Ab initio computations of atomic nuclei

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International School of Physics “Enrico Fermi”

Course 213 - Nuclear Structure and Reactions from a Broad Perspective

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Ricardo Broglia (1939-2022)

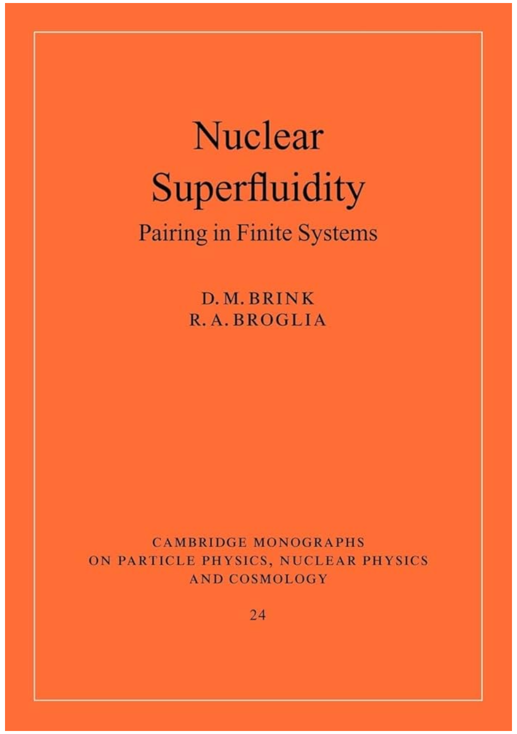
Physics Reports
Volume 30, Issue 4, May 1977, Pages 305-360

Nuclear field theory ☆

P.F. Bortignon **, R.A. Broglia [a b], D.R. Bes ****, R. Liotta

Pairing fluctuations in rapidly rotating nuclei

Y. R. Shimizu, J. D. Garrett, R. A. Broglia, M. Gallardo, and E. Vigezzi
Rev. Mod. Phys. **61**, 131 – Published 1 January 1989



These lectures builds on many insights from Ricardo Broglia.
His works and writings have been an inspiration.

Energy scales and relevant degrees of freedom

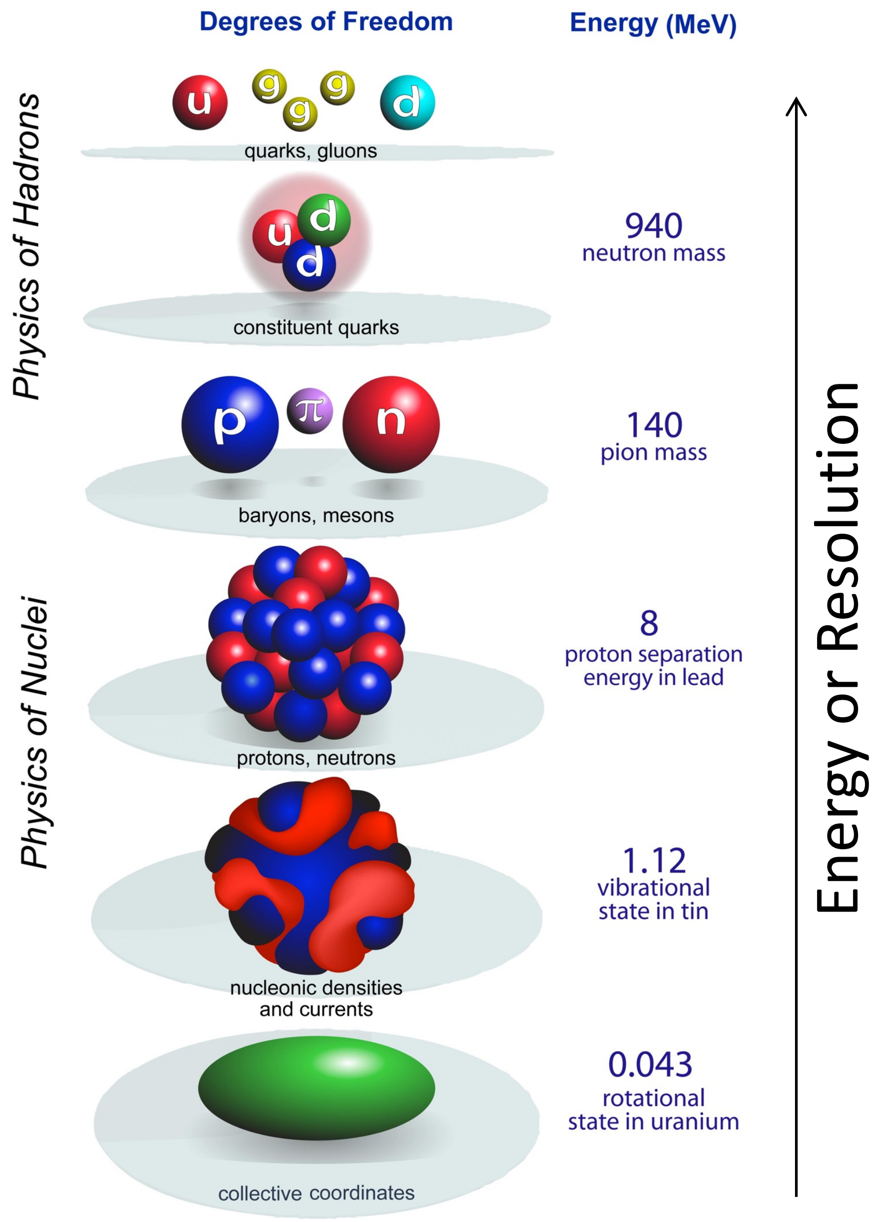


Fig.: Bertsch, Dean, Nazarewicz (2007)

- Physics of atomic nuclei spans several orders of magnitude
- Scales are well separated
- Which degrees of freedom are active depends on the resolution scale
- Many opportunities to construct effective field theories!

Energy scales and relevant degrees of freedom

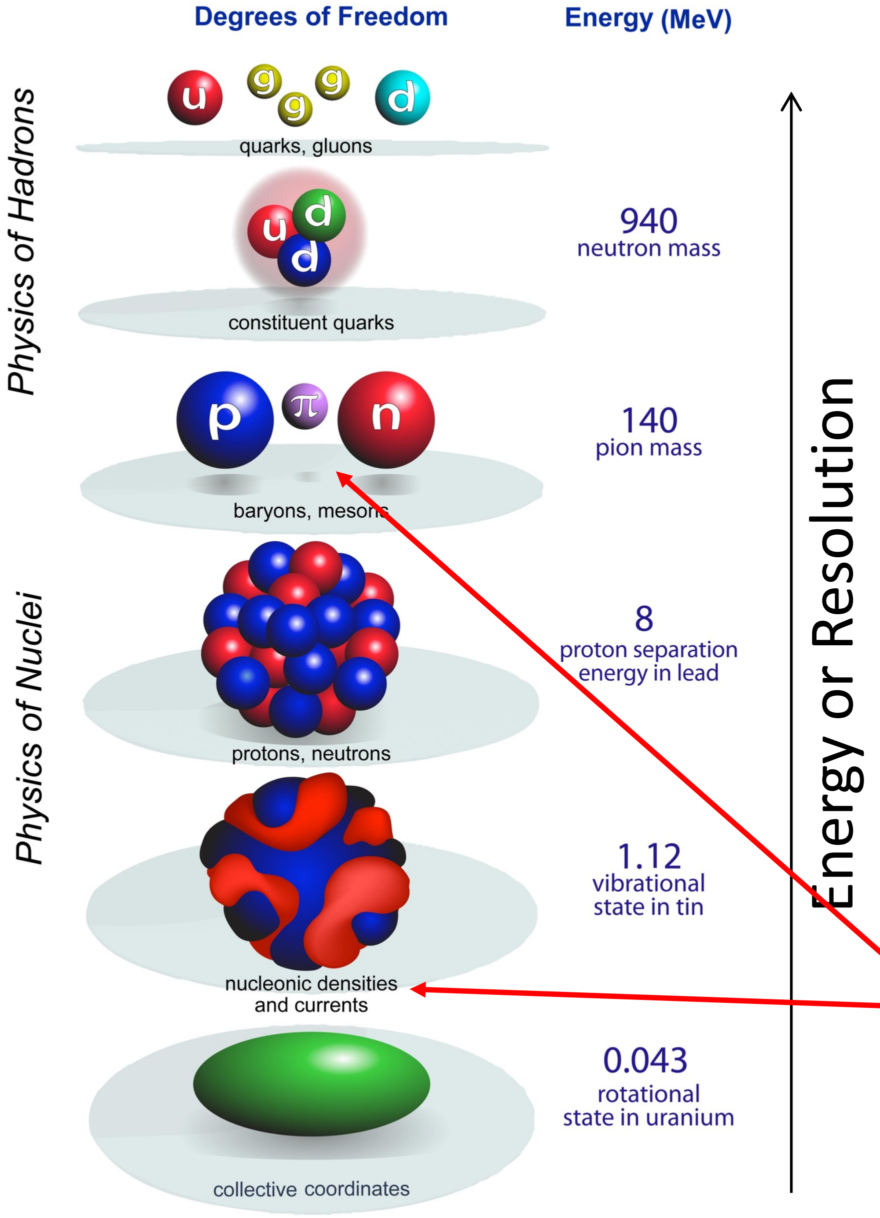


Fig.: Bertsch, Dean, Nazarewicz (2007)

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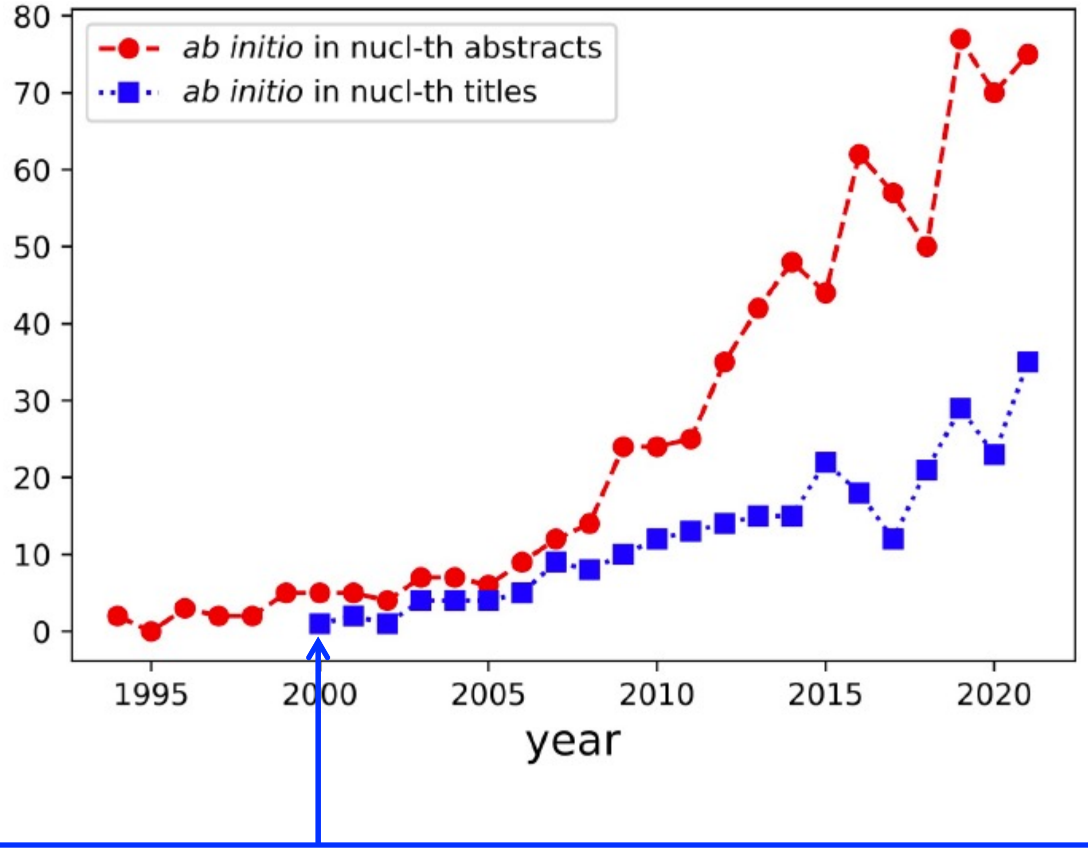
Elena Litvinova's lectures:
Relativistic nuclear field theory
based on meson exchange

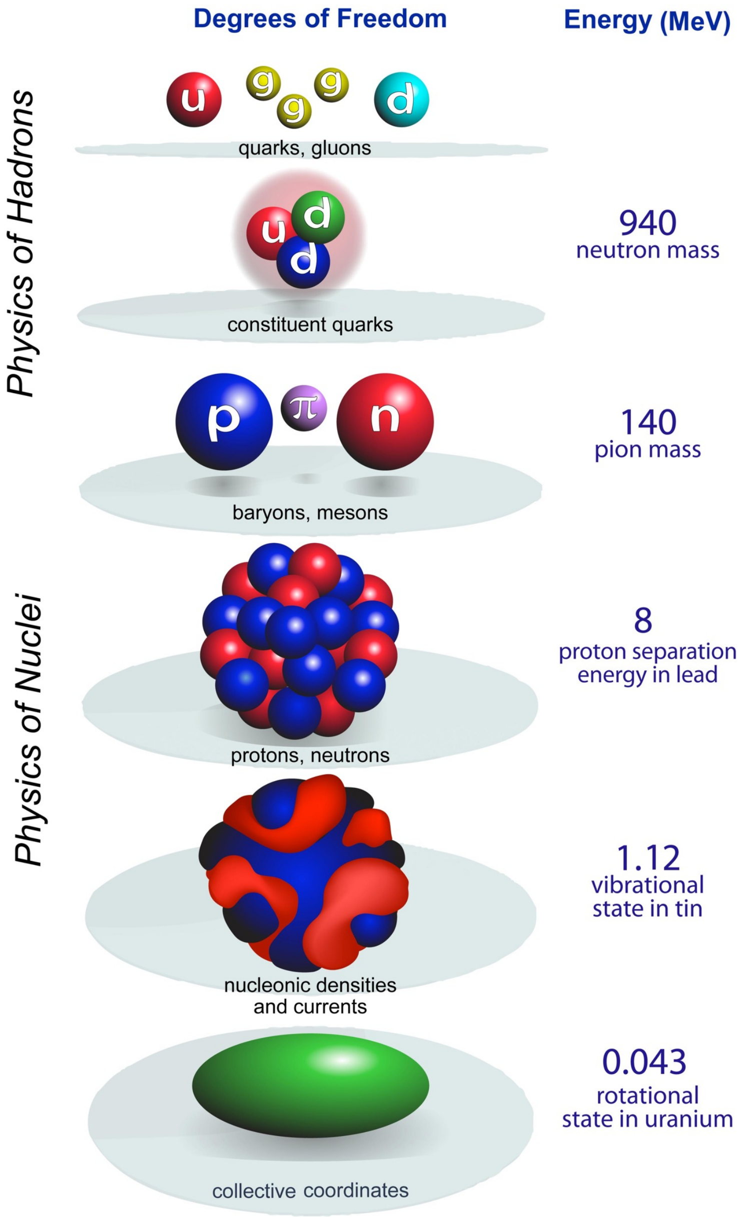
What is ab initio?



