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In collaboration with Serdar Elhatisari, Ulf-G. Meißner, NLEFT and JSC

Outline

- Motivation
 - ▶ Introduction to NLEFT
 - ▶ Wavefunction Matching
 - ▶ Calculations near the Sn Dripline
 - ▶ Extension to Hypernuclei
- Summary

-
- The diagram illustrates the vast range of scales in physics, from the smallest particles to the largest structures in the universe. The logarithmic scale ranges from 10^{-20} to 10^{24} meters. Key features include:
- Scale Labels:** 10^{24} , 10^{20} , 10^{16} , 10^{12} , 10^8 , 10^4 , 10^0 , 10^{-4} , 10^{-8} , 10^{-12} , 10^{-16} , 10^{-20} , meter.
 - Objects and Phenomena:**
 - Galaxy:** Represented by a yellow starry field at 10^{24} m.
 - Planets:** Represented by a large grey sphere with a ring at 10^{16} m.
 - Onion:** Represented by a purple onion at 10^0 m.
 - Cell:** Represented by a grey cell with a blue nucleus at 10^{-4} m.
 - Genetic material DNA:** Represented by a blue double helix at 10^{-8} m.
 - Atom:** Represented by a red sphere with a blue nucleus at 10^{-10} m.
 - Atomic nucleus:** Represented by a cluster of blue and yellow spheres at 10^{-14} m.
 - Hadrons:** Represented by a grey sphere at 10^{-16} m.
 - Quarks:** Represented by three small colored spheres (red, blue, green) at 10^{-18} m.
 - Area of Interest:** Two blue arrows point to the top and bottom of the scale, indicating the range of scales covered by the research.
 - Left Side Images:** A series of images connected by lines to the scale, showing the progression from large-scale astronomy (radio telescope, building) to human vision (eye) and then to microscopic scales (microscopes).
 - Logos:** COSY, CERN, and DESY logos are displayed at the bottom left.

The nuclear chart

proton number

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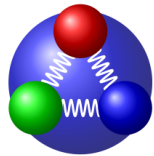
- Limits of stability
- Three-body forces
- Cluster structures
- Neutron stars

- Mitglied der Helmholtz-Gemeinschaft

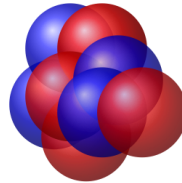
Dominant interactions at different scales



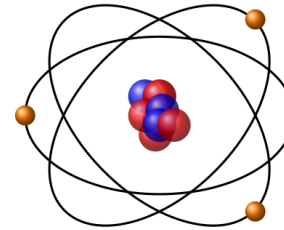
Quarks
 $< 10^{-16}$



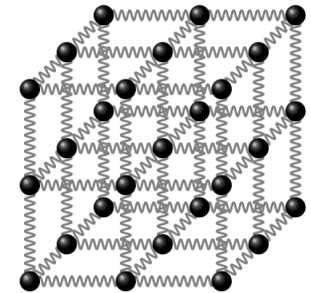
Nucleons
 $\sim 10^{-13}$



Nucleus
 $\sim 10^{-12}$



Atoms
 $\sim 10^{-8}$ cm



Matter

(Fig. S.Elhatisari)



strong force



nuclear force



electromagnetic force
sometimes gravity

Utilize this separation! There is no need to consider things that are not relevant at a specific scale

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

*This is not Lattice QCD,
no quarks or gluons!*

construct effective field
theory

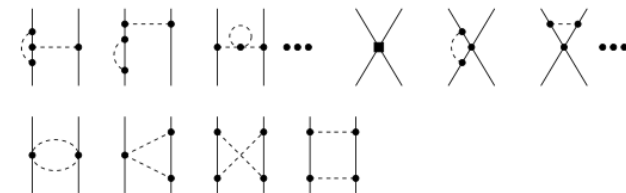
- Low energy chiral effective field theory of QCD
 - No model, systematic improvement is possible due to a hierarchy of forces
 - Systematic error analysis possible
 - Typical nuclear systems are far away from breakdown scale

