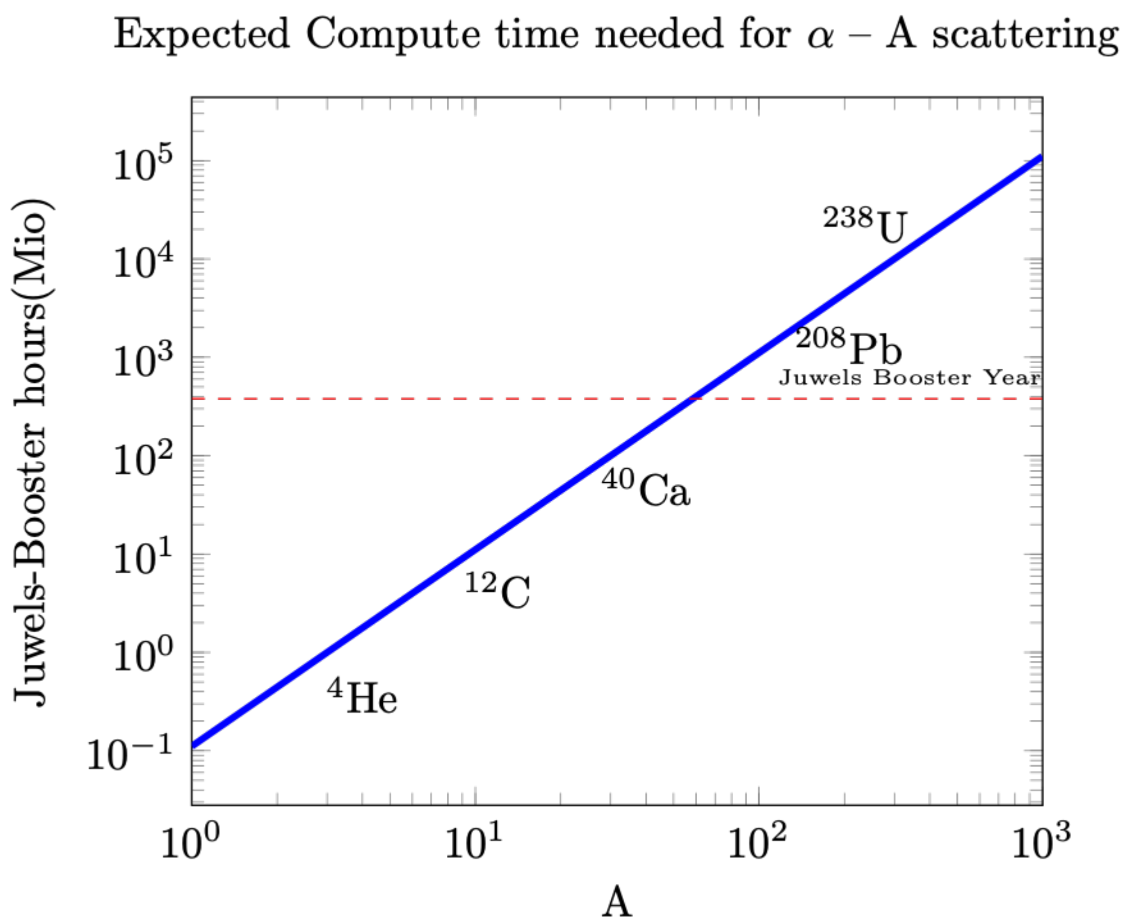
(S.Elhatisari,…,FH, et al. Nature 630(2024))

How does exascale change the game?

- JUWELS Booster (current Rank 48)
- Although not for structure calculation illustrates the scaling of the code
- Result shown before are years of allocations on machines all over the world
- NLEFT Code scales rather mildly with A

What changes with Exascale systems?