Navrátil, Vary, Barrett, *Properties of ^{12}C in the ab initio nuclear shell model*, Phys. Rev. Lett. 84, 5728 (2000)

Ekström, Forssén, Hagen, Jansen, Jiang, TP, Front. Phys. (2023); Google "ab initio" and "gruyere" to find the paper

What is ab initio in nuclear theory?



Ekström et al. *Front. Phys.* (2023) "interpret the ab initio method to be a systematically improvable approach for quantitatively describing nuclei using the finest resolution scale possible while maximizing its predictive capabilities."

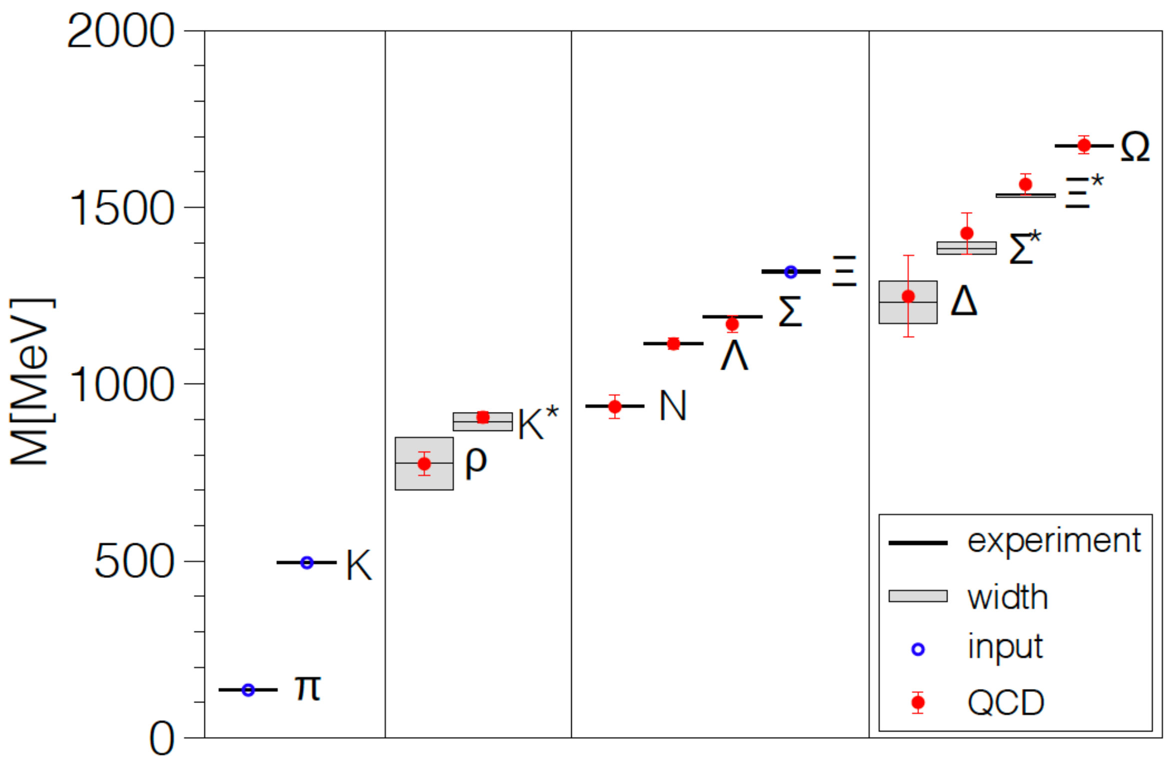
Q: What does this mean for computing atomic nuclei?

A1: Ab initio means starting from quantum chromodynamics, the fundamental theory of the strong nuclear force.

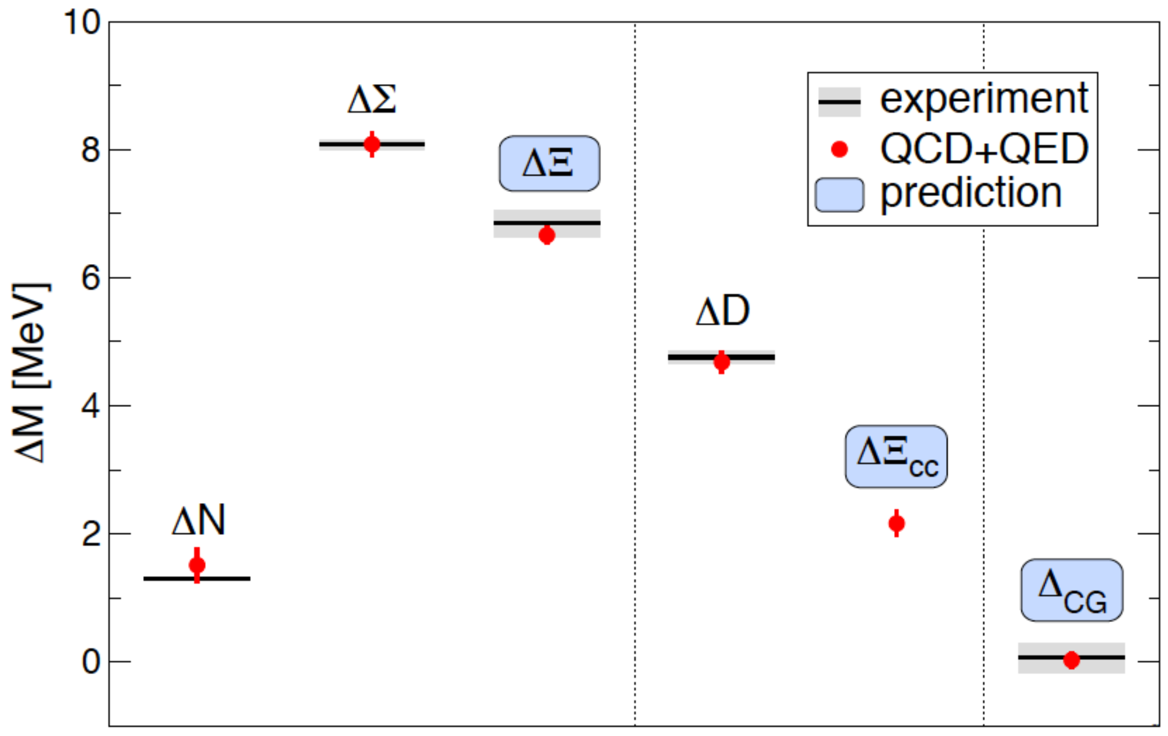
A2: Ab initio means starting from nucleons and the interactions between them.

A3: Ab initio means starting from nuclear energy density functionals.

Precision computations from lattice QCD



Hadron mass spectrum from lattice QCD.
Dürr et al., Science (2009); arXiv:0906.3599



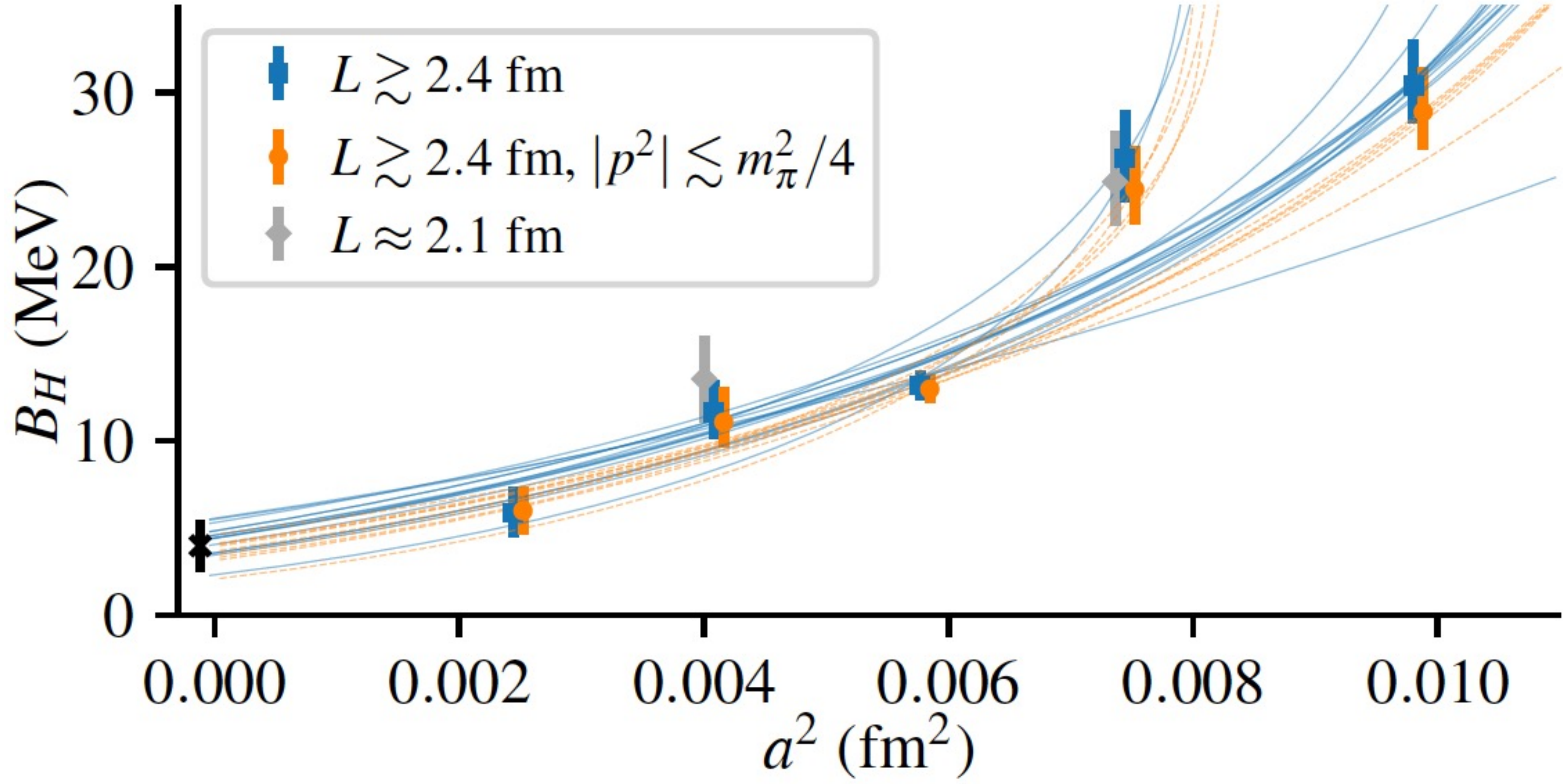
Proton-neutron mass splittings from lattice QCD & QED.
Borsanyi et al., Science (2015); arXiv:1406.4088

Lattice QCD very precise for hadrons, but what about nuclei as bound states of hadrons?

Towards Lattice QCD computations of hadron bound states

H-baryon, hypothetical six-quark bound state *uuddss*, computed at $m_\pi = m_K = 420$ MeV

$a =$ lattice spacing; $B_H =$ H-baryon binding energy



Challenges:

- Continuum limit ✓
- Physical meson masses ✗

$B_H = 3.97 \pm 1.16 \pm 0.86$ MeV

Jeremy R. Green, Andrew D. Hanlon, Parikshit M. Junnarkar, Hartmut Wittig, arXiv: 2103.01054

Computing nuclei to QCD

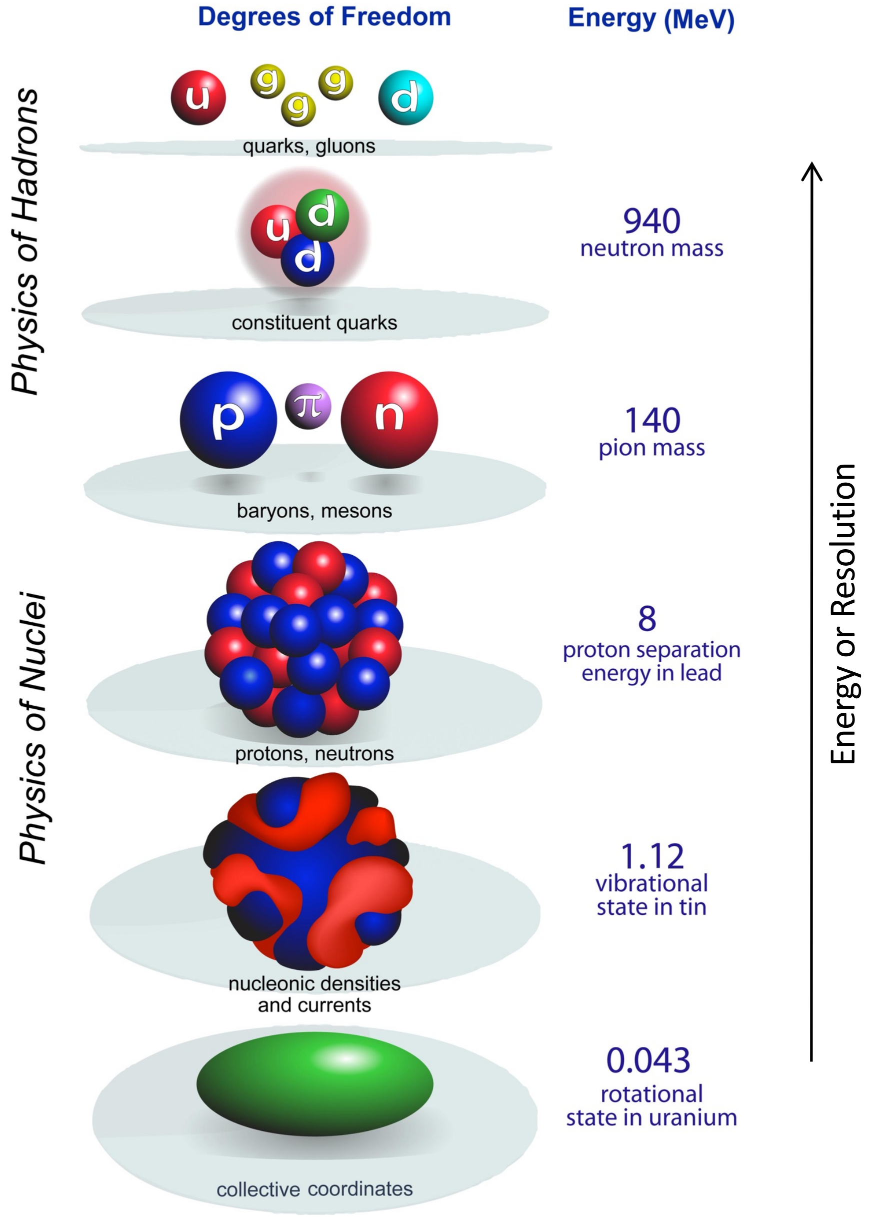
The computation of light nuclei from lattice QCD is controversial, see discussion in [Drischler, Haxton, McElvain, Mereghetti, Nicholson, Vranas, Walker-Loud, arXiv:1910.07961]

There was a controversy about whether nuclear binding increases with increasing pion mass [see, e.g., NPLQCD collaboration] or whether it decreases [see, e.g., HAL QCD collaboration]; it seems that there is a resolution [Amy Nicholson et al, arXiv:2112.04569] in favor of the latter.