combine with lattice
methods

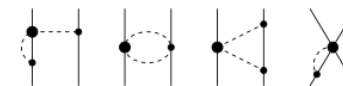
Leading order



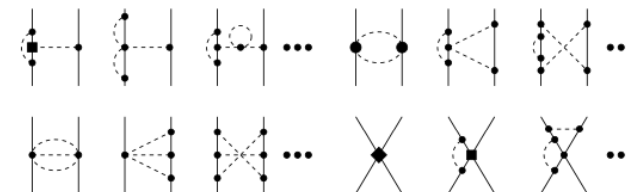
Next-to-leading order



Next-to-next-to-leading order



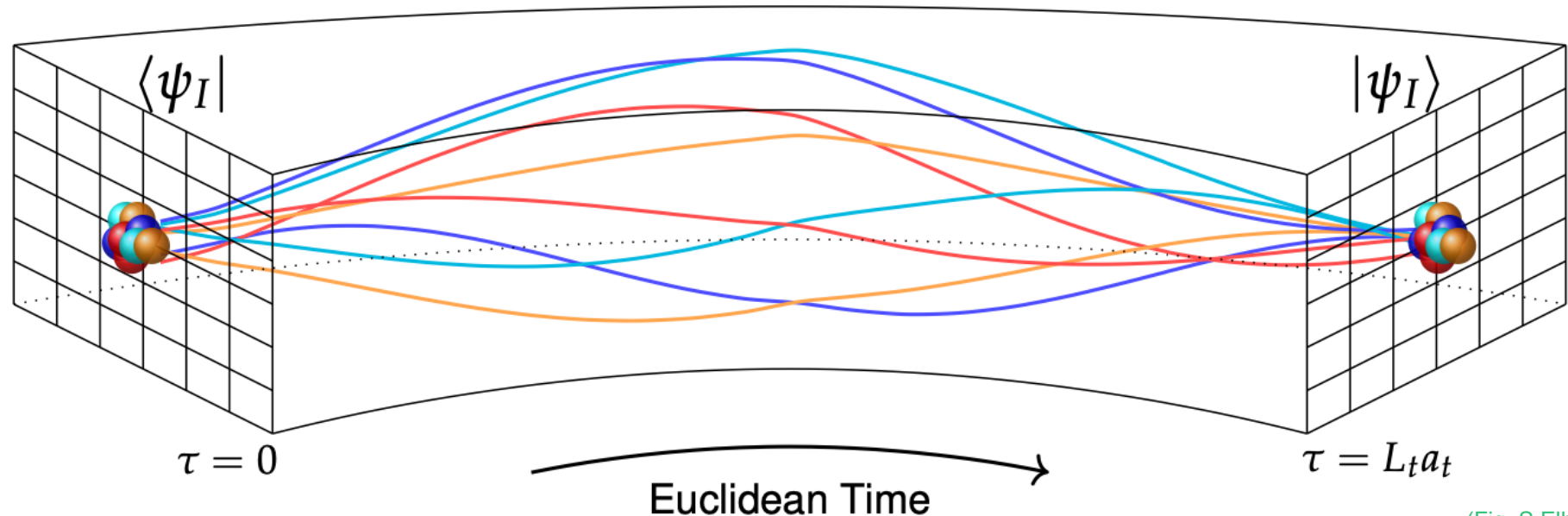
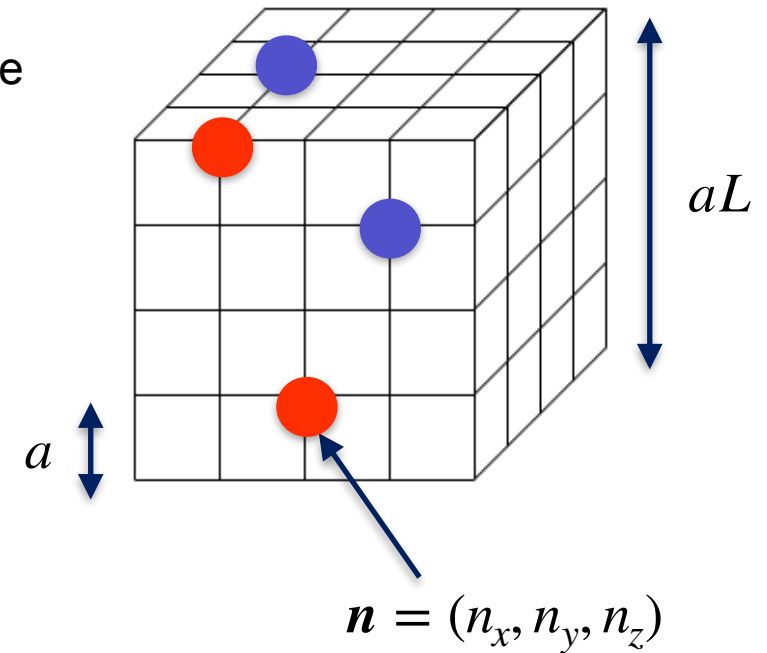
Next-to-next-to-next-to-leading order



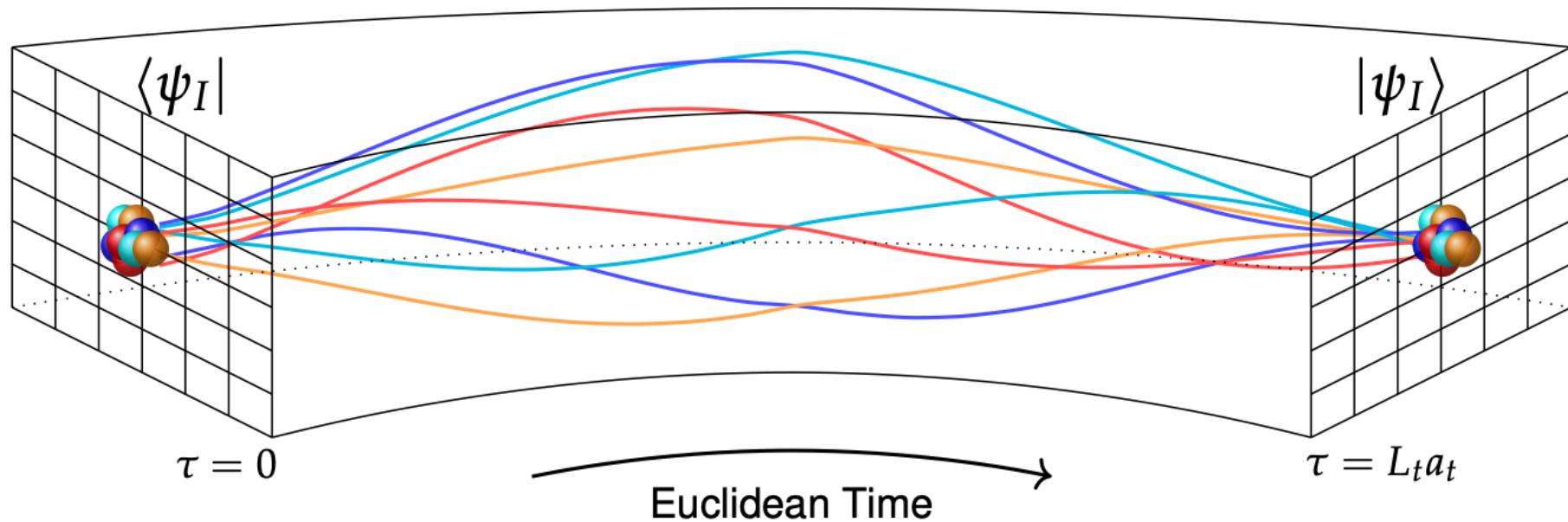
(Epelbaum et al. RevModPhys.81.1773)

Method: Lattice Monte Carlo

- Lattice $\Rightarrow$ cubic volume of size $(La)^3$ with discrete lattice site
- Discretized chiral potentials, contact interactions
one-pion exchange, Coulomb (Epelbaum et al.)
- Do Euclidean time evolution and extract i.e. energies
as transient energy $E = -\frac{d}{d\tau} \ln(Z(\tau))$



(Fig. S.Elhatisari)



(Fig. S.Elhatisari)

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

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

Since nucleons only interact with an auxiliary field $\Rightarrow$ perfect for parallel computing

The Challenge : Sign Problem

- Sign problem in a nutshell : makes life hard!

fermionic 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



*some aspects of
nuclear structure are
well described*

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

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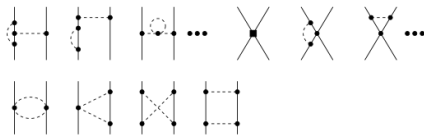
same particle with different quantum number isospin

but we want and need:

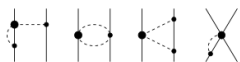
Leading order



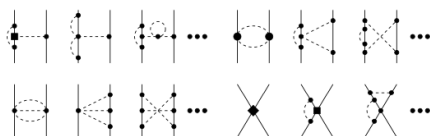
Next-to-leading order



Next-to-next-to-leading order



Next-to-next-to-next-to-leading order



Need improved perturbation theory to go beyond N2LO



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



some aspects of nuclear structure are well described

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

Wavefunction Matching!

