Nuclear Structure: Ab initio computations of atomic nuclei

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Thomas Papenbrock, The University of Tennessee & Oak Ridge National Laboratory

National Nuclear Physics Summer School
Bloomington, IN, July 15-26, 2024

Work supported by the US Department of Energy

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$$H\Psi = E\Psi$$

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Energy scales and relevant degrees of freedom

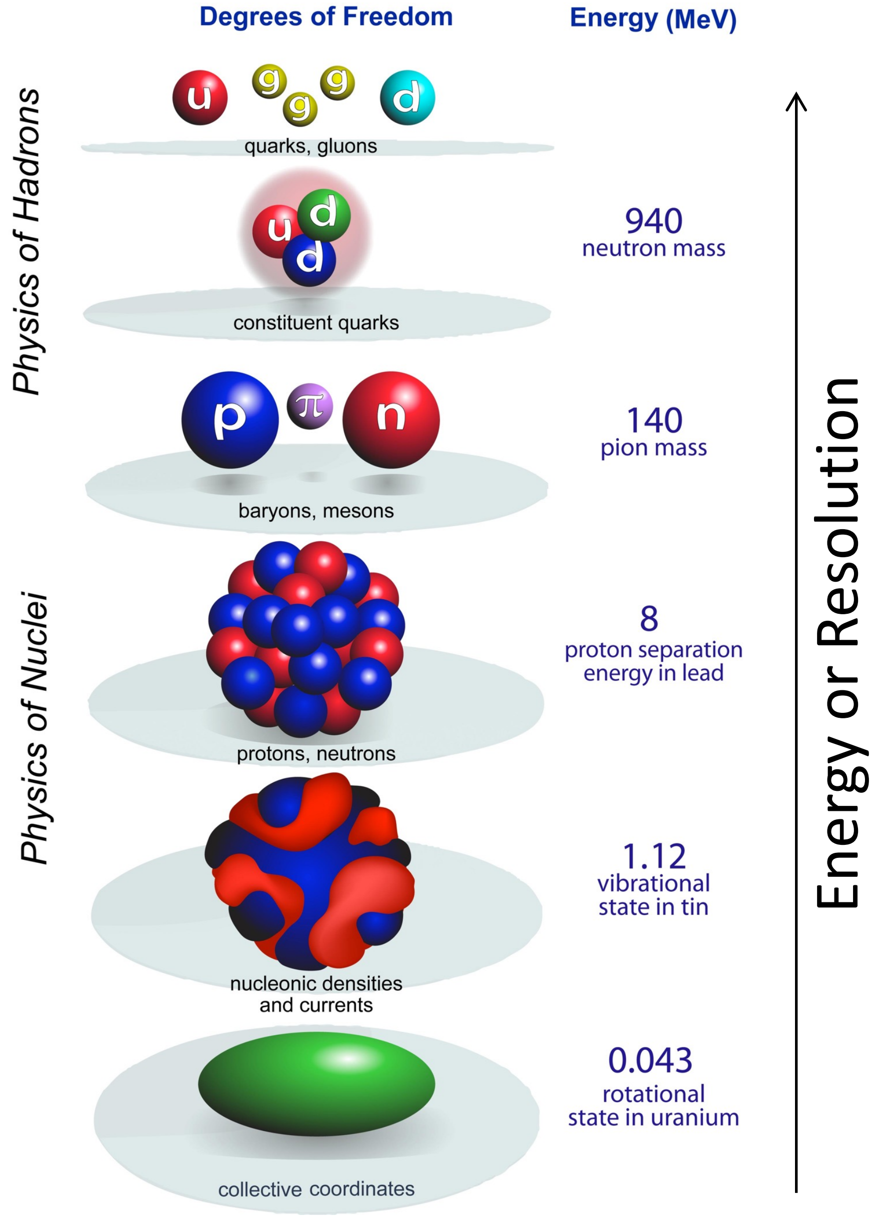
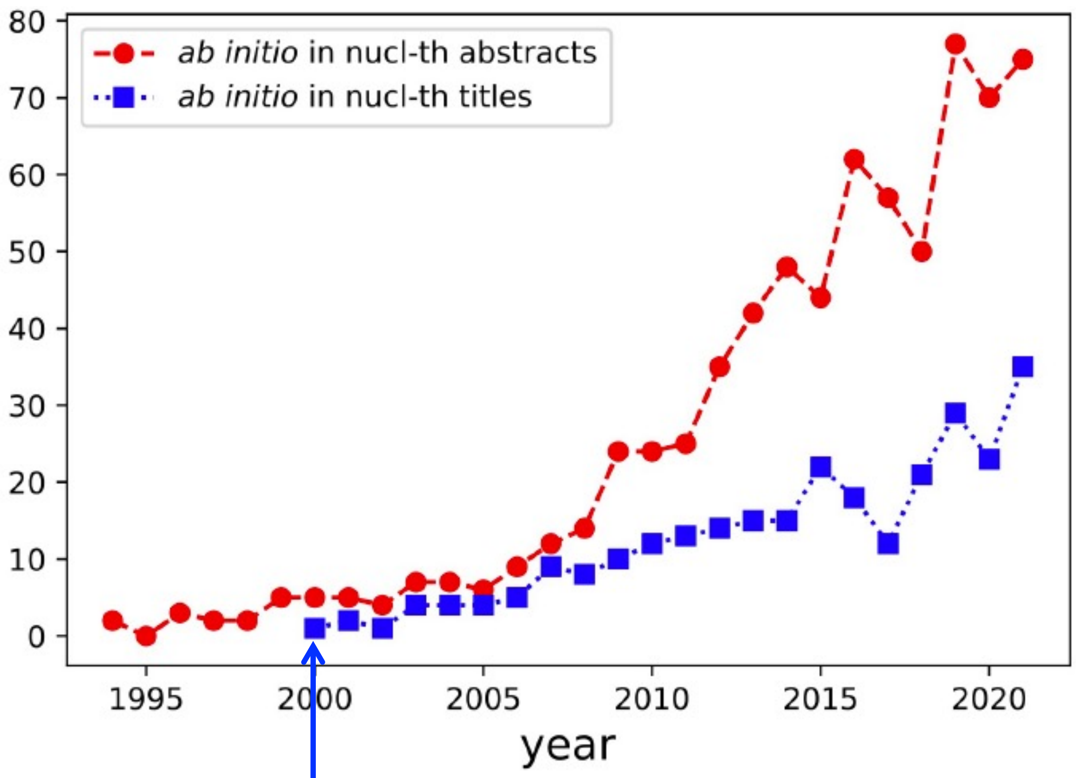