Theorists are ready to match effective field theories to lattice QCD data, and compute nuclei as heavy as ^{40}Ca, see [Barnea et al, Phys. Rev. Lett. (2015); Contessi et al, Phys. Lett. B (2017); C. McIlroy et al Phys. Rev C (2018); Bansal *et al*., Phys. Rev. C 98, 054301 (2018)]

Enter effective field theories …

Energy scales and relevant degrees of freedom

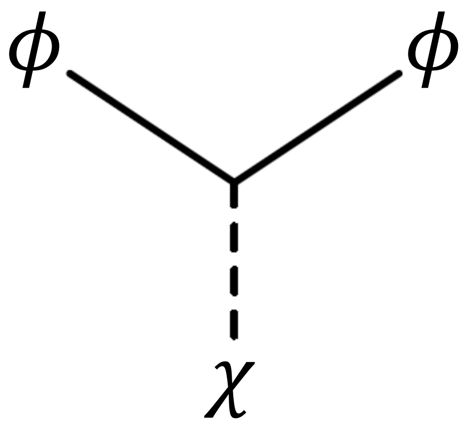


Chiral EFT

Fig.: Bertsch, Dean, Nazarewicz (2007)

Effective field theories: ideas

Fields ϕ, χ. Interaction via exchange of a heavy meson χ with mass M_{hi}

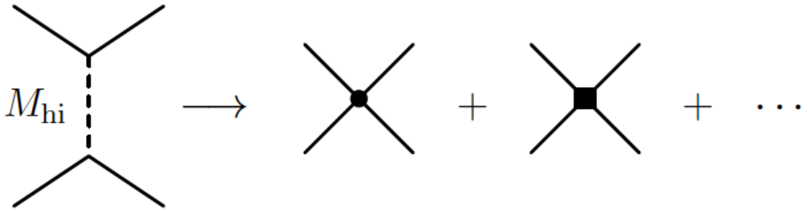


$$\mathscr{L}_{\text{int}} = g\left(\chi^\dagger \phi\phi + \phi^\dagger\phi^\dagger\chi\right)$$

Amplitude at small momenta $q \ll M_{hi}$ (introduce separation of scales)

$$T \sim \frac{g^2}{M_{\text{hi}}^2 - q^2} = \frac{g^2}{M_{\text{hi}}^2} + \frac{g^2 q^2}{M_{\text{hi}}^4} + \cdots$$

Note: this is a sum of increasingly singular terms; regularization (e.g. via cutoff) and renormalization required



Result: A systematic improvable theory, valid at low momenta $q \ll M_{hi}$, in powers of q/M_{hi}

$$\mathscr{L}_{\text{int}} = -\frac{C_0}{4}\left(\phi^\dagger\phi\right)^2 - \frac{C_2}{4}\left(\nabla(\phi^\dagger\phi)\right)^2 + \cdots$$

Nice pedagogical lectures on this topic: H.-W. Hammer, Sebastian König, arXiv:1610.02961

Lepage: How to renormalize the Schrödinger equation

Hamiltonian: Coulomb potential $V = -\alpha/r$ plus an unknown short-range part.

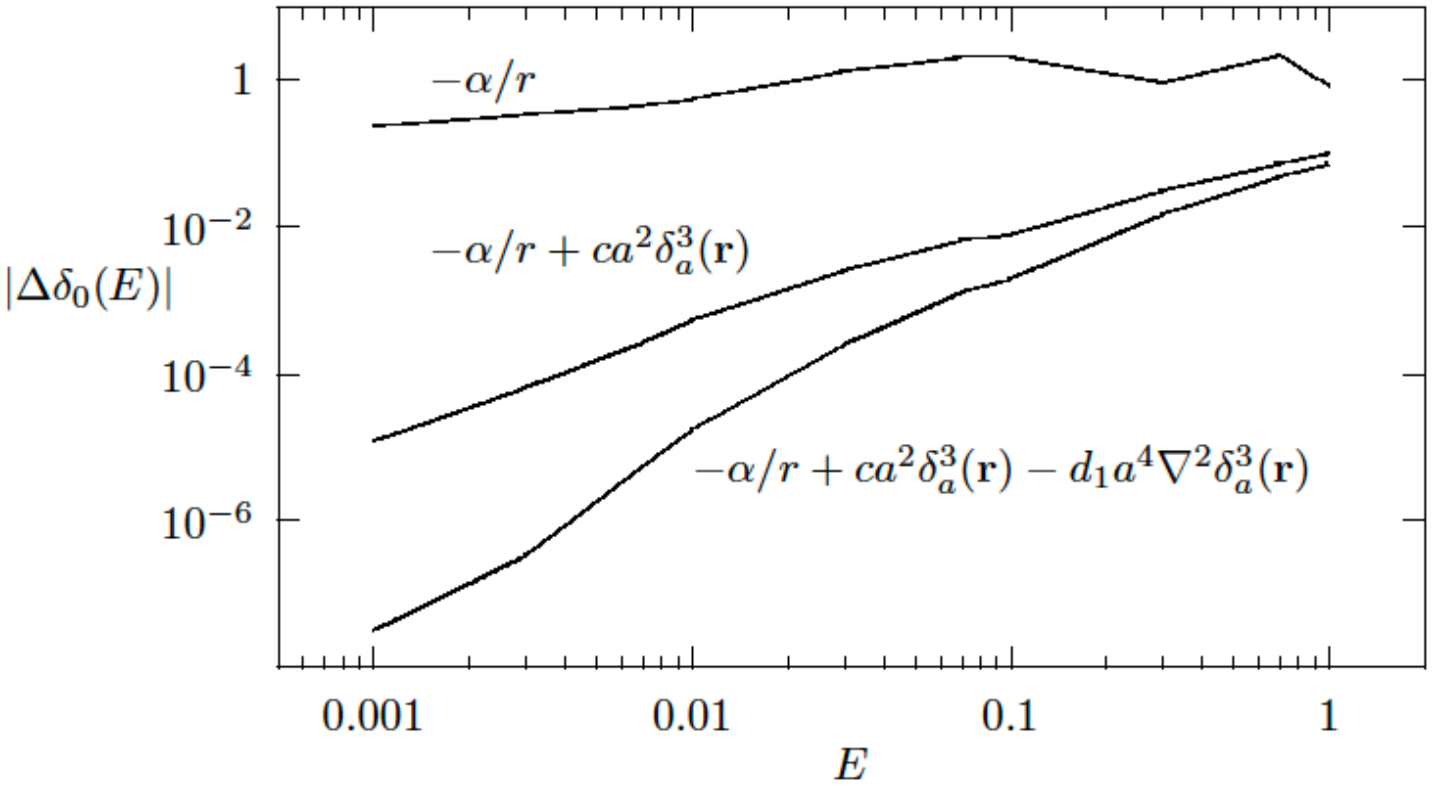
Q: How to reproduce available scattering data for this potential?

A: Use series of singular potentials:

$$V = -\frac{\alpha}{r} + ca^2\delta_a^{(3)}(r) - d_1 a^4 \nabla^2 \delta_a^{(3)}(r) + \cdots$$

(Here, a is a small but finite range, so π/a is a momentum cutoff; c and d_1 are dimensionless low-energy constants.)

Note: the series will not approximate the true short-range potential but rather only mimic its effect at low energies



Q: Do you see the power counting at work?
Q: Can you verify this quantitatively?
Q: What is the breakdown energy?

Peter Lepage., arXiv:nucl-th/9706029

Effective field theories: ideas

We do not need to know all the details (i.e. short-range physics) of the strong interaction to compute nuclei.

Effective field theories provide us with a systematically improvable approach that is valid up to some breakdown scale (in energy or momenta)

Effective field theories are particularly constrained in case of spontaneous symmetry breaking

Chiral effective field theory

[Weinberg; van Kolck; Epelbaum, Gloeckle, Krebs, Meissner; Entem & Machleidt; Kievsky, Marcucci, Viviani; Piarulli; Ekström, …]

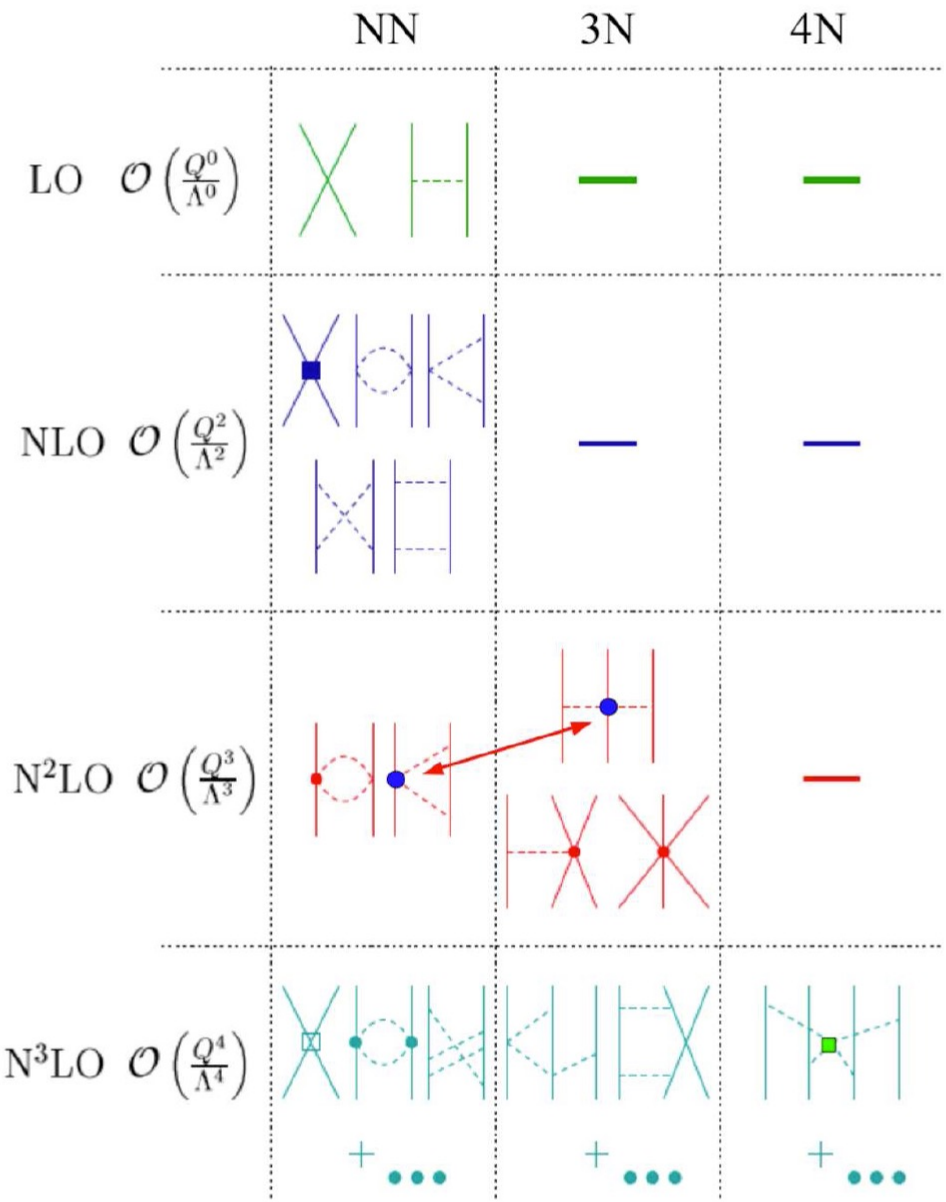
- The pion is the Nambu-Goldstone boson of the spontaneously broken chiral symmetry
  - Severely constrains the form of the nucleon-pion interaction ☺
  - Interactions between Nambu-Goldstone bosons are weak ☺
  - Provides the connection to QCD via chiral perturbation theory
- Pion exchange constitutes the long-range part of the nuclear force
- Everything else (presumably unknown/short ranged) is captured by contact interactions and derivatives thereof
- Power counting orders contributions

One-pion exchange potential: $V(q) = -\frac{g_A^2}{4f_\pi^2}\frac{(\sigma_1\cdot q)\,(\sigma_2\cdot q)}{m_\pi^2+q^2}\tau_1\cdot\tau_2$

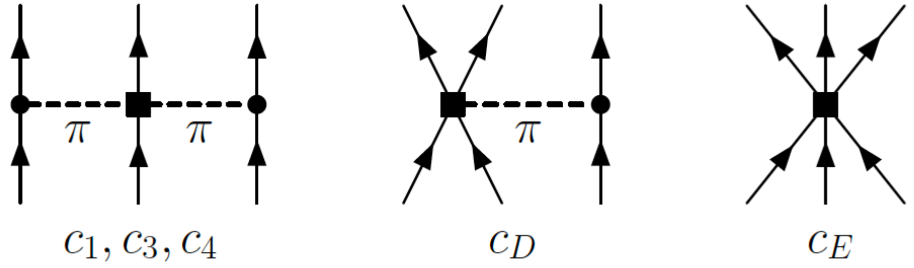
There are clouds in paradise (e.g. questions regarding the power counting), but these lectures will not dwell on them

Chiral effective field theory

[Weinberg; van Kolck; Epelbaum, Gloeckle, Krebs, Meissner; Entem & Machleidt; Kievsky, Marcucci, Viviani; Piarulli; Ekström, …]



Q: Why three-nucleon forces?