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

- New method to solve the quantum many-body problem
- In principle applicable in many different fields

starting point : H_S which has acceptable sign problem and can be simulated

How to connect?

target : H which has a severe sign problem

lowest eigenstate $|\psi_s^0\rangle$

projected and normalised :

$$|\phi_s^0\rangle = \mathcal{P}|\psi_s^0\rangle / ||\psi_s^0||$$

map $|\psi_s^0\rangle$ on $|\psi^0\rangle$

lowest eigenstate $|\psi^0\rangle$

projected and normalised :

$$|\phi^0\rangle = \mathcal{P}|\psi^0\rangle / ||\psi^0||$$

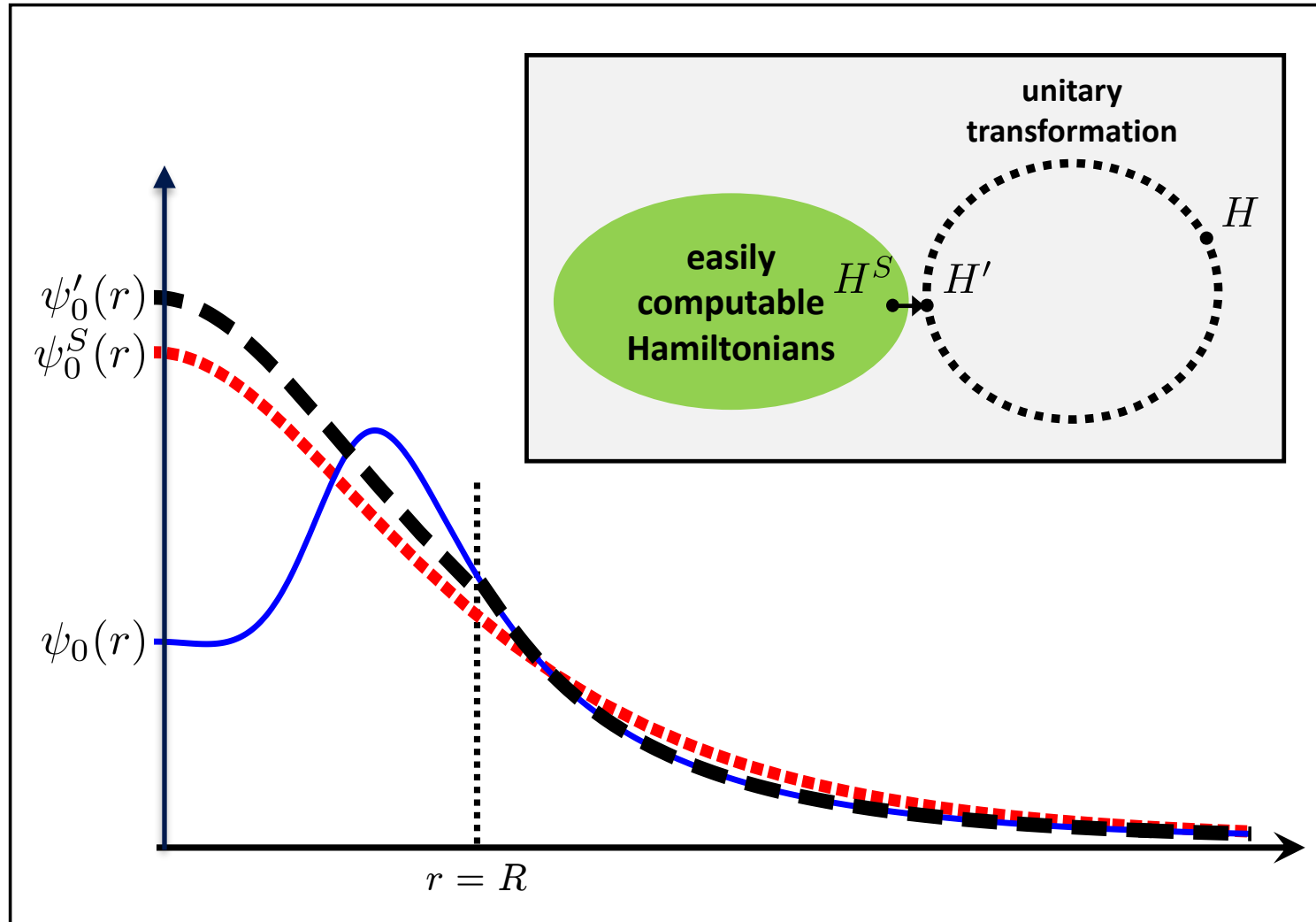
$$U = \begin{cases} 1 & r > R \\ |\phi^\perp\rangle\langle\phi_s^\perp| & r < R \end{cases}$$

Unitary trafo with finite range

$$H' = U^\dagger H U$$

perturbation theory now works from H_S to H'

Wavefunction Matching II !



- Use H^S for non-perturbative part and do perturbation theory to H'
- Direct use of H' , no reconstruction of higher order forces needed!

This is not a
renormalization group
transformation

How does exascale change the game?

- JUWELS Booster (current Rank 58)
- Although not for structure calculation illustrates the scaling of the code
- NLEFT Code scales rather mildly with A
What changes with Exascale systems?



JUPITER(current Rank 5)