JUPITER(current Rank 4)



- ~ 15 times more compute
- Higher GPU Memory

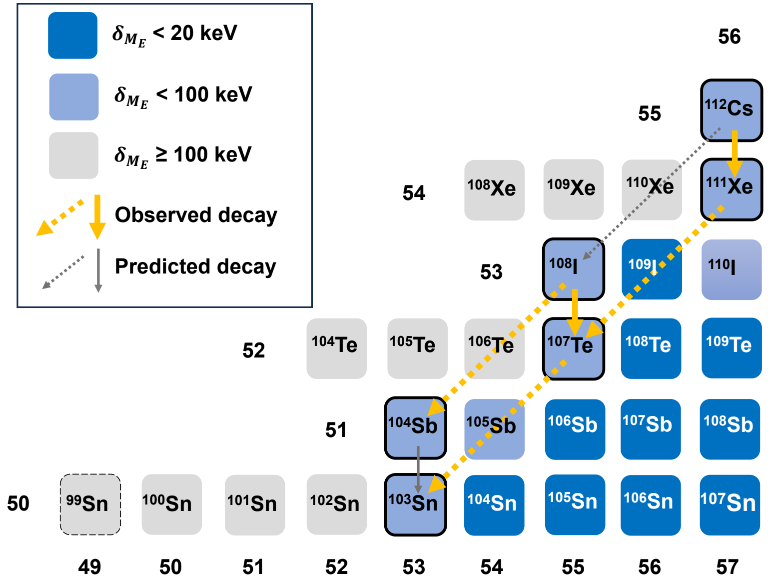
→

- More efficient sampling
- Rather Compute then memory bound now

→ Results about to show are $\sim$ 15 days of JUWELS Booster in pre-access time on JUPITER

Calculations around the proton dripline for Sn

- The tinline is a prime example to study to benchmark interactions to go to even heavier systems
- Even N=Z system hit/are close to the proton dripline
- Allows to study the dripline close to the ideal calculation region for NLEFT
- Finally within reach with the newest generation of supercomputers arriving at JSC
- Current efforts to pin down the dripline are based on extrapolation



(C.M. Ireland et al. PRC(2025) 111 014314)

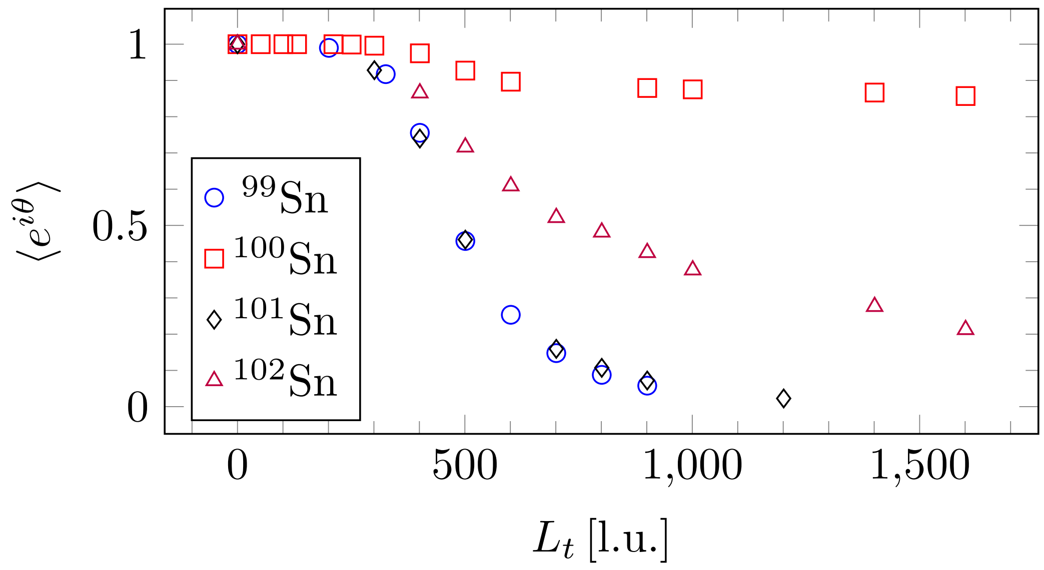
- Inconsistency between 2020 AME launched new experiments by ISOLTRAP and LEBIT

(L. Nies al. PRC (2025) 111, 014315)