Chiral effective field theory

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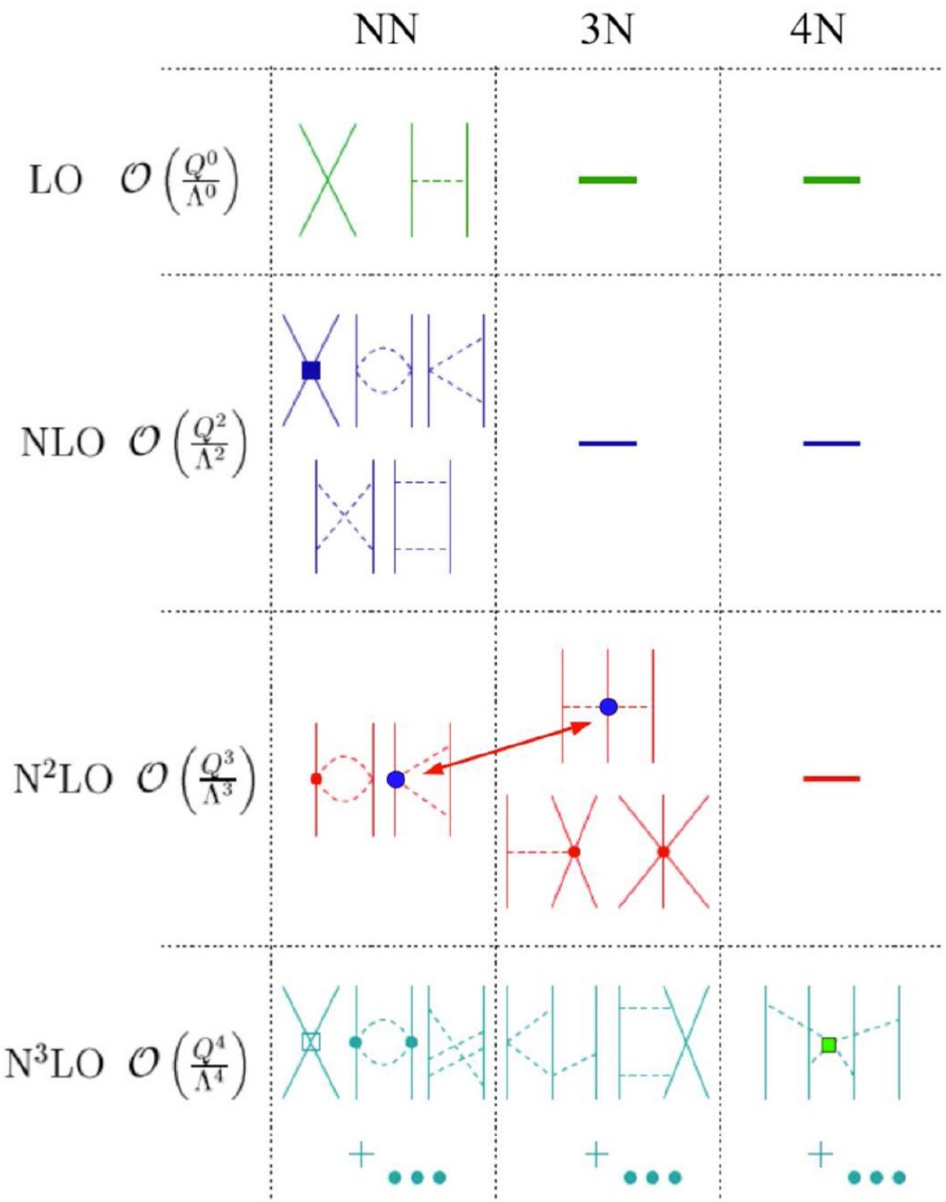

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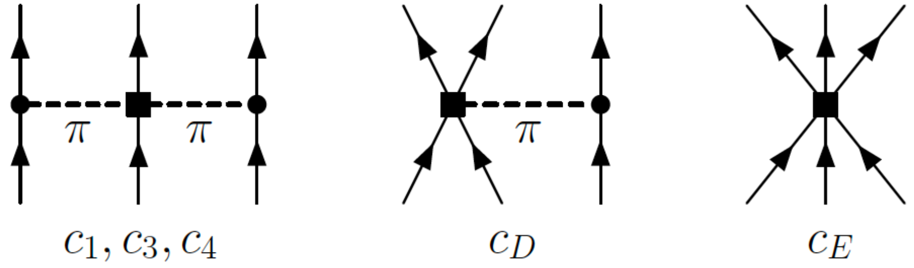

A1: In an EFT, one writes down everything that is allowed by symmetries and then orders according to a power counting

A2: Nucleons are composite particles, and many-body forces arise when treating them as point particles, i.e. when removing high-momentum “stiff” degrees of freedom

A3: all of the above

Three nucleon forces

- How do 3NFs arise in nuclear physics?
- What are omitted degrees of freedom? Can you draw diagrams that explain the origin of three nucleon forces?

Three nucleon forces

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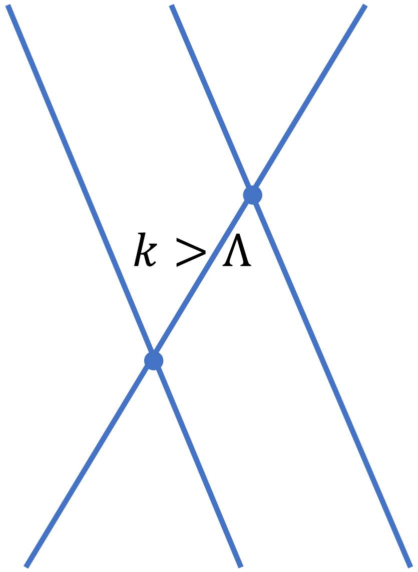
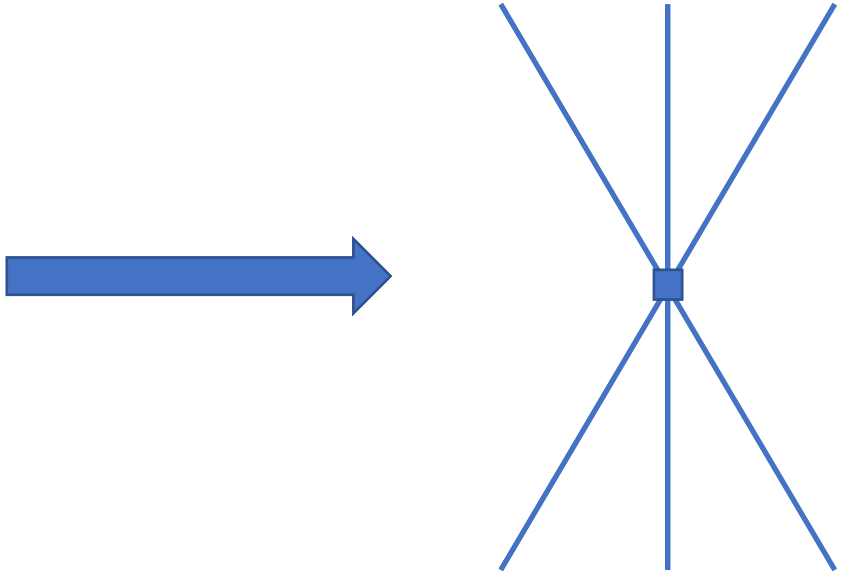
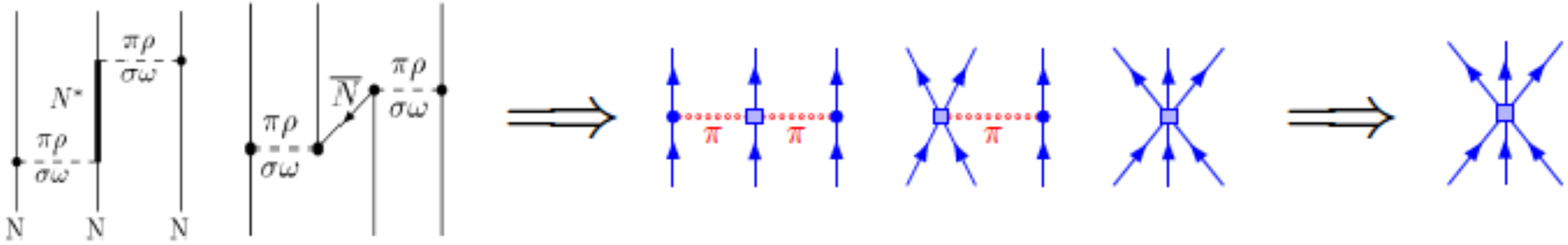
- What are omitted degrees of freedom? Can you draw diagrams that explain the origin of three nucleon forces?





Removal (or omission) of high-energy degrees of freedom leads to new interactions.

3NFs in a theory with pions

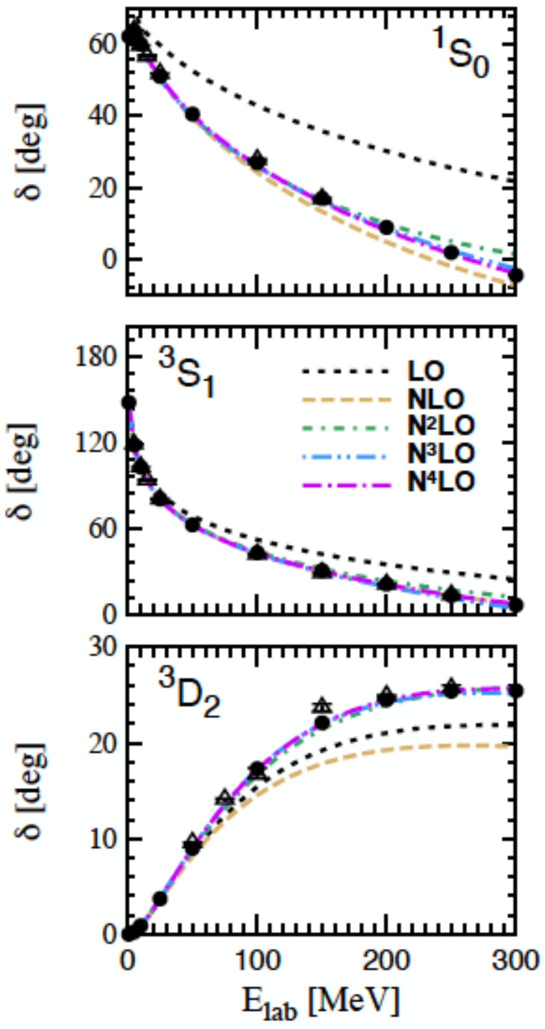


The essential rationale is:
Nuclei are extended objects, i.e. they have intrinsic degrees of freedom. They have excited states, can be deformed etc.
We treat nuclei as point particles, i.e. we neglect their intrinsic structure. While this is justified at low energies (low resolution), it comes with a price tag of 3NFs, 4NFs, …

Summary EFT Intro / three-nucleon forces

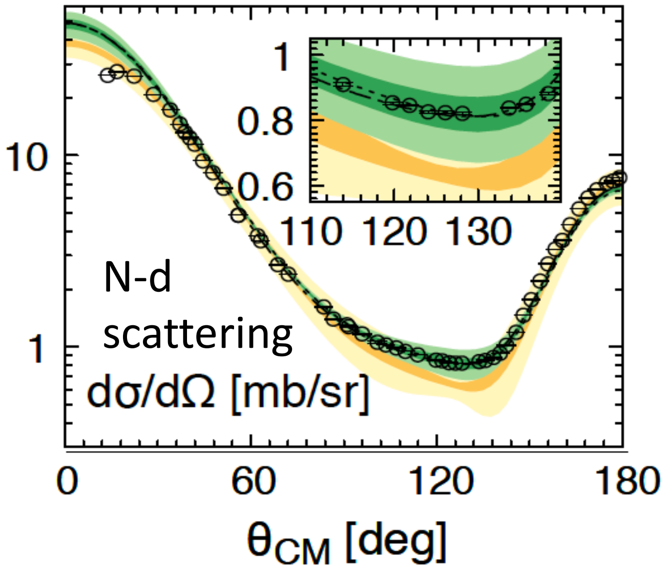
- Lattice QCD not yet there to compute nuclei
  - Even when that day arrives, the physical degrees of freedom are colorless hadrons
- Effective field theories can, in principle, be matched to QCD input
  - Meanwhile, we use data from nuclei
- Three-nucleon forces naturally arise as high-energy degrees of freedom are removed ("integrated out")

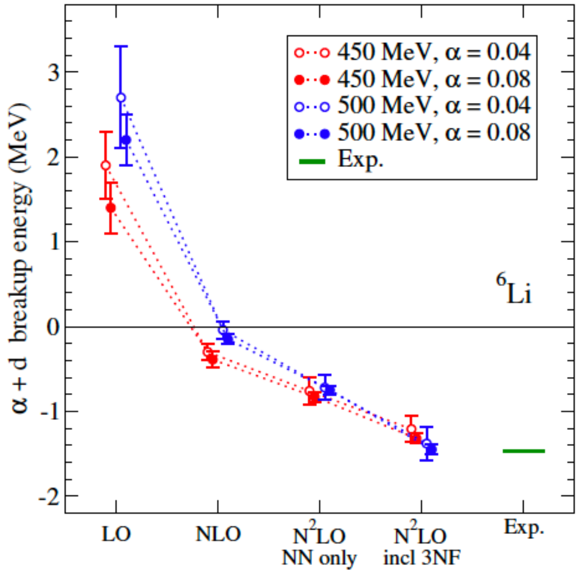
Chiral effective field theory: state of the art



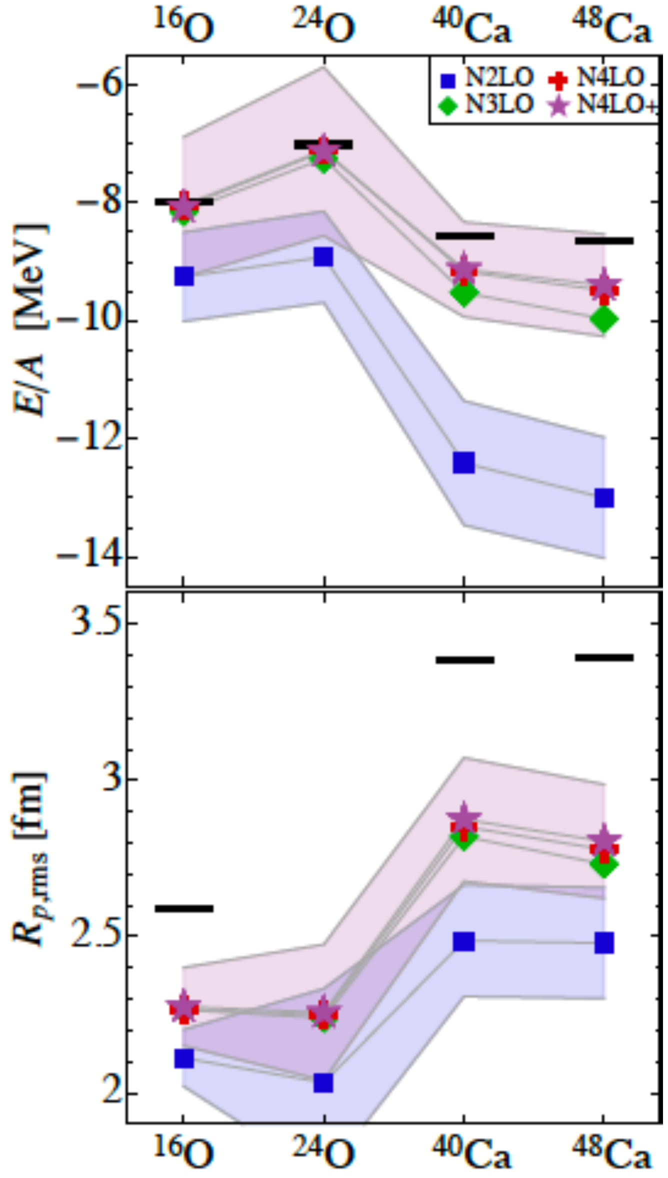
Reinert, Krebs, Epelbaum, Eur. Phys. J. A 54, 86 (2018)

Maris et al., Phys. Rev. C 103, 054001 (2021)





Maris et al., Phys. Rev. C 106, 064002 (2022)



Q: Can you spot successes and failures?