- ~ 15 times more compute

- Higher GPU Memory

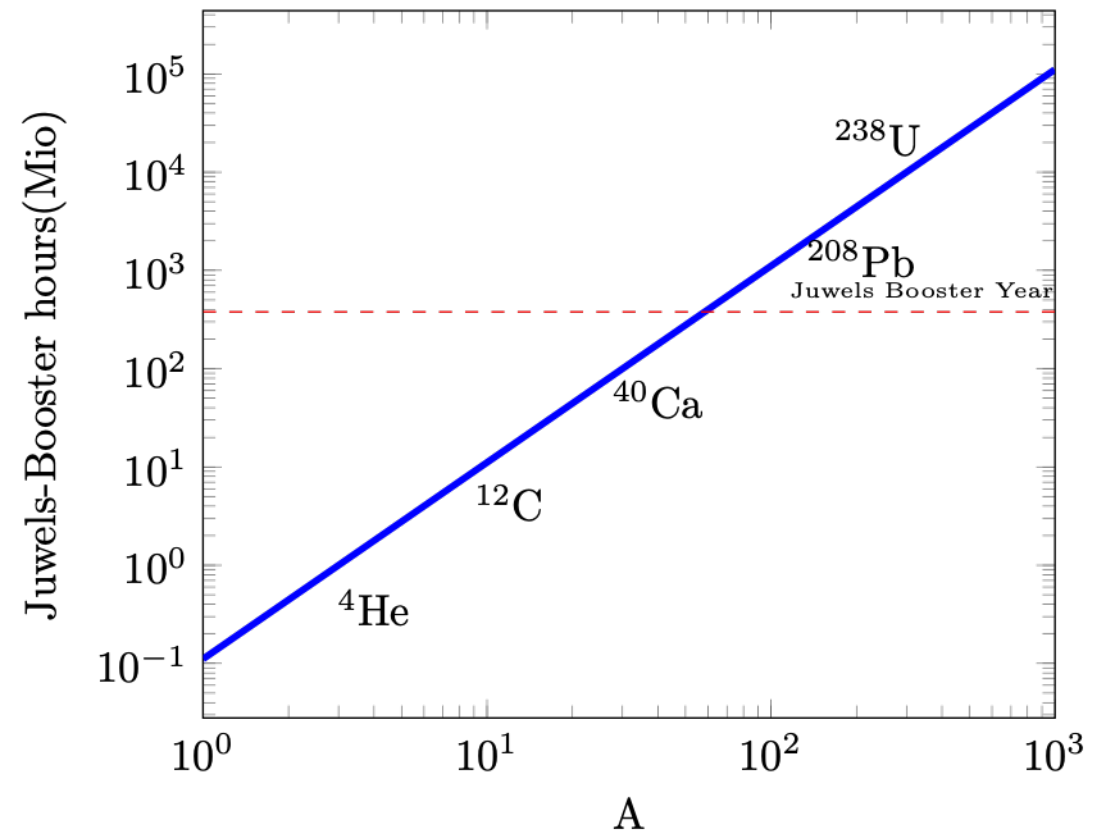


- More efficient sampling
- Rather Compute then memory bound now



Results about to show are ~ 15 days of JUWELS Booster
in pre-access time on JUPITER

Expected Compute time needed for $\alpha - A$ scattering



- Expectation values of observables $\mathcal{O}$ in path integral formalism

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}\mathcal{O} e^{-S_E[s]}$$

Euclidean action

- However the fermion determinant $\det M$ is in general not positive definite. Hence, we use in practice:

$$\langle \mathcal{O} \rangle \approx \frac{\sum_{\{s\}} e^{i\theta[s]} \mathcal{O} e^{-\tilde{S}_E[s]}}{\sum_{\{s\}} e^{i\theta[s]} e^{-\tilde{S}_E[s]}}$$

- Where we define the complex phase to be

$$e^{i\theta[s]} = \frac{\det M}{|\det M|}$$



This is part of the observable



Indicator how bad the sign problem is

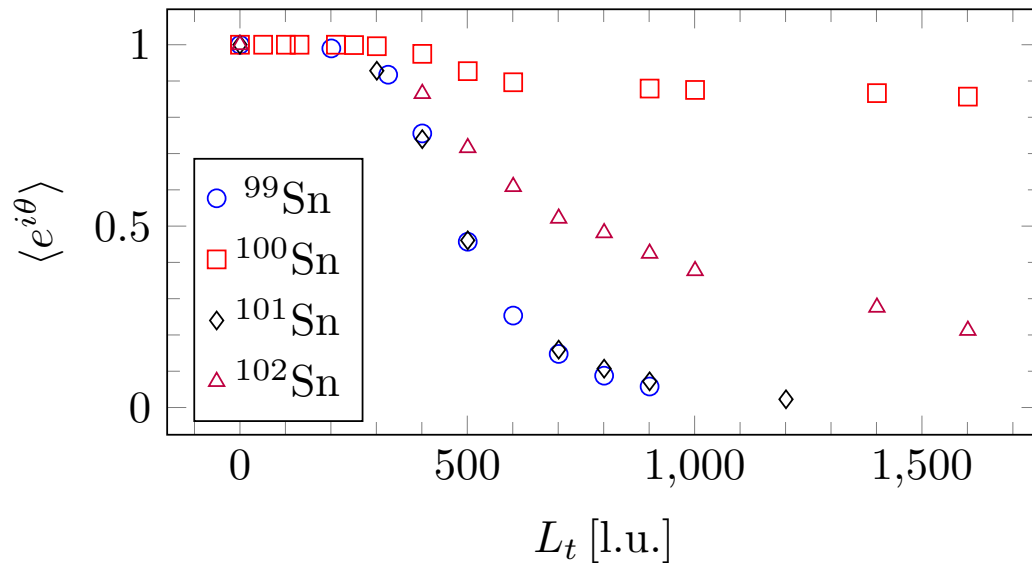
- The Tinline is a prime example to study to benchmark interactions to go to even heavier systems
- Even $N=Z$ system hit/are close to the proton dripline
- Allows to study the dripline close to the ideal calculation region for NLEFT
- Finally within reach with the newest generation of supercomputers arriving at JSC
- Inconsistency between 2020 AME launched new experiments by ISOLTRAP and LEBIT

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

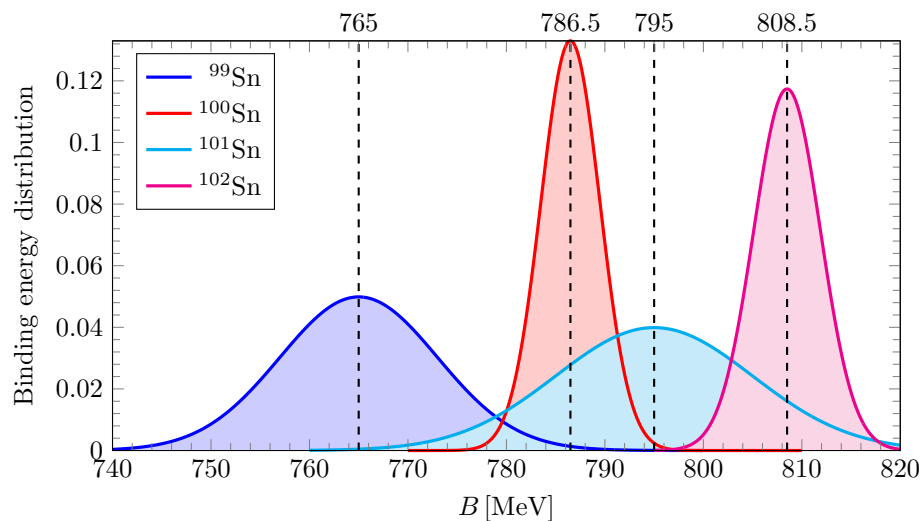
(C.M. Ireland et al. *Phys.Rev.C* 113 (2026) 2, L021302)
- Current experimental efforts to pin down the dripline are based on extrapolation