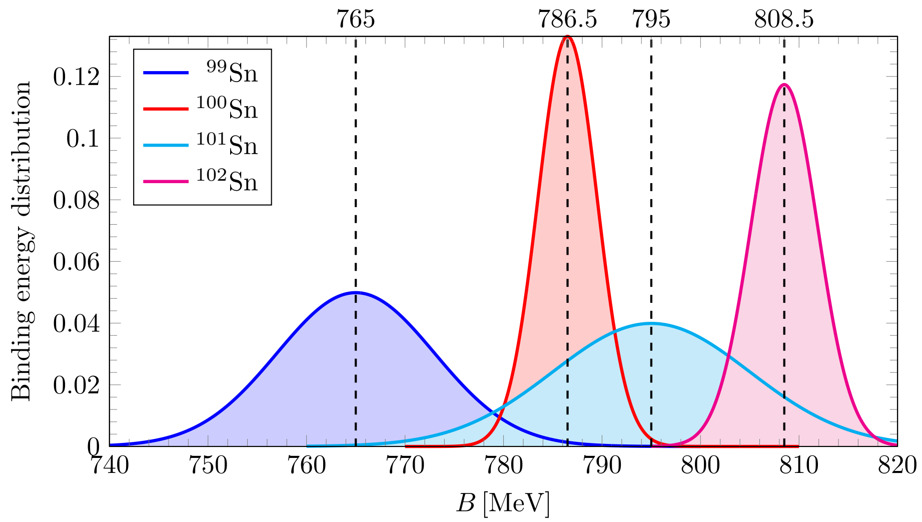
(C.M. Ireland et al. arxiv 2510.11815)

Calculations around the proton dripline for Sn

(FH et al. PRL 136 (2026) 6 065209)



- Phase drops quickly for odd nuclei
- Phase for even-even nuclei much more stable
- Expected small modifications to the three-body force needed to describe experimental data



Nucleus	N^3LO [24]	N^3LO^*	Exp.
^{99}Sn	765 ± 8	804 ± 8	807.9 ± 0.6
^{100}Sn	786.5 ± 3.0	825.2 ± 3.0	825.16 ± 0.24
^{101}Sn	795 ± 10	834 ± 10	836.39 ± 0.30
^{102}Sn	808.5 ± 3.4	848.1 ± 3.4	849.09 ± 0.10

Calculations around the proton dripline for Sn

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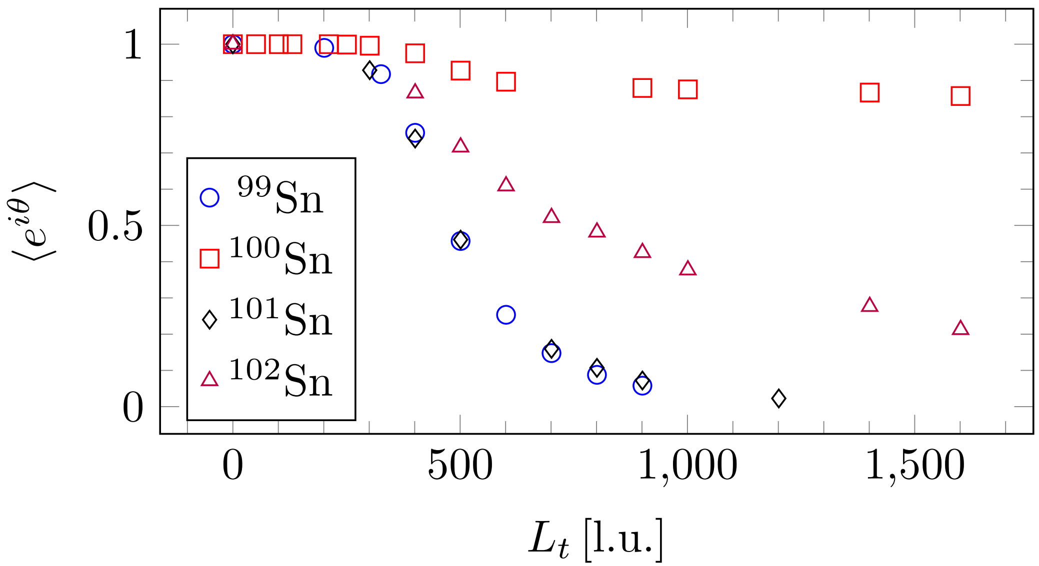