Chiral effective field theory: state of the art

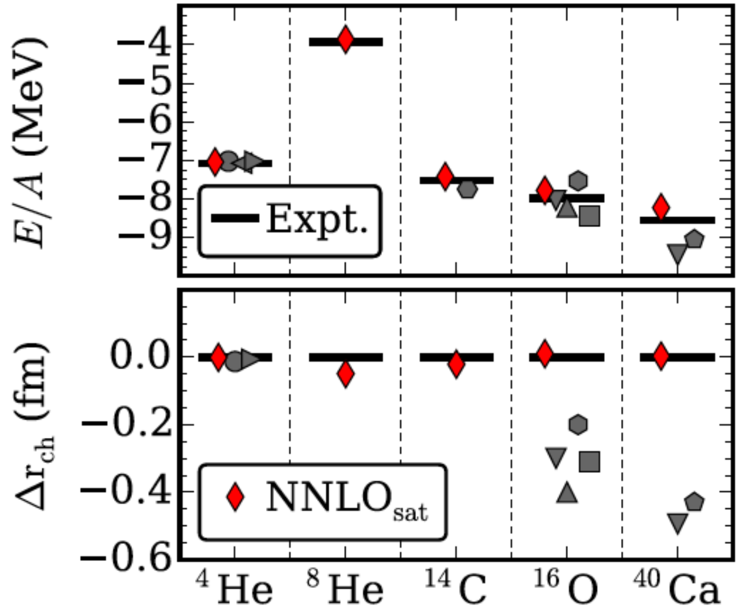
Problems:

- Inspection shows that the theory at leading order is cutoff dependent (not properly renormalized), see [Nogga, Timmermans, van Kolck, Phys. Rev. C 72, 054006 (2005)]
- So far, interactions from chiral effective field theory that were constrained in two- and three-nucleon systems, have failed accurately reproduce binding energies and charge radii in medium-mass nuclei.

Proposed solution: Optimize low-energy coefficient by also using data from medium-mass nuclei

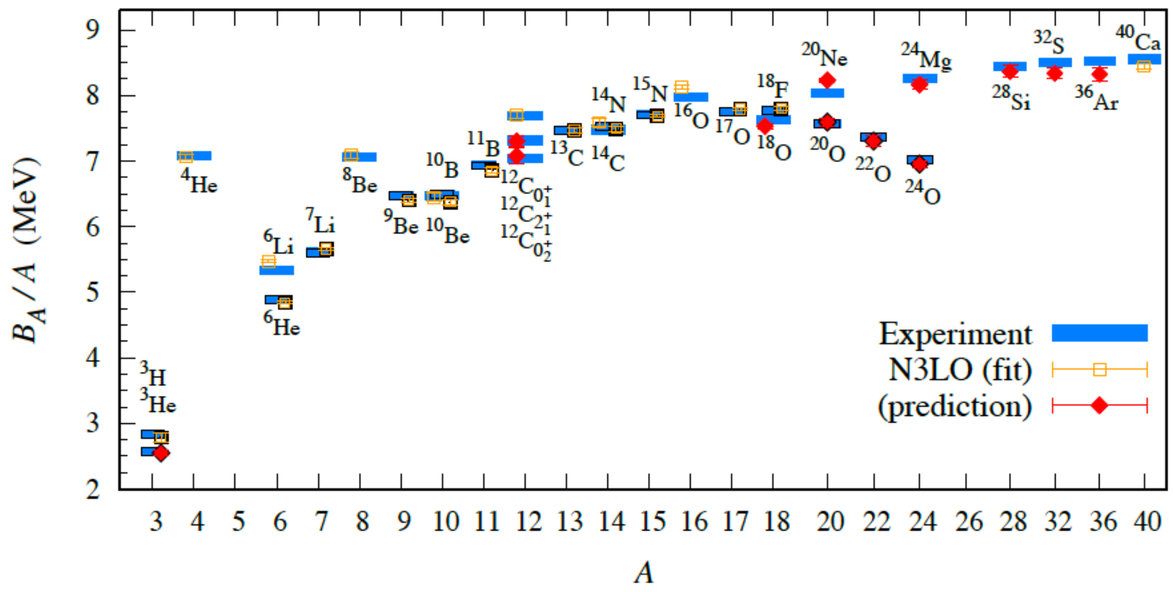
TABLE I. Binding energies (in MeV) and charge radii (in fm) for ^{3}H, ^{3,4}He, ^{14}C, and ^{16,22,23,24,25}O employed in the optimization of NNLO$_{\text{sat}}$.

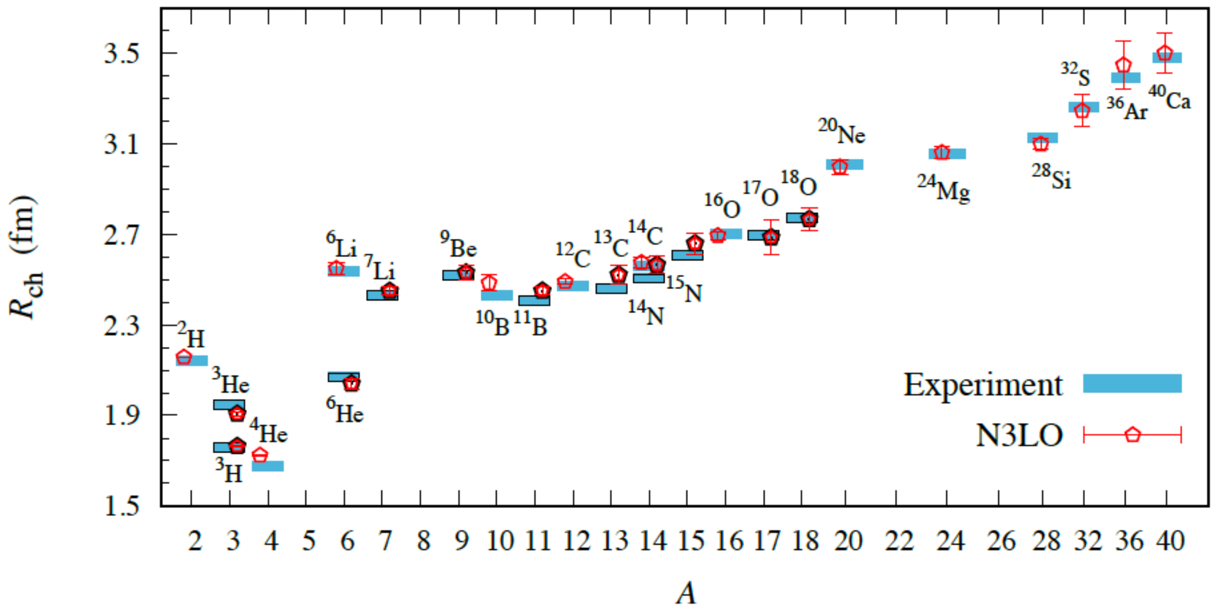
	$E_{\text{g.s.}}$	Expt. [69]	r_{ch}	Expt. [65,66]
^{3}H	8.52	8.482	1.78	1.7591(363)
^{3}He	7.76	7.718	1.99	1.9661(30)
^{4}He	28.43	28.296	1.70	1.6755(28)
^{14}C	103.6	105.285	2.48	2.5025(87)
^{16}O	124.4	127.619	2.71	2.6991(52)
^{22}O	160.8	162.028(57)		
^{24}O	168.1	168.96(12)		
^{25}O	167.4	168.18(10)		



Ekström et al., Phys. Rev. C 91, 051301(R) (2015)

Chiral effective field theory: state of the art





Chiral EFT inspired interaction

Used 4 three-body contacts (instead of 2 in chiral EFT)

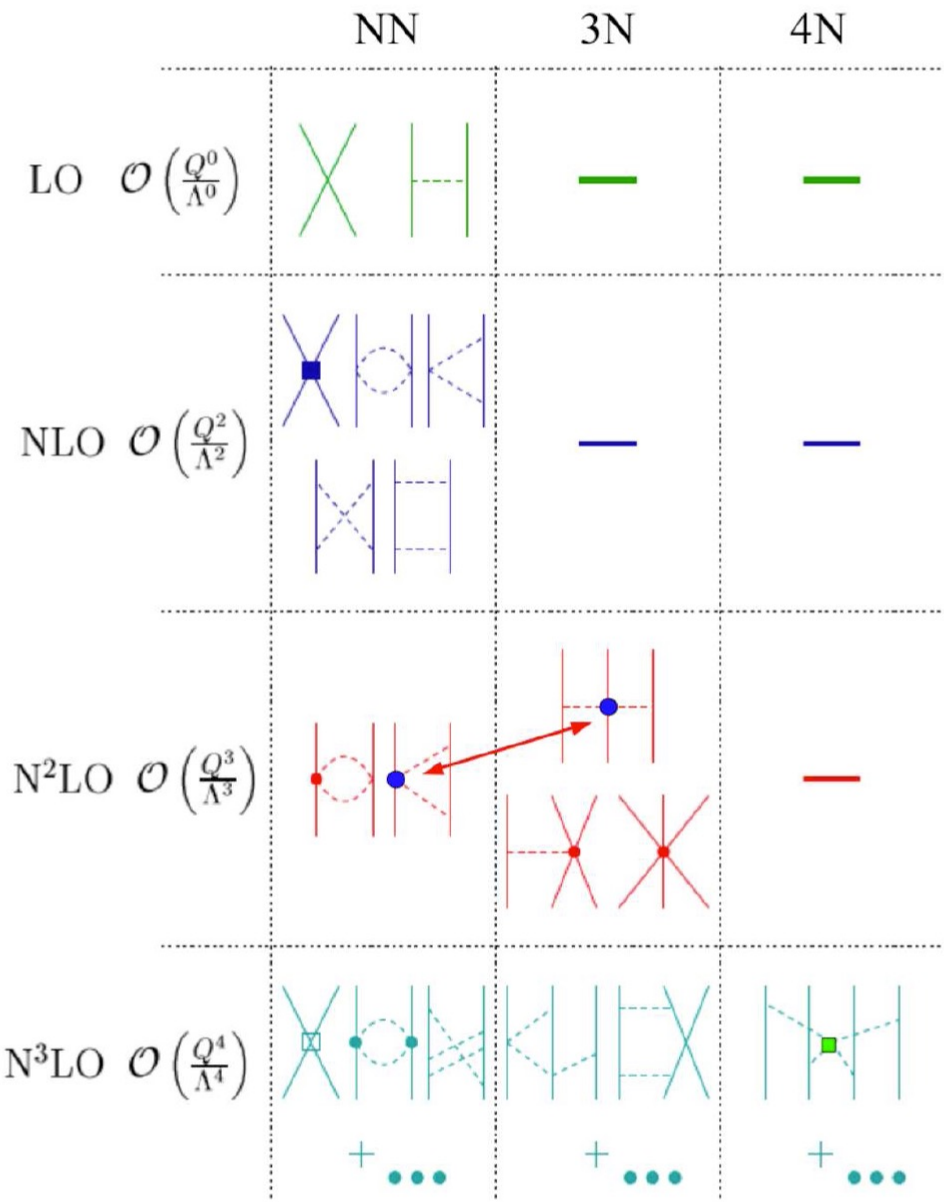
Adjusted energies of cluster states
(e.g. ^{8}Be = ^{4}He + ^{4}He, Hoyle state in ^{12}C = ^{4}He + ^{4}He + ^{4}He)

Result: accurate charge radii come out

Elhatisari et al., Nature 630, 59 (2024), arXiv:2210.17488

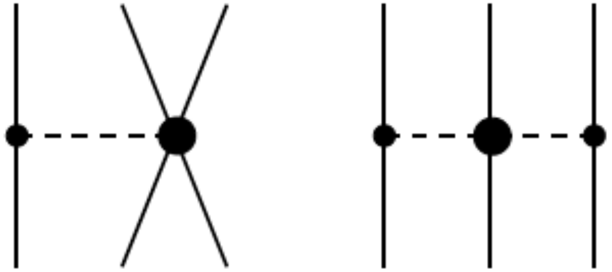
Chiral effective field theory: consistency of currents and interactions

[Weinberg; van Kolck; Epelbaum, Gloeckle, Krebs, Meissner; Entem & Machleidt; Ekström, …]



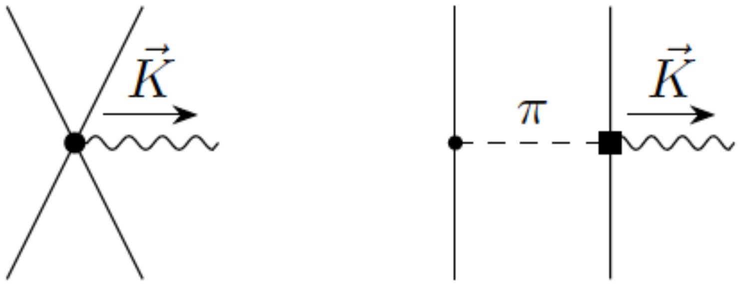
Effective field theories provide us with a consist formulation of

interactions



and

currents:



Three-body forces go hand in hand with two-body currents.