Calculations around the proton dripline at Sn=100

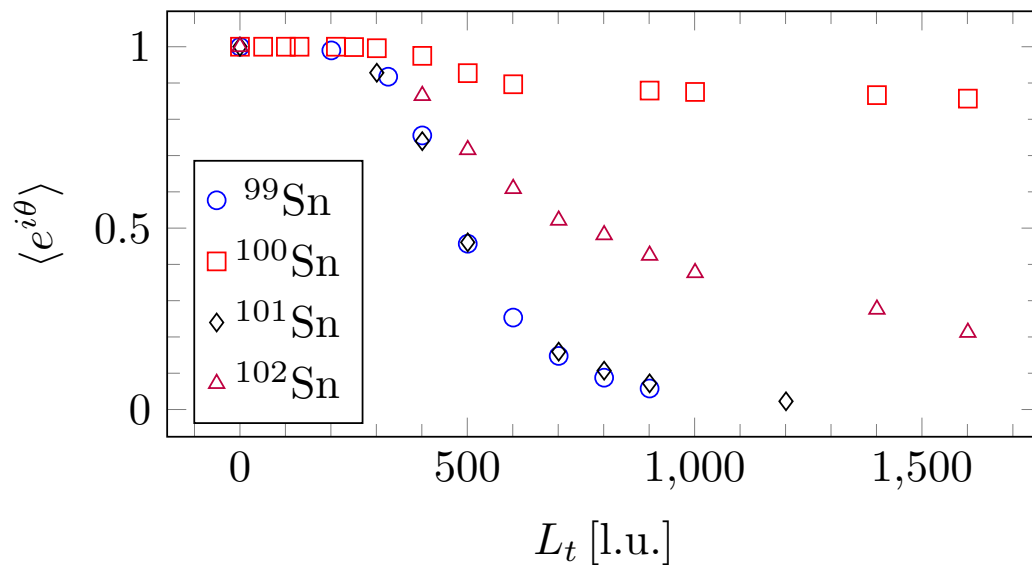
(FH et al. PRL 136 (2026) 6, 062501)



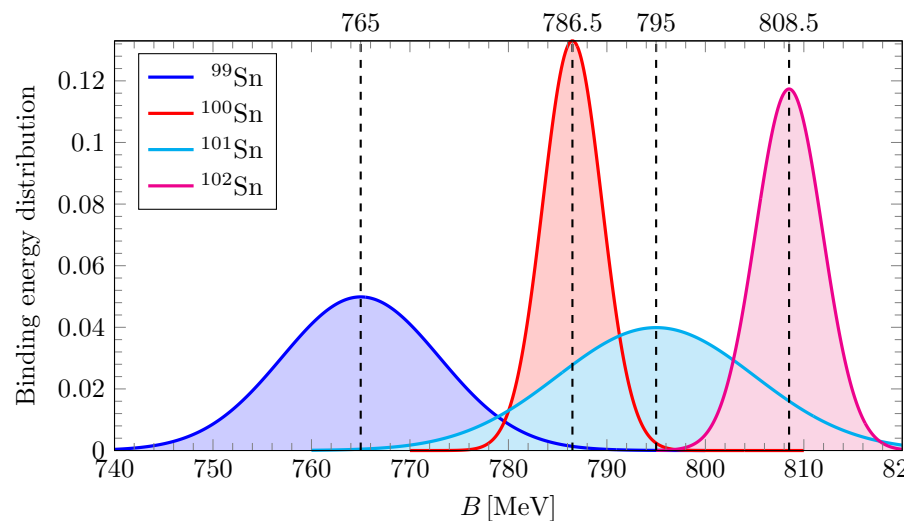
- Phase drops quickly for odd nuclei
- Phase for even-even nuclei much more stable
- Expected small modifications to the three-body force needed to describe experimental data



Nucleus	N ³ LO [24]	N ³ LO*	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

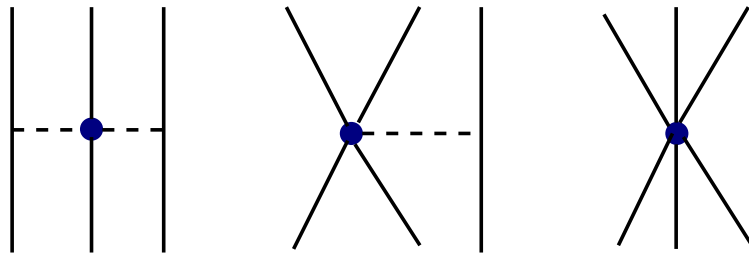


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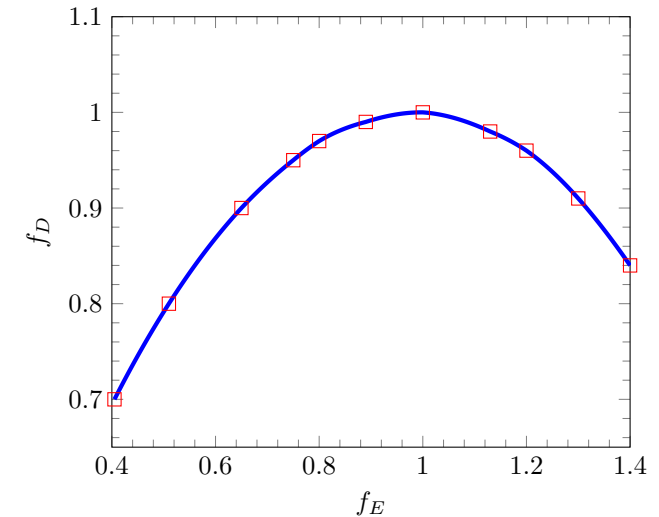


Isotopes	N ³ LO	N ³ LO*	Exp.
102-101	13.5 ± 10.6	14.1 ± 10.6	12.7 ± 0.3
102-100*	22.5 ± 4.6	22.9 ± 4.6	23.9 ± 0.3
102-99	43.5 ± 8.7	44.1 ± 8.7	41.2 ± 0.6
101-100	8.5 ± 10.4	8.9 ± 10.4	11.2 ± 0.4
101-99*	30.0 ± 12.8	30.1 ± 12.8	28.5 ± 0.7
100-99	21.5 ± 8.6	21.2 ± 8.6	17.3 ± 0.7

- Typical input to three-body forces in other approaches
- Exact full non-perturbative (two-body and three-body) GPU Lanczos calculation
- Does not rely on WFM, test ground beyond the two-body level