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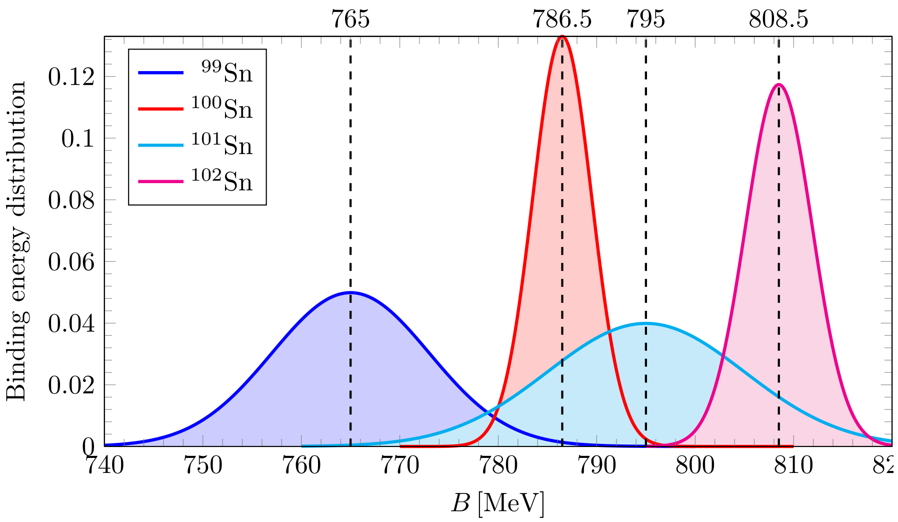
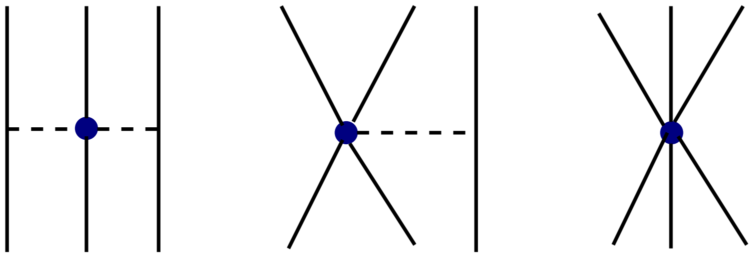


Isotopes	N^3LO	N^3LO*	Exp.
102-101	13.5 ± 10.6	14.1 ± 10.6	12.7 ± 0.3
102-100*	22.5 ± 4.6	22.9 ± 4.6	23.9 ± 0.3
102-99	43.5 ± 8.7	44.1 ± 8.7	41.2 ± 0.6
101-100	8.5 ± 10.4	8.9 ± 10.4	11.2 ± 0.4
101-99*	30.0 ± 12.8	30.1 ± 12.8	28.5 ± 0.7
100-99	21.5 ± 8.6	21.2 ± 8.6	17.3 ± 0.7

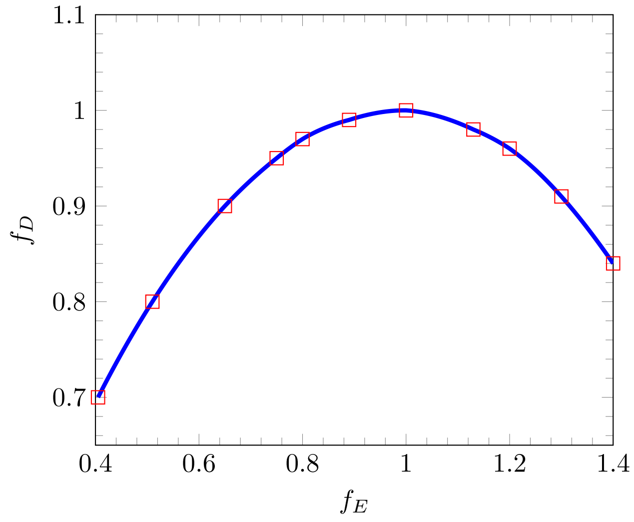
More on Three-body forces: Triton-beta-decay

(Elhatisari, FH, Meißner *PLB* 859 (2024)139086)

- Typical input to three-body forces in other approaches
- Exact full non-perturbative (two-body and three-body) GPU Lanczos calculation