Heavy meson exchange c_D

Pion exchange c_3, c_4

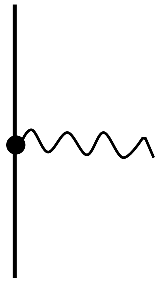
Consistency between Hamiltonians and currents
example: electromagnetic interactions

Heisenberg Eq. of motion $\frac{d\rho}{dt} = \frac{i}{\hbar}[H,\rho]$

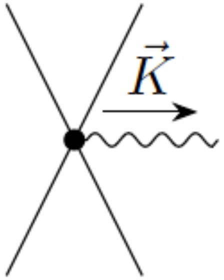
Continuity equation $\frac{d\rho}{dt} = -\nabla \cdot j$

We see that Hamiltonians and currents must fulfill $\frac{i}{\hbar}[H,\rho] + \nabla \cdot j = 0$
As EFT Hamiltonians contain momentum-dependent interactions, this is a non-trivial constraint on the current operator

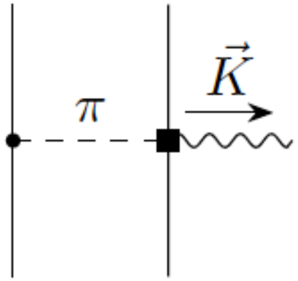
Leading order: 1-body current



Subleading corrections: 2-body currents
a.k.a. "meson-exchange currents"



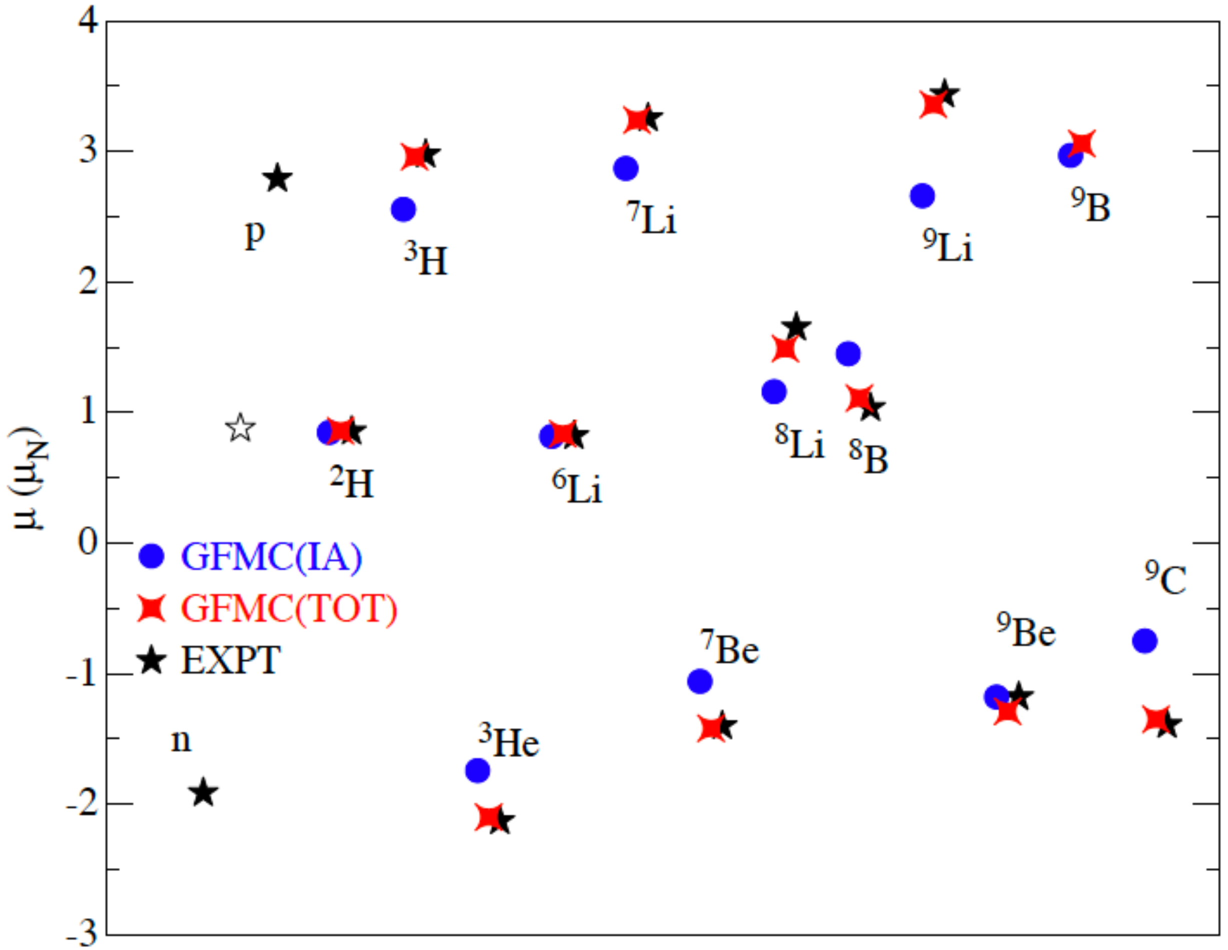
Heavy meson exchange
c_D



Pion exchange
$c_3,\ c_4$

Role of two-body currents: magnetic moments

The magnetic moment is a short-range operator, so we expect significant contributions from two-body currents

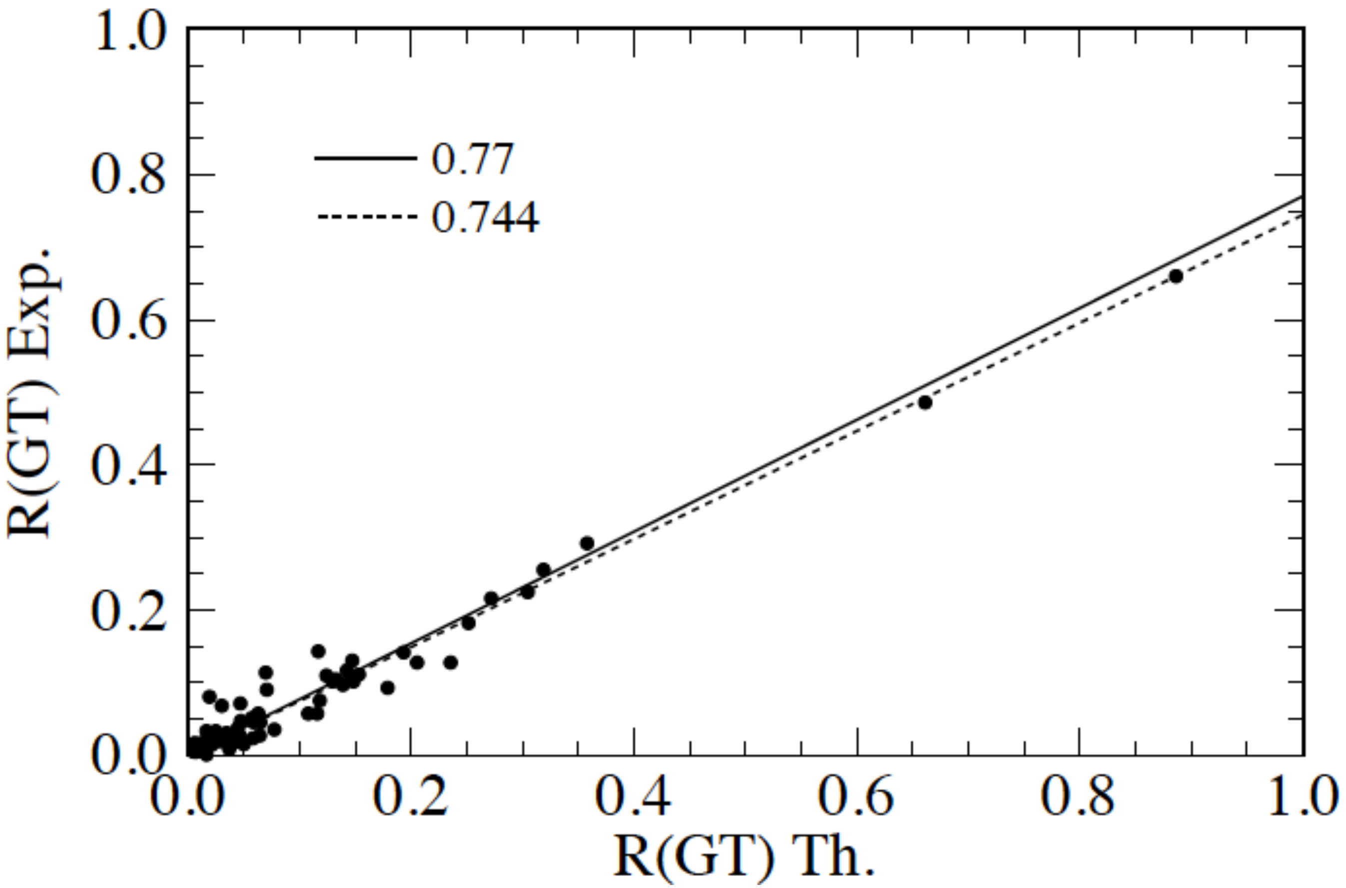


S. Pastore, Steven C. Pieper, R. Schiavilla, R. B. Wiringa, Phys. Rev. C 87, 035503 (2013); arXiv:1212.3375

Two-body currents solve 50-year-old puzzle of quenched β-decays

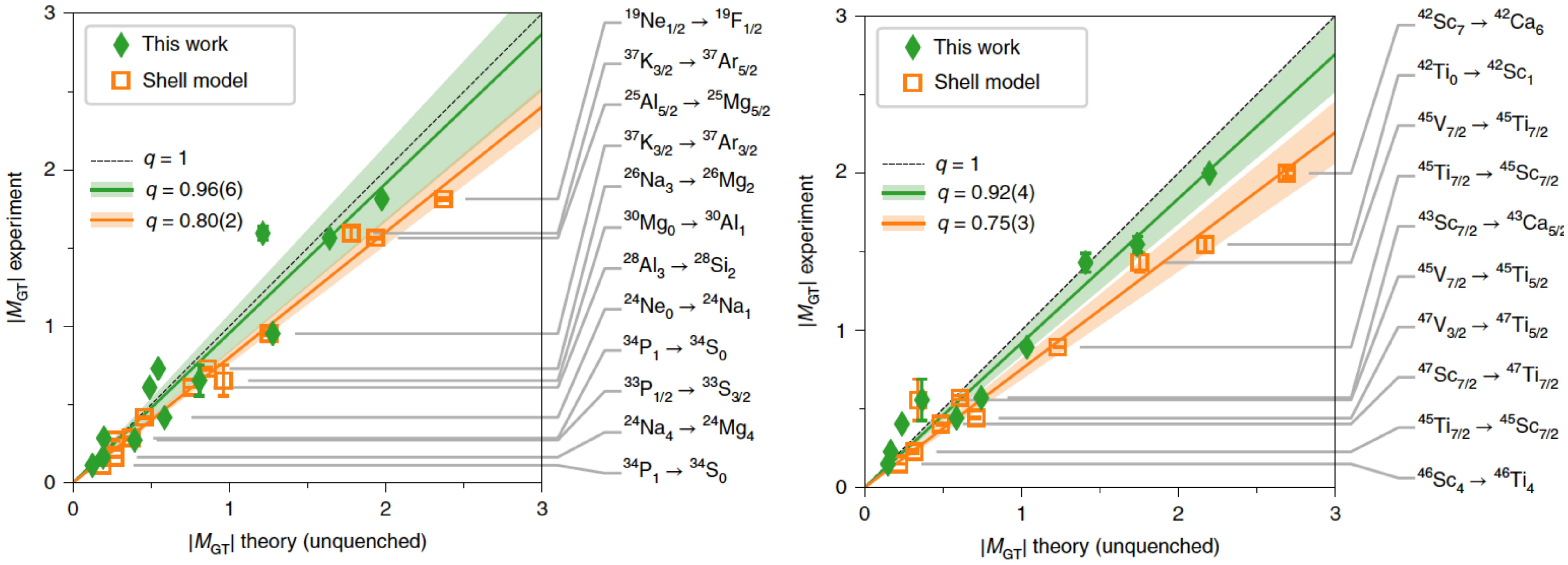
Puzzle: The strengths of Gamow-Teller transitions (operator $\propto g_A\vec{\sigma}\tau^{\pm}$) in nuclei are smaller ("quenched") than what is expected from the β-decay of the free neutron.

- Wilkinson (1973): quenching factor $q^2 \approx 0.90$ for nuclei with $A = 17 \ldots 21$
- Brown & Wildenthal (1985): quenching factor $q^2 \approx 0.77$ for nuclei with $A = 17 \ldots 40$
- Martinez-Pinedo et al. (1996): quenching factor $q^2 \approx 0.74$ for nuclei with $A = 40 \ldots 60$



Martinez-Pinedo, Poves, Caurier, and Zuker, Phys. Rev. C **53**, R2602 (1996)

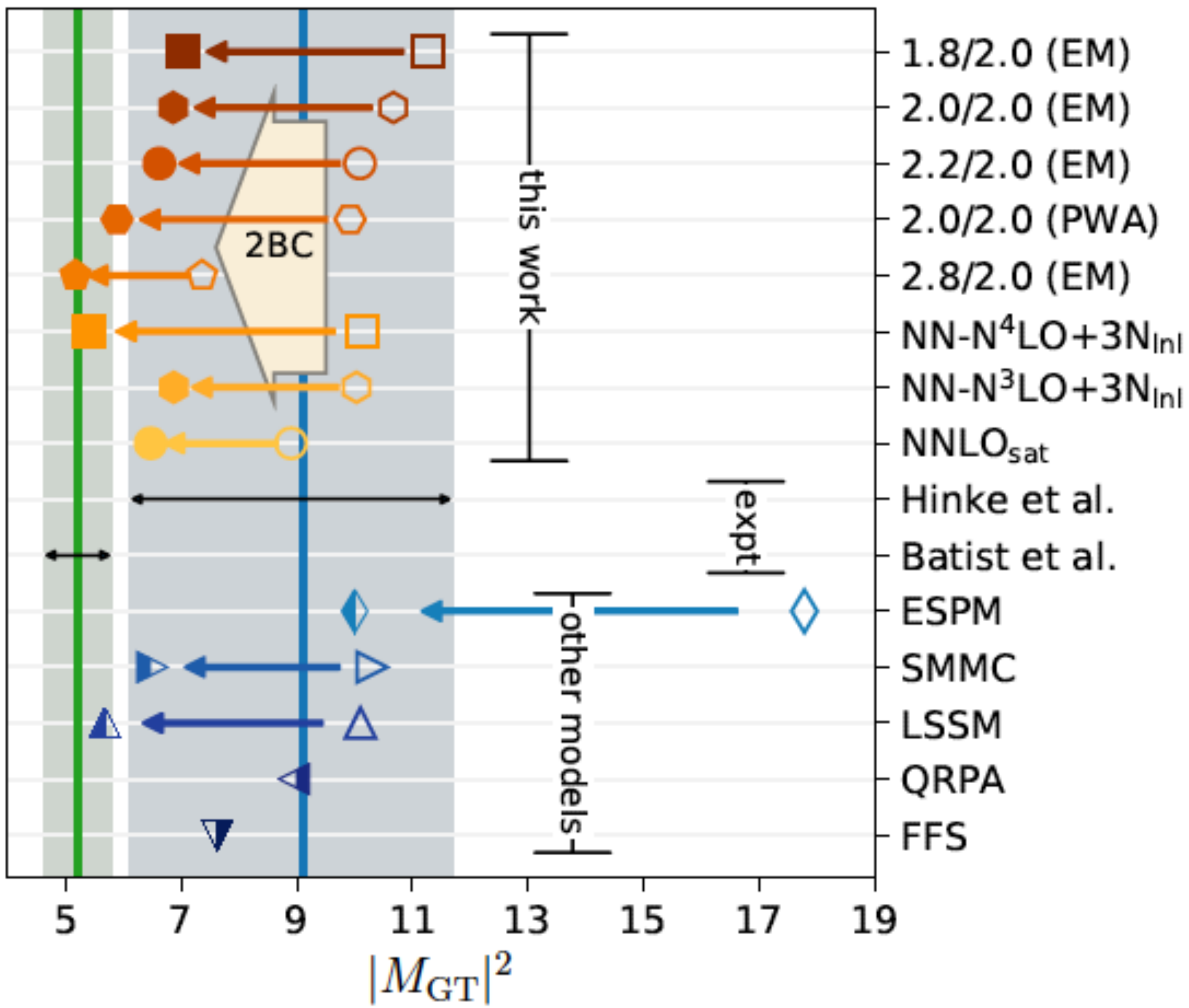
β decays in medium-mass nuclei, including two-body currents



IMSRG computations with NN-N^{4}LO + 3NlnI interaction

Gysbers, Hagen, Holt, Jansen, Morris, Navratil, TP, Quaglioni, Schwenk, Stroberg & Wendt, Nature Physics (2019); arXiv:1212.3375

β decay of ^{100}Sn, including two-body currents



Coupled-cluster computations based on various potentials from chiral EFT

Open symbols: no two-body currents

Full symbols: with two-body currents

Two-body currents reduce the systematic uncertainty from the set of chiral interactions.