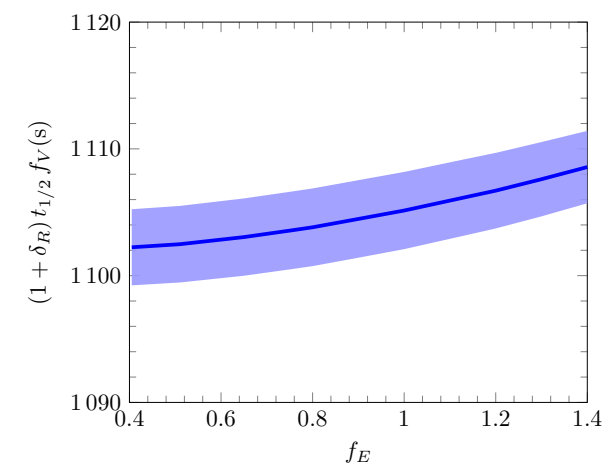
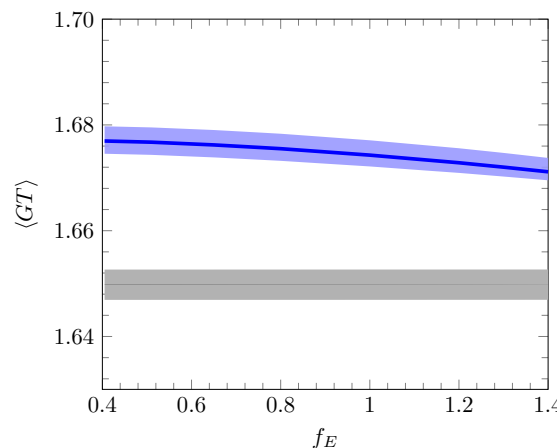
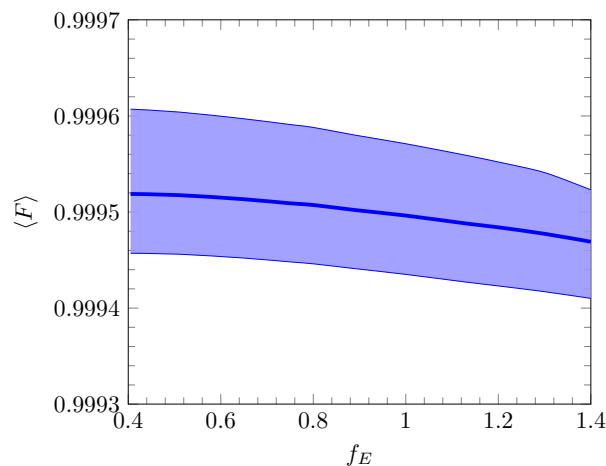
Curve of constant binding energy



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

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

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

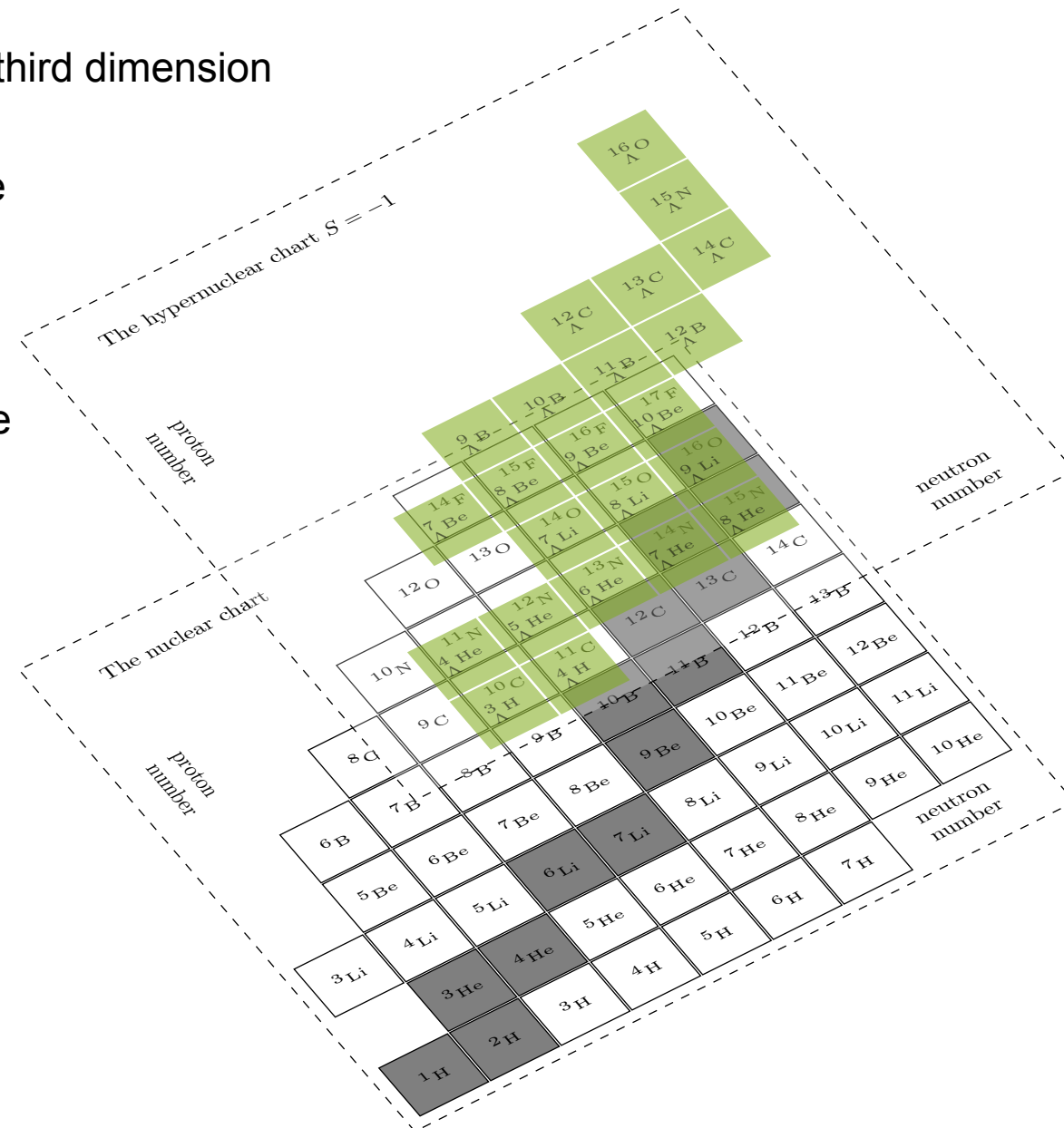
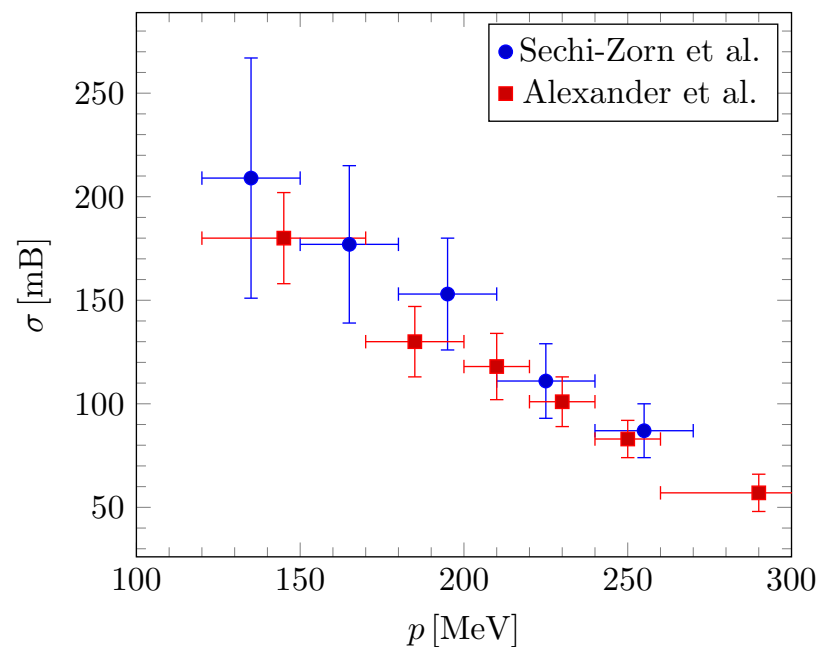