Fig.: Bertsch, Dean, Nazarewicz (2007)

- 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!

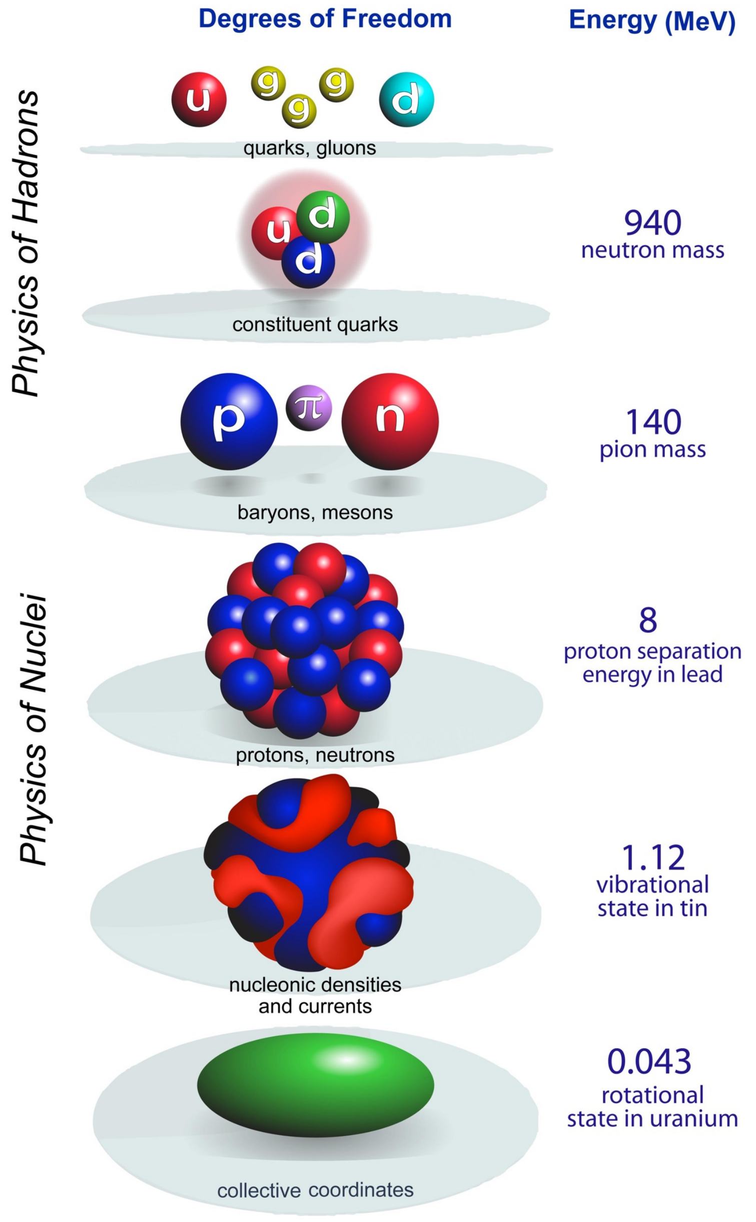
What is ab initio?



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."

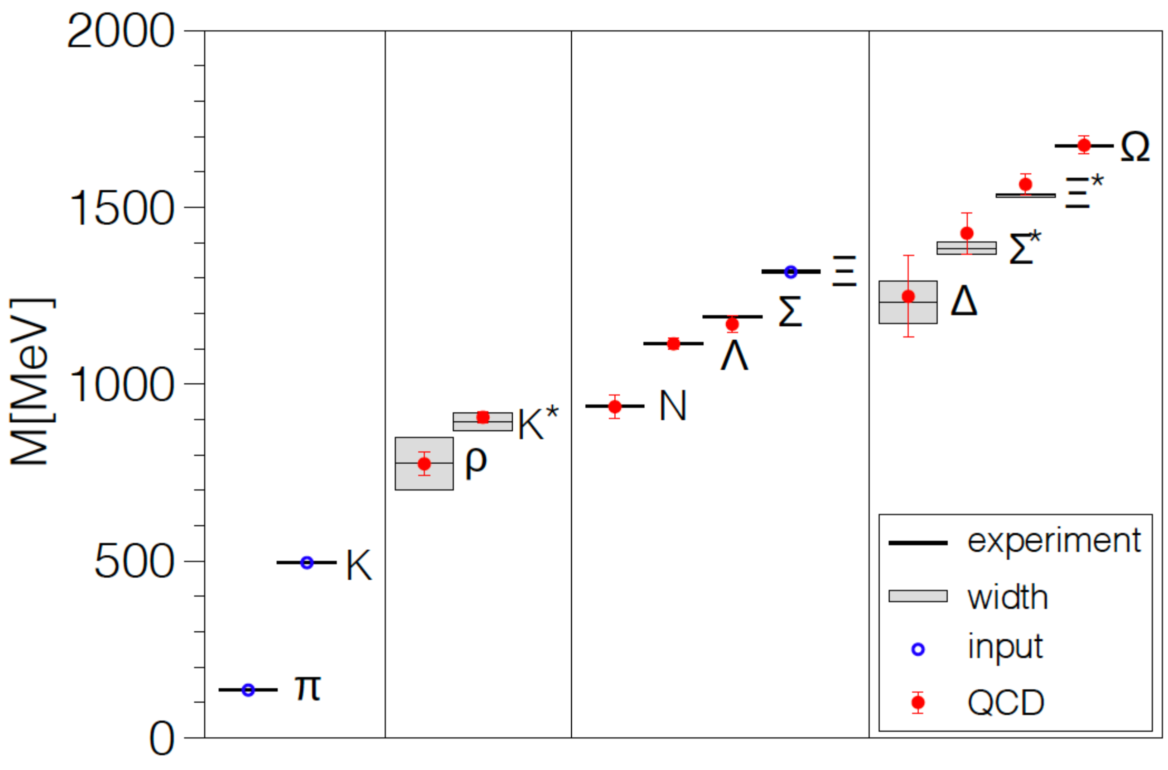
Q: What does this mean for computing atomic nuclei?

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

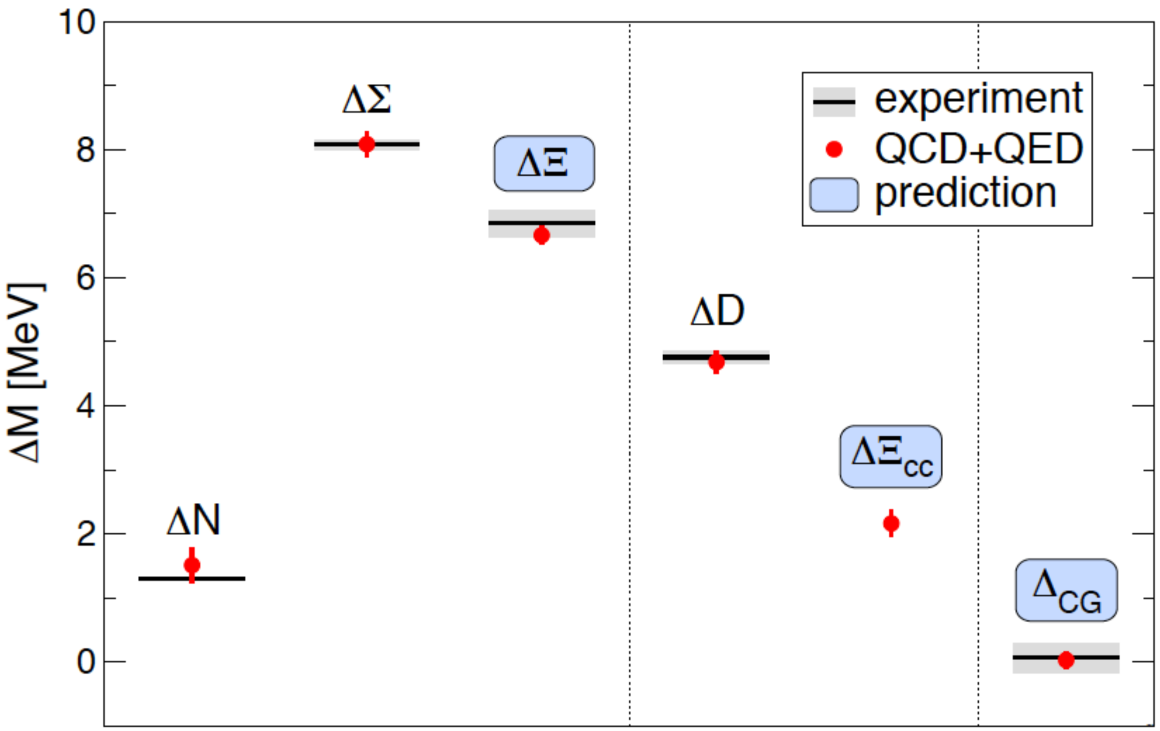
A2: Ab initio means starting from nucleons and the interactions between them.

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



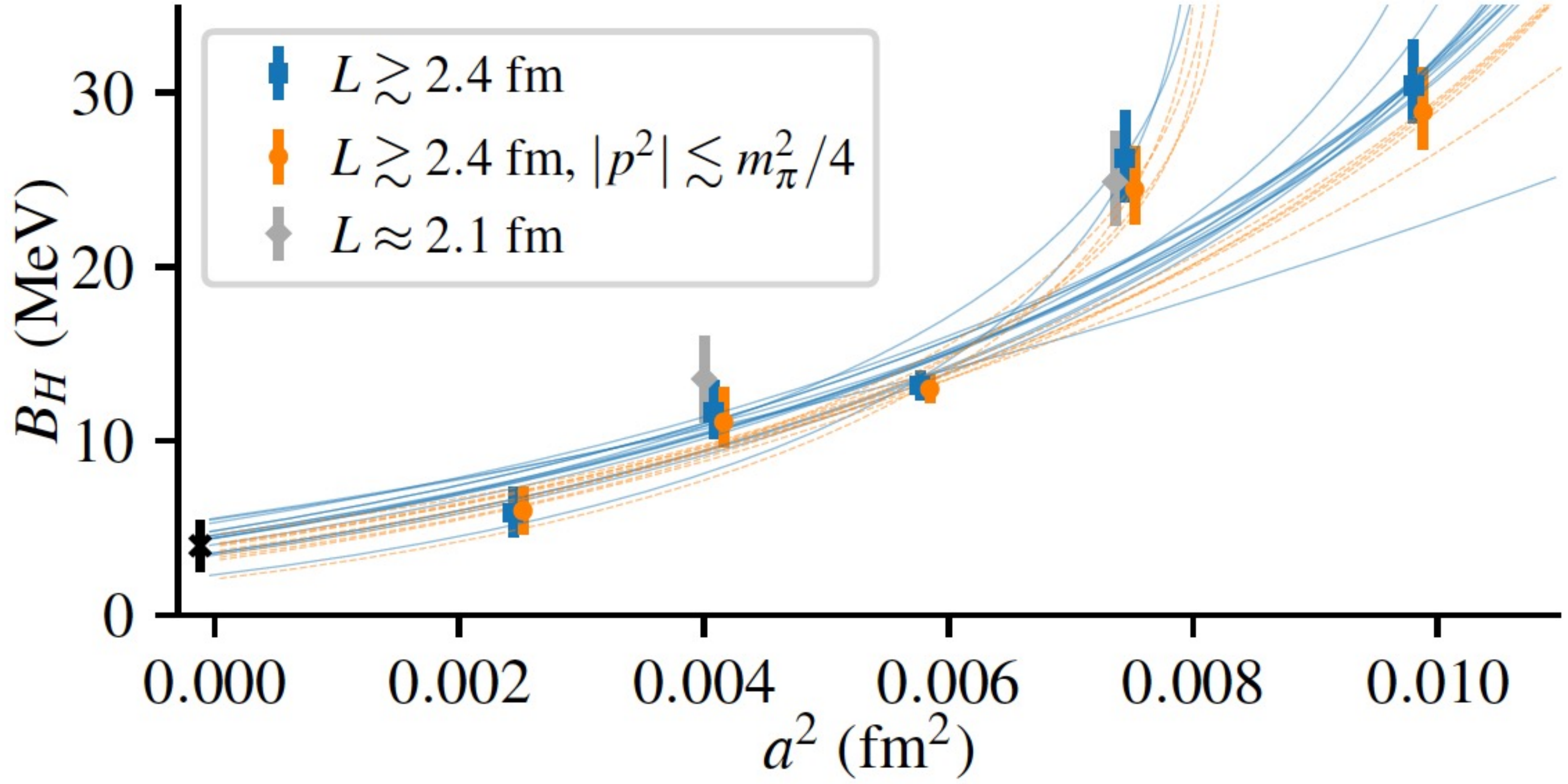
Proton-neutron mass splittings from lattice QCD & QED.
Borsanyi et al., Science (2015); arXiv:1406.4088

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 ✗

$$B_H = 3.97 \pm 1.16 \pm 0.86 \text{ MeV}$$

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

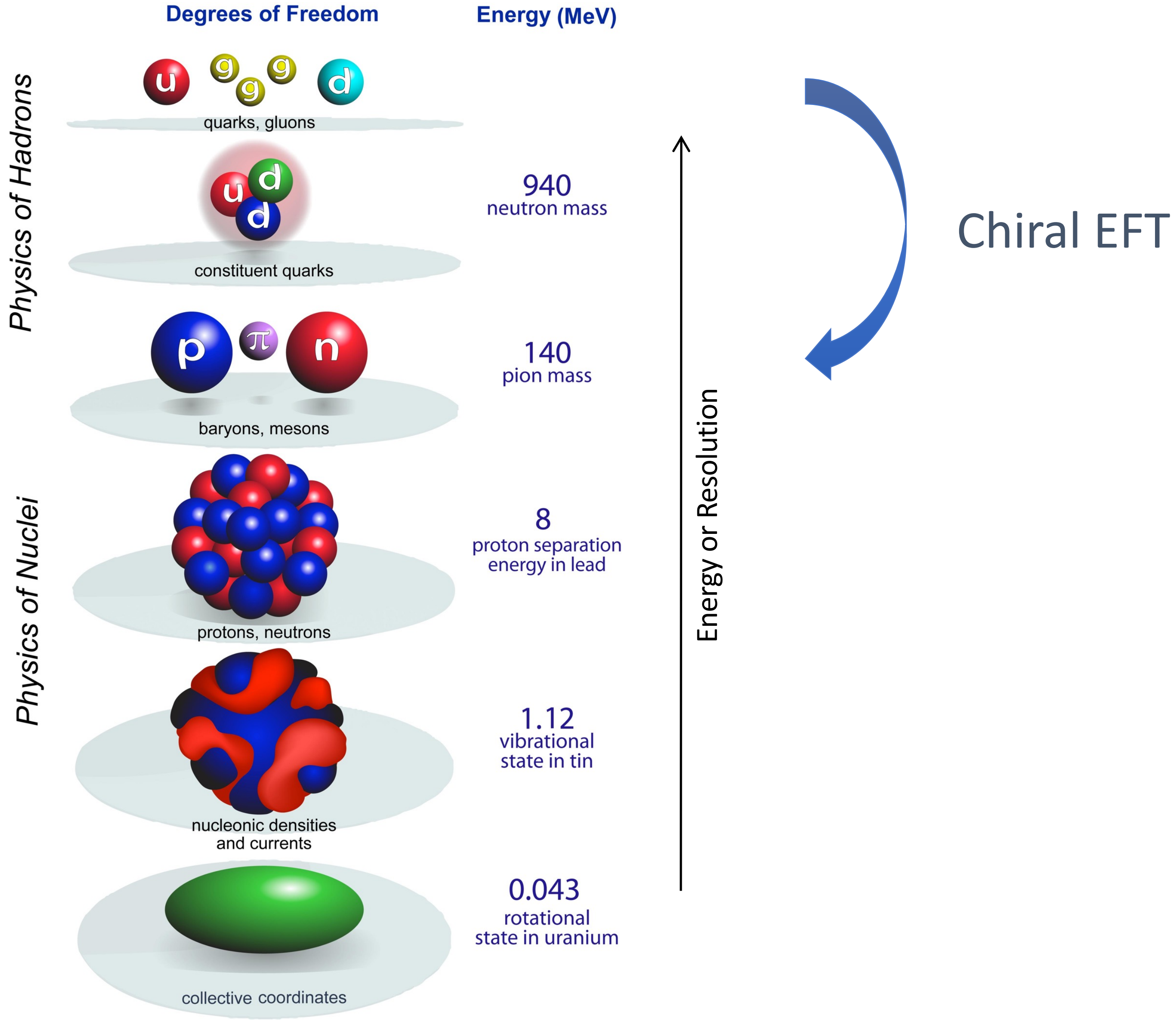
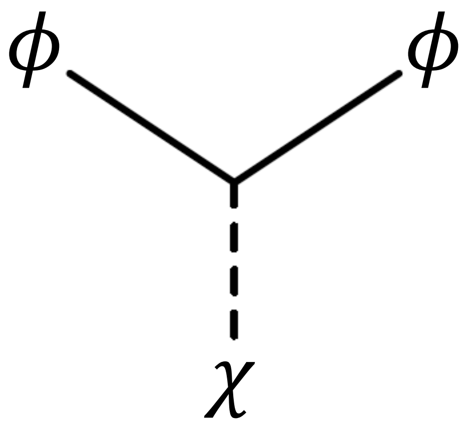


Fig.: Bertsch, Dean, Nazarewicz (2007)

Effective field theories: ideas

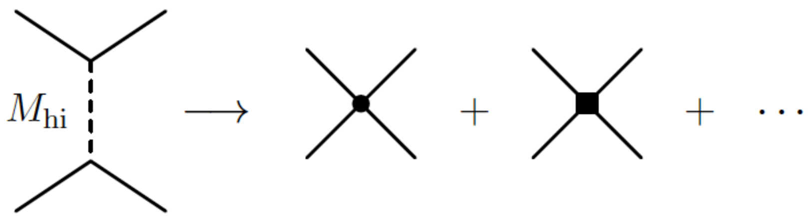
Fields ϕ, χ. Interaction via exchange of a heavy meson χ with mass M_{hi}



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

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.

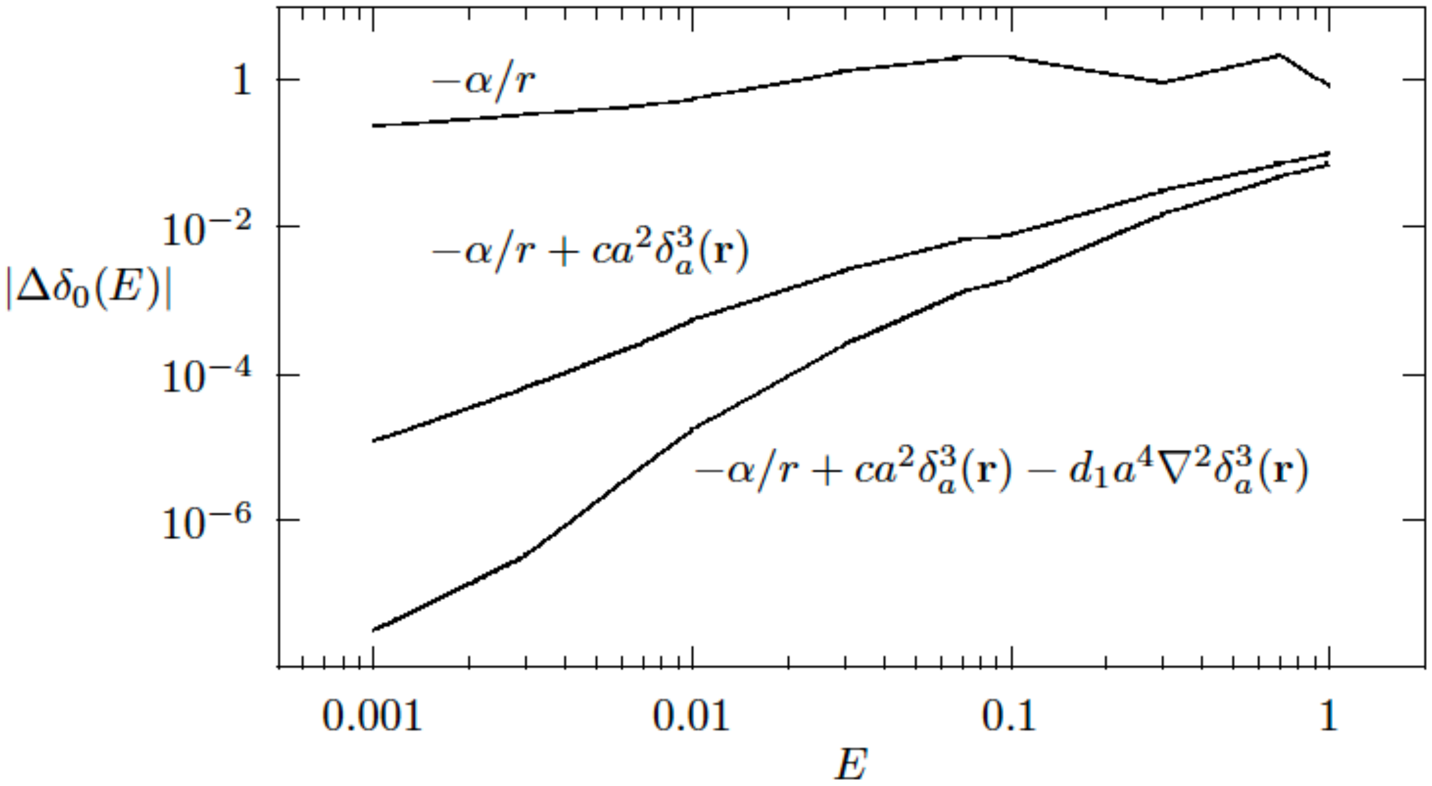
Q: How to reproduce available scattering data for this potential?

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.

Short-range physics is not resolved at low energies.

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, …]