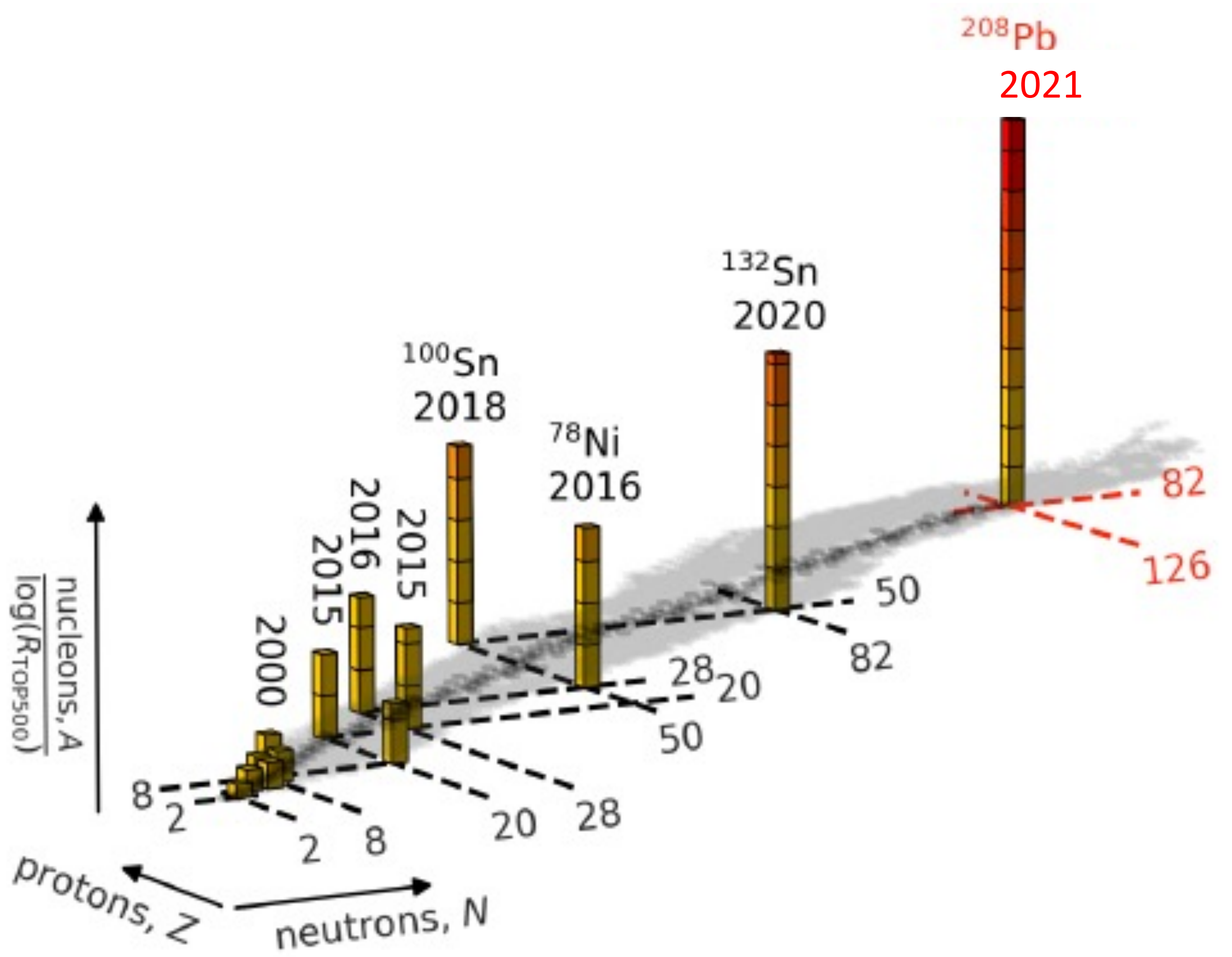
Traditional models need quenching factors to describe data.
(open symbols: no quenching).

Gysbers, Hagen, Holt, Jansen, Morris, Navratil, TP, Quaglioni, Schwenk, Stroberg & Wendt, Nature Physics (2019); arXiv:1212.3375

Summary two-body currents

- Two-body currents (2BCs) naturally arise in theories with three-body forces
  - In chiral EFTs, these are subleading corrections
- 2BCs deliver visible contributions to nuclear magnetic moments
- 2BCs provide us with a solution to the long-standing puzzle of quenched β decays

Progress in computing nuclei from EFT Hamiltonians



Tremendous progress

- Ideas from EFT and RG
- Methods that scale polynomially with mass number
- Ever-increasing computing powers

1. Ab initio methods not limited to light nuclei
2. Computing of (most) nuclei only exponentially hard if one chooses so
3. Why solve approximate Hamiltonians exactly?

Symmetries of the single-particle basis

Q: What are the relevant symmetries when computing nuclei?

A1:

A2:

A3:

Symmetries of the single-particle basis

Q: What are the relevant symmetries when computing nuclei?
A1: Translational invariance
A2: Rotational invariance
A3: Parity

(Isospin is conserved by the strong force but broken by the Coulomb force)

Symmetries of the single-particle basis

Bases:

1. Lattice in position space with periodic boundary conditions (L^3 sites, lattice spacing a)
   - Conserved quantities:
   - Lacking/not conserved:
   - IR/UV cutoffs:
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Symmetries of the single-particle basis

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   - Conserved quantities: angular momentum, parity
   - Lacking/not conserved: momentum
   - IR/UV cutoffs: $\Lambda_{IR} \approx \left(2(N + \frac{3}{2})\right)^{-\frac{1}{2}} \pi/b$, $\Lambda_{UV} \approx \left((2N + \frac{3}{2})\right)^{\frac{1}{2}} \pi/b$

   In other words: $La \approx \left(2(N + \frac{3}{2})\right)^{\frac{1}{2}} b$, and $a \approx \left(2(N + \frac{3}{2})\right)^{-\frac{1}{2}} b$

Comments on bases and symmetries

- One could work with (relative) Jacobi coordinates and have all relevant symmetries respected in the basis.
  - Antisymmetrization of the wave function increases exponentially with increasing mass number; approach limited to few-body systems
- One could work in the no-core shell model, i.e. using all Slater determinants up to $\left(N+\frac{3}{2}\right)\hbar\omega$; the center-of-mass wave function then is a Gaussian with frequency $\hbar\omega$.
  - Cost of exact diagonalization increases exponentially with mass number; limited to light nuclei

- Instead: Use angular-momentum projection for the lattice and intrinsic Hamiltonian $H = T - T_{CoM} + V$ in the harmonic oscillator basis.

Efficient computations of atomic nuclei

Question: How much effort does it take to compute a nucleus?

To answer this question, assume that we want to compute a nucleus with mass number A and using an interaction with a momentum cutoff Λ.

Q: Taking a 3D lattice in position space, how many lattice sites do we need (as a function of A and Λ.

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Q: Taking a 3D lattice in position space (or a spherical harmonic oscillator basis), how many lattice sites (states) do we need (as a function of A and Λ.

A: Simple answer: the nucleus has to fit into the basis in position space, i.e. $La > R \propto A^{1/3}$ and in momentum space, i.e. $\frac{\pi}{a} > \Lambda$.

One can work this out in more detail and finds

- Number of single-particle states $n_s \propto (R\Lambda)^3$
- Number of single-particle states $n_s \approx c_{geom} A \left(\frac{\Lambda}{k_F}\right)^3$ with $c_{geom} \sim O(1)$.

Interactions with smaller cutoffs require much smaller spaces!

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A: Let us work this out:

- A nucleus with mass number A occupies a volume $V = A/\rho_0$ with the nuclear saturation density $\rho_0 \approx 0.16$ fm^{-3}.
- The lattice spacing is $a = \frac{\pi}{\Lambda}$, and the number of states per unit volume is $\frac{n_s}{V} = \frac{g}{a^3} = \frac{g\Lambda^3}{\pi^3}$ where $g = 4$ is the spin-isospin degeneracy.
- Thus we need $n_s = \frac{4\Lambda^3}{\pi^3 \rho_0} A$ single-particle states.
- One can make this prettier: use $\rho_0 \propto k_F^3$ and get $n_s \approx c_{geom} A \left(\frac{\Lambda}{k_F}\right)^3$ with $c_{geom} \sim O(1)$.
- For a momentum cutoff of $\Lambda = 2$fm^{-1}, one gets $n_s \approx (3 \ldots 6)A$ single-particle states.

Similarity renormalization group (SRG) transformation

Glazek, & Wilson, PRD **48** (1993) 5863; **49** (1994) 4214; Wegner, Ann. Phys. **3** (1994) 77; Perry, Bogner, & Furnstahl (2007)

Main idea: decouple low from high momenta via a (unitary) similarity transformation

Unitary transformation

$$\widehat{H}(s) = U(s)\widehat{H}U^\dagger(s) = U(s)\left(\widehat{T}+\widehat{V}\right)U^\dagger(s)$$

Evolution equation

$$\frac{d\widehat{H}(s)}{ds} = \left[\eta(s), \widehat{H}(s)\right] \qquad \text{with} \qquad \eta(s) \equiv \frac{dU(s)}{ds}U^\dagger(s) = -\eta^\dagger(s)$$

Choice of unitary transformation through (one does not need to construct U explicitly).

$$\eta(s) = \left[\widehat{T}, \widehat{H}(s)\right]$$

yields scale-dependent potential that becomes more and more diagonal

$$\widehat{H}(s) = \widehat{T} + \widehat{V}(s)$$

Note: Baker-Campbell-Hausdorff expansion implies that SRG of 2-body force generates many-body forces

$$e^{-\eta}\widehat{H}e^{\eta} = \widehat{H} + \left[\widehat{H},\eta\right] + \frac{1}{2!}\left[\left[\widehat{H},\eta\right],\eta\right] + \dots$$

SRG evolution of a chiral potential

(use cutoff $\lambda \equiv s^{-1/4}$ as evolution variable)

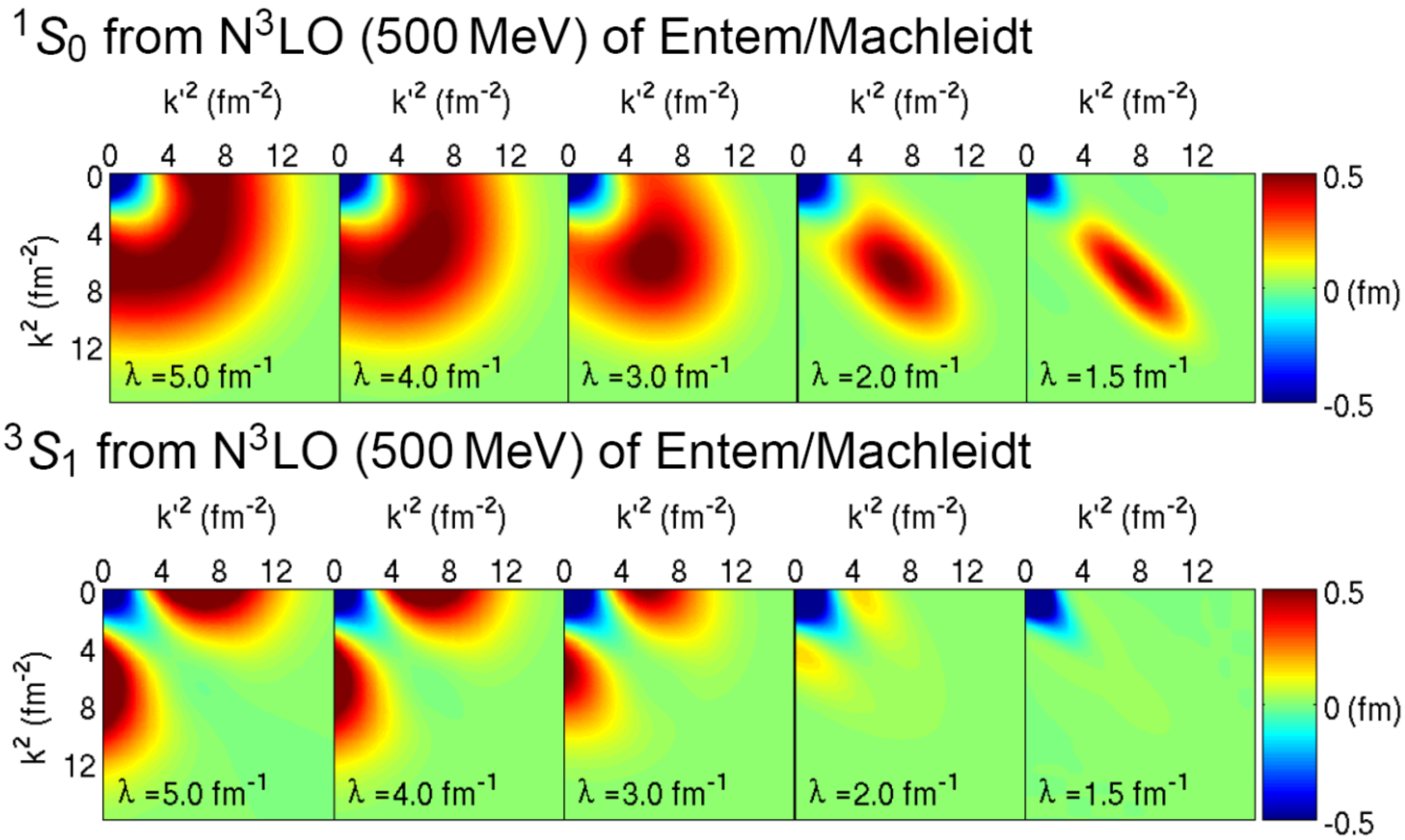
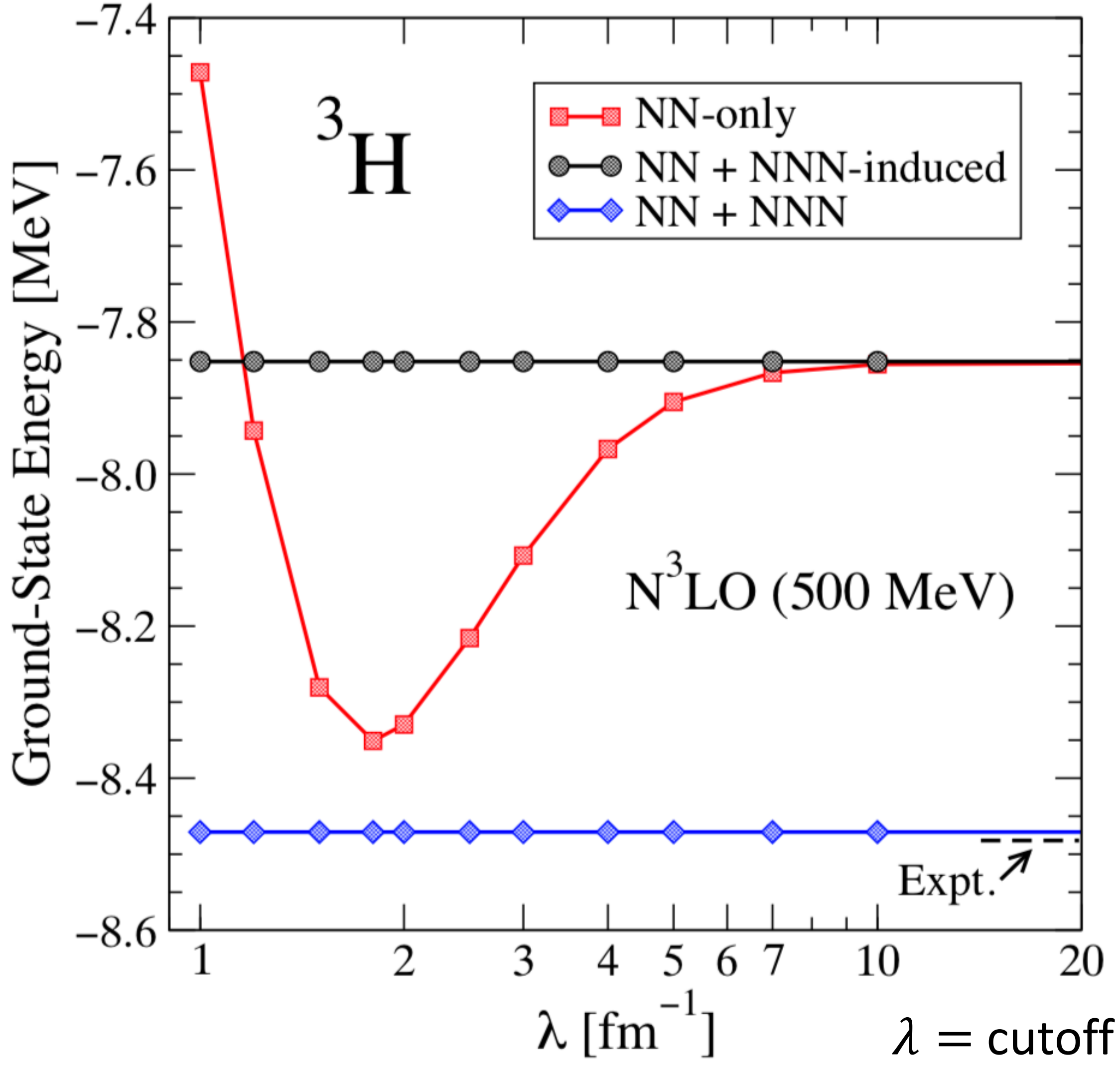
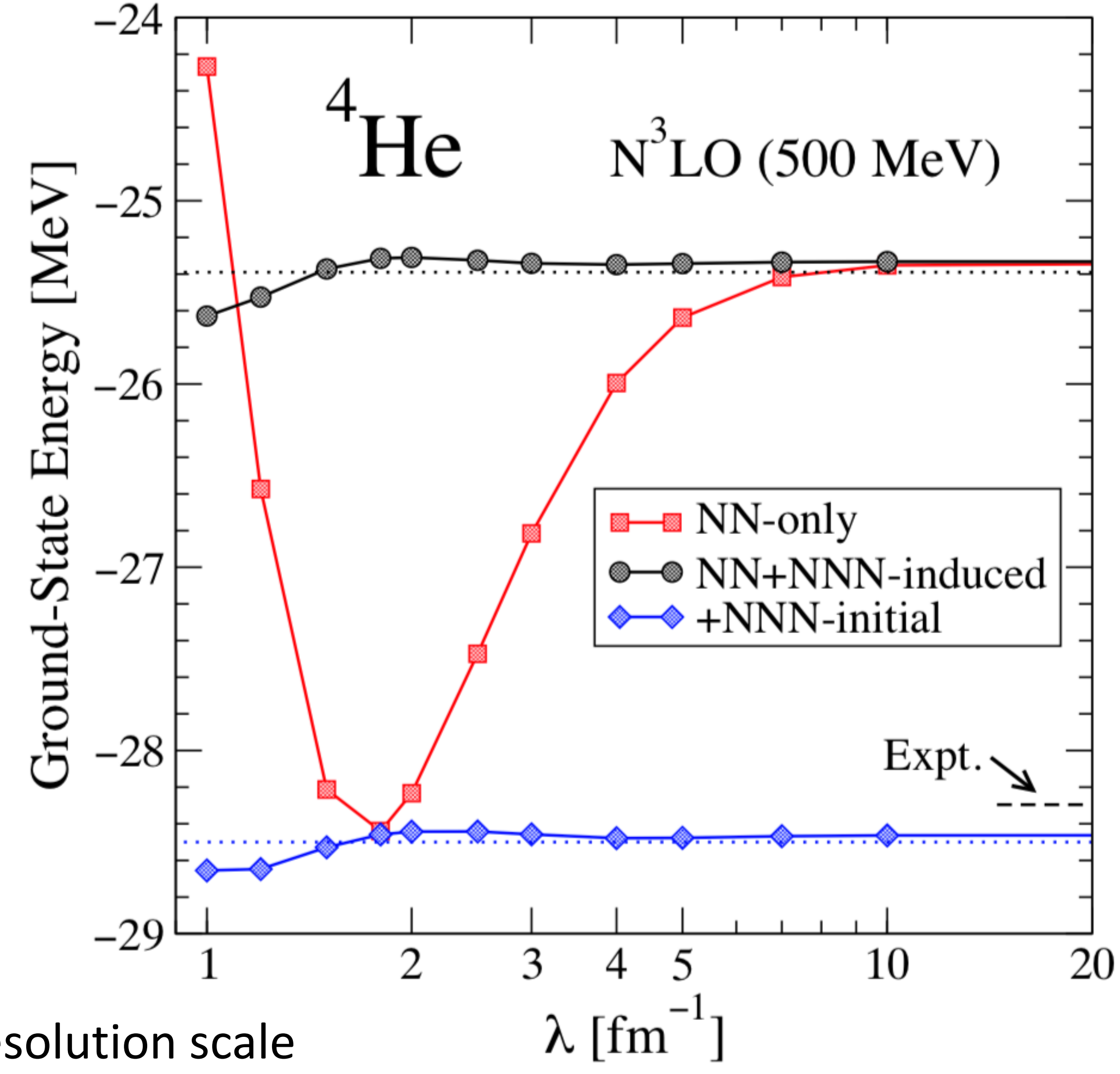


Fig.: Bogner & Furnstahl. See http://www.physics.ohio-state.edu/~ntg/srg

RG Evolution of Nuclear Many-Body Forces





λ = cutoff or resolution scale

Jurgenson, Furnstahl, Navratil, Phys. Rev. Lett. 103, 082501 (2009); arXiv:0905.1873

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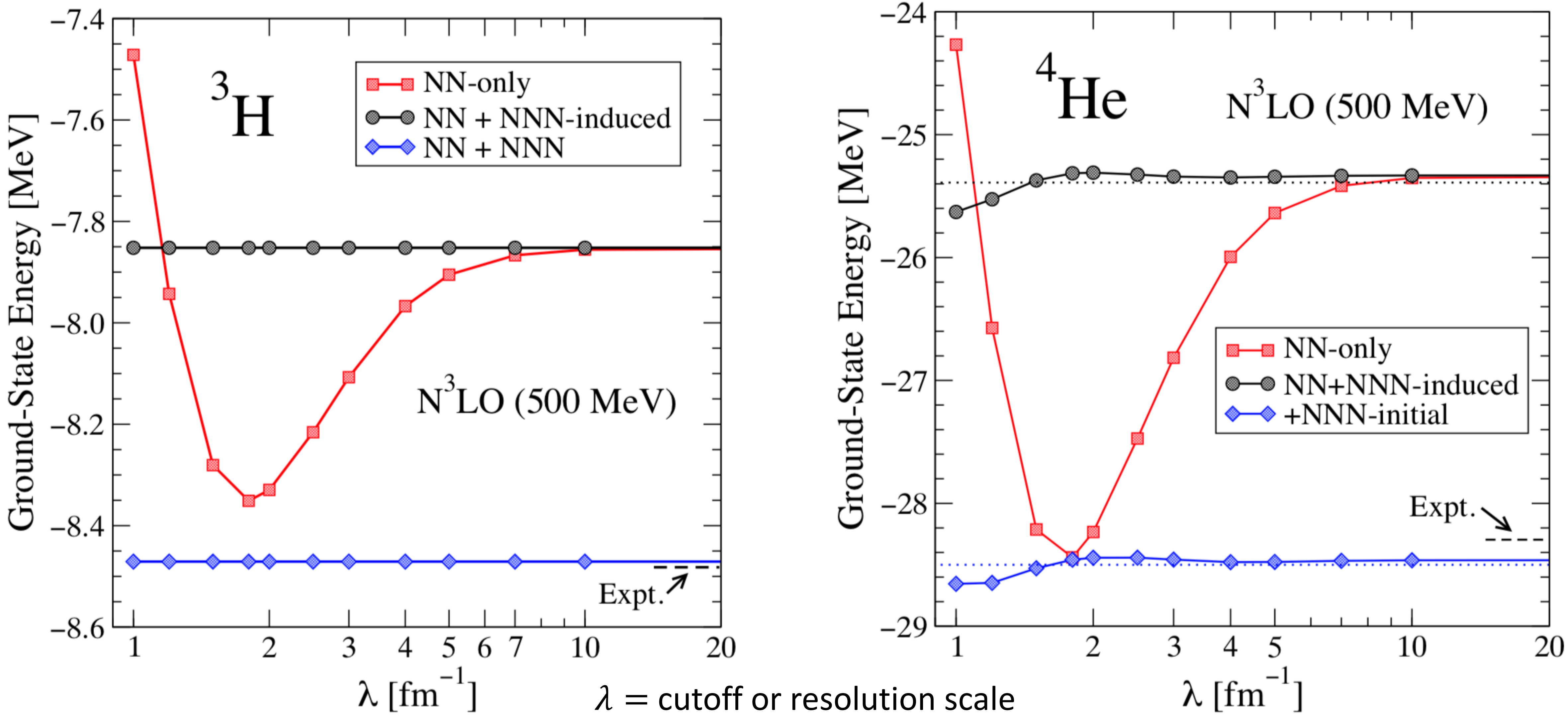

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Q: How large are (omitted in this calculation) four-nucleon forces?

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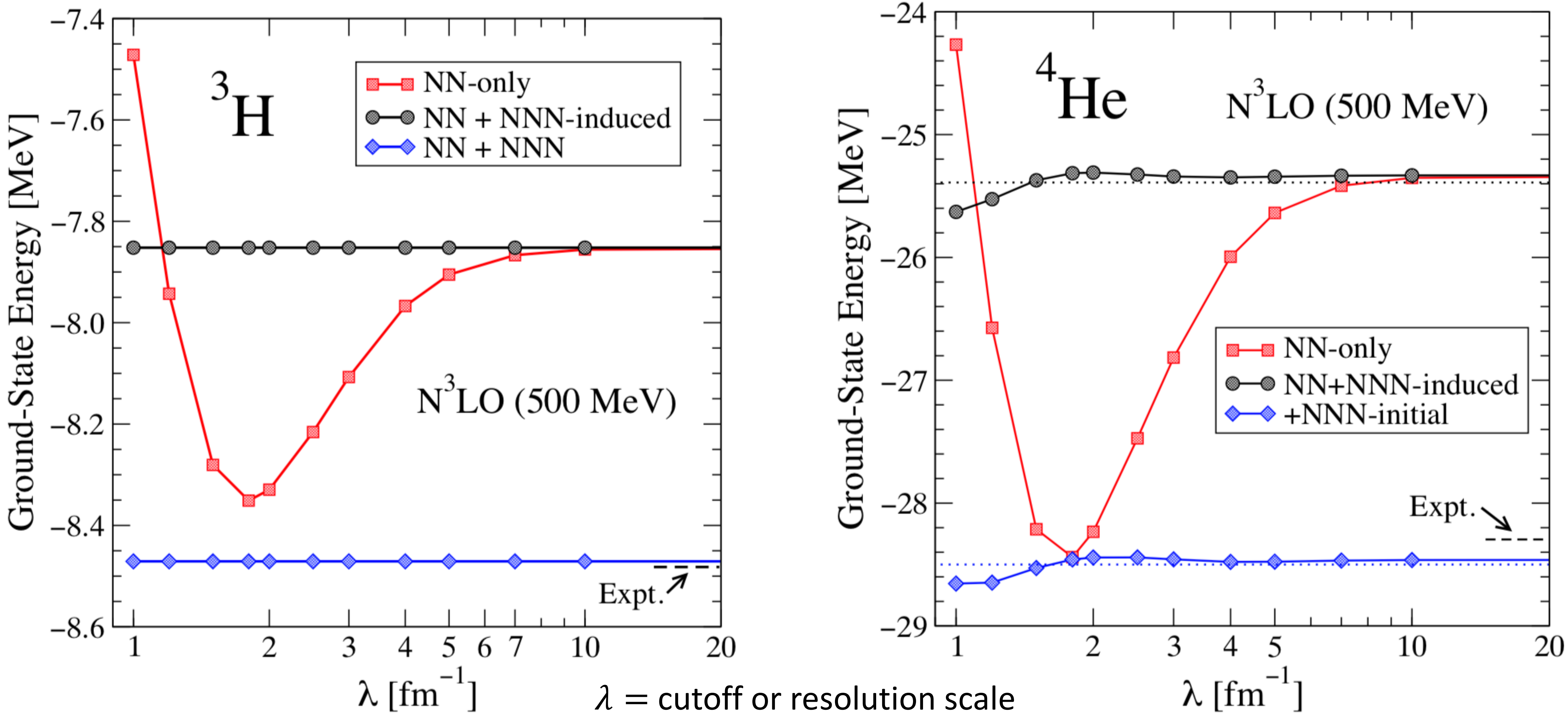

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A: The four-body system does not meet data; difference is about 0.2 MeV ⟷ 1% of binding energy

Size of Hilbert space in many-body calculations

Question: Once the single-particle basis is chosen, what is the dimension of the Hilbert space?

To answer this question, assume that we want to compute a nucleus with mass number A and using an interaction with a momentum cutoff Λ. [For $\Lambda = 2\text{fm}^{-1}$, one gets $n_s \approx (3 \dots 6)A$]

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Exact solution has exponential cost: Hilbert space dimension

- $\binom{2A}{A} \approx \left(\frac{1}{\pi A}\right)^{\frac{1}{2}} 4^A$ for $A \gg 1$.
- $\binom{3A}{A} \approx \left(\frac{3}{4\pi A}\right)^{\frac{1}{2}} \left(\frac{27}{4}\right)^A$ for $A \gg 1$.

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Q: Why solve an approximate Hamiltonian exactly?

Summary Hilbert spaces

- Simple arguments tie the nucleus and interaction under consideration to the dimension of Hilbert space
  - Smaller cutoffs are a big deal: they require much smaller bases
- The exact solution of the nuclear many-body computation is exponentially expensive