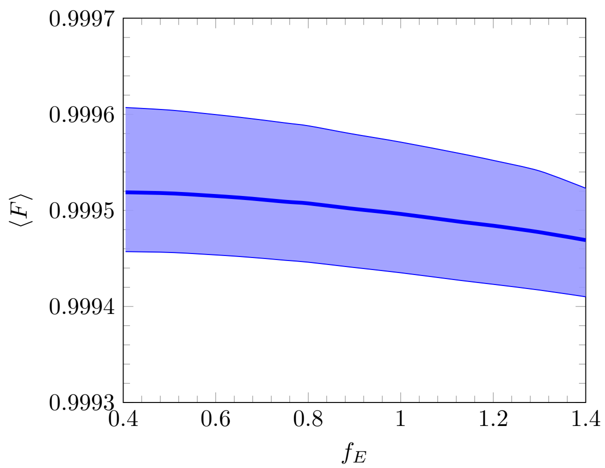
Curve of constant binding energy

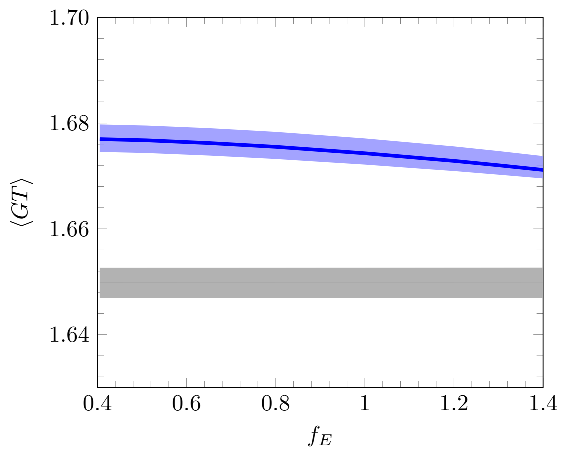


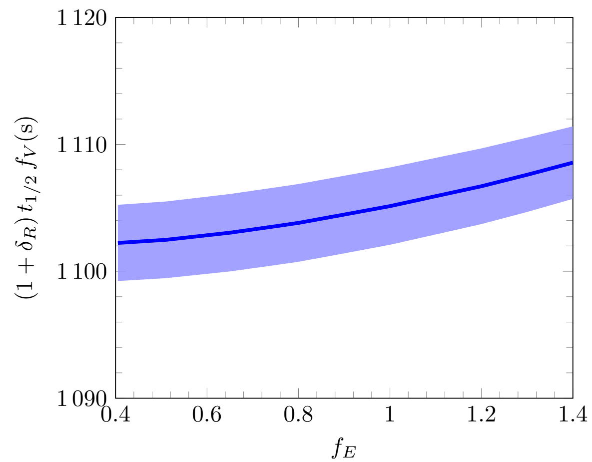
$$\langle F \rangle = \sum_{n=1}^{3} \langle {}^3\mathrm{He} \| \tau_{n,+} \| {}^3\mathrm{H} \rangle = 0.9998$$

$$\langle GT \rangle = \sum_{n=1}^{3} \langle {}^3\mathrm{He} \,||\, \sigma_n \tau_{n,+} \,||\, {}^3\mathrm{H} \rangle = 1.6497(23)$$

$$(1+\delta_R)\, t_{1/2}\, f_V = 1132.1(25)s$$







- First step to study β decay in the framework of NLEFT

Further NLEFT Study:

(T Wang et al. RRC 112 (2025) 2, 025502)

Summary

- Introduced Nuclear Lattice Effective Field Theory
  - Relevant degrees of freedoms are neutrons and protons
  - Combine effective field theory with lattice methods
- Showed first results for the heavy mass region
  - Slight modifications of three-body forces needed
  - Within the uncertainties we can extract ground state properties and separation Energies
  - Can confirm the shell closure at N=50
- Presented first application of β-decay in NLEFT
  - Full non-perturbative calculation
  - Allows consistent extraction of the Fermi and Gamow-Teller matrix elements

What is next?

- Calculations near the proton dripline
    - Structure Calculations, e.g. charge radii for the Sn Isotopes
    - Need significant more compute ~ factor 10-20, but within reach with JUPITER
- Improvement of the nuclear interaction
    - Refinement of three-body forces
    - Explicit inclusion of two-pion-exchange forces
    - Inclusion of consistent currents at N3LO accuracy