- First step to study β decay in the framework of NLEFT

Hypernuclear physics in a nutshell

- Strangeness extends the nuclear chart to a third dimension
- Unique opportunity to study the strong force
Without the Pauli principle
- Typical approach from nuclear physics
does not work since two-body data is sparse

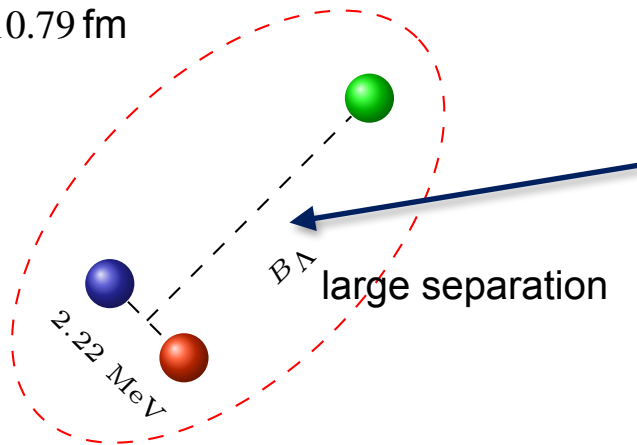
$$\Lambda p \rightarrow \Lambda p$$



- Gateway : **Three-Body Systems**

Construction of a first Lattice ΛN interaction

$$\sqrt{\langle r_{\Lambda d}^2 \rangle} \approx 10.79 \text{ fm}$$



Emulsion:

$$B_{\Lambda} = 0.130 \pm 0.050 \text{ MeV} \text{ Juric 1973}$$

Heavy Ion:

$$B_{\Lambda} = 0.406 \pm 0.120 \text{ MeV} \text{ Star 2020}$$

$$B_{\Lambda} = 0.102 \pm 0.063 \text{ MeV} \text{ Alice 2023}$$

World Average:

$$B_{\Lambda} = 0.113 \pm 0.029 \text{ MeV} \text{ Mainz 2025}$$

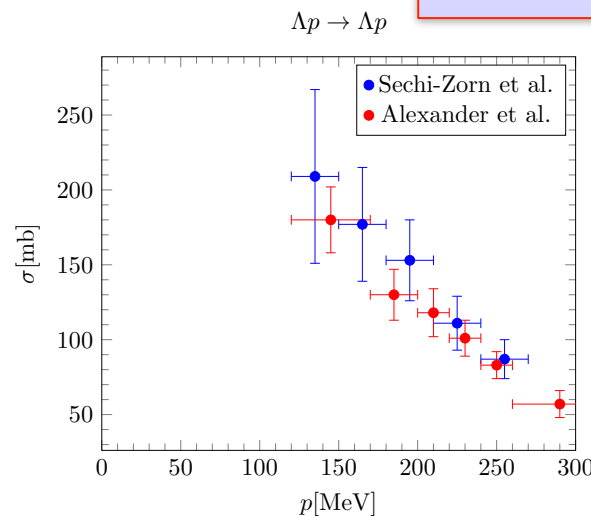
Shallow S-Wave State

$$J^P = \frac{1}{2}^+$$

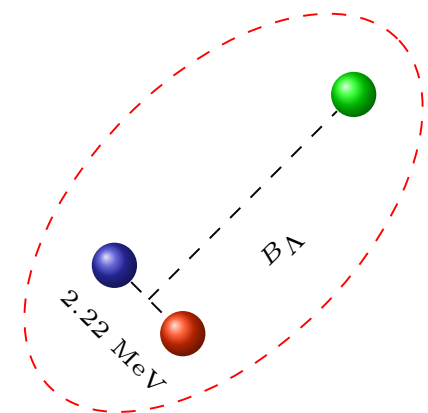
Distinguishable

$$I = 0 \Rightarrow \frac{1}{\sqrt{2}}(pn - np)\Lambda$$

Combine 2-Body data
with hypertriton in
exact calculation

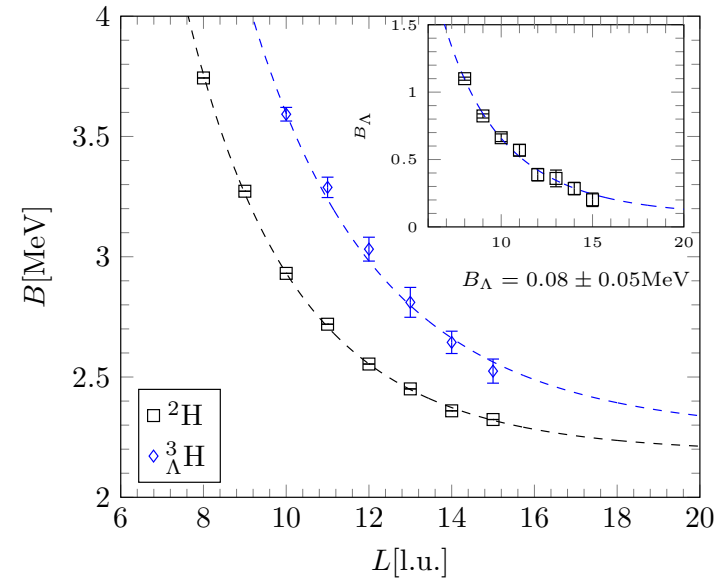
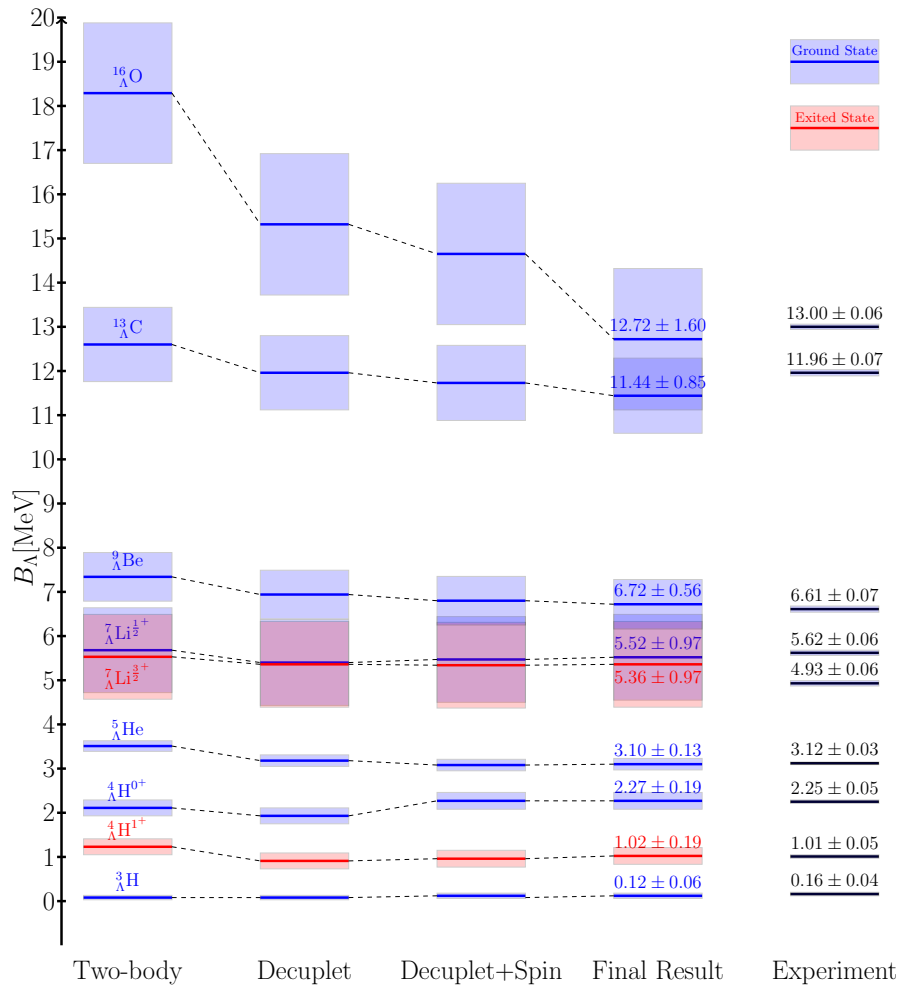


+



Results for hypernuclei

(FH et al., *Eur.Phys.J.A* 60 (2024) 10, 215)



Proper extrapolation:

$$B_\Lambda(^3_\Lambda\text{H}) = 0.08 \pm 0.05 \text{ MeV}$$

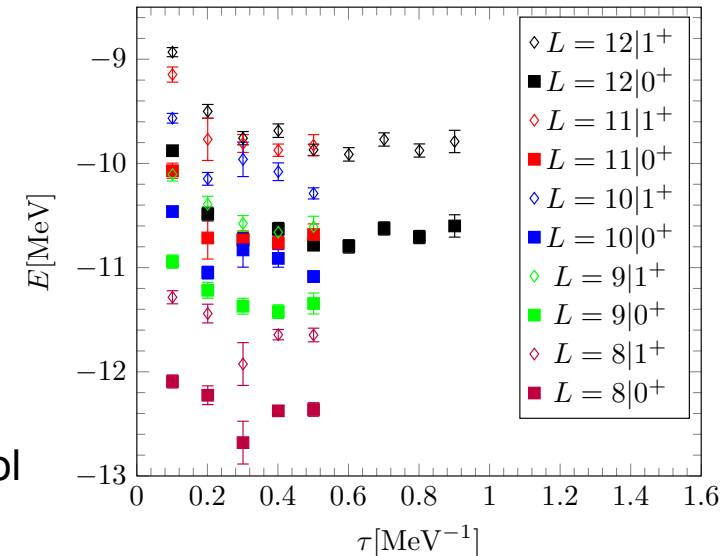
Experiment

$$0.113 \pm 0.029 \text{ MeV}$$

- Hypertriton has large Λ separation of $\sim 11 \text{ fm}$

$$V_{ct}^{\Lambda NN} = C_1(1 - \sigma_2 \cdot \sigma_3)(3 + \tau_2 \cdot \tau_3) + C_2\sigma_1 \cdot (\sigma_2 + \sigma_3)(1 - \tau_2 \cdot \tau_3) + C_3(3 + \sigma_2 \cdot \sigma_3)(1 - \tau_2 \cdot \tau_3)$$

Finite Box under control



- Introduced Nuclear Lattice Effective Field Theory
 - Relevant degrees of freedoms are neutrons and protons
 - Combine effective field theory with lattice methods
- Presented a new approach to solve the quantum many-body problem:
 - Wavefunction Matching
 - Makes a whole set of new calculations available
 - High precision consistent calculation of matter radii and binding energies
- Showed first results for the heavy mass region
- Presented an extension to the hypernuclear chart and results for light to medium mass hypernuclei

What is next?

- Improve the interaction in the hypernuclear sector
 - Typical problems go away by calculations beyond leading order
 - Inclusion of other hyperons
- Calculations near the proton dripline
 - Experimental extrapolations now available for $A=96-98$
 - Tin isotopes are typically studied from Cd and Indium isotopes
 - Structure Calculations, e.g. charge radii for the Sn Isotopes ~ is on the way
 - Need significant more compute ~ factor 10-20, but within reach with JUPITER
- Move to the neutron drip line
 - Tin isotopes are within reach for even isotopes, improvement on initial waves
 - Complementary study of super neutron rich calcium isotopes
- Improvement of the nuclear interaction
 - Refinement of three-body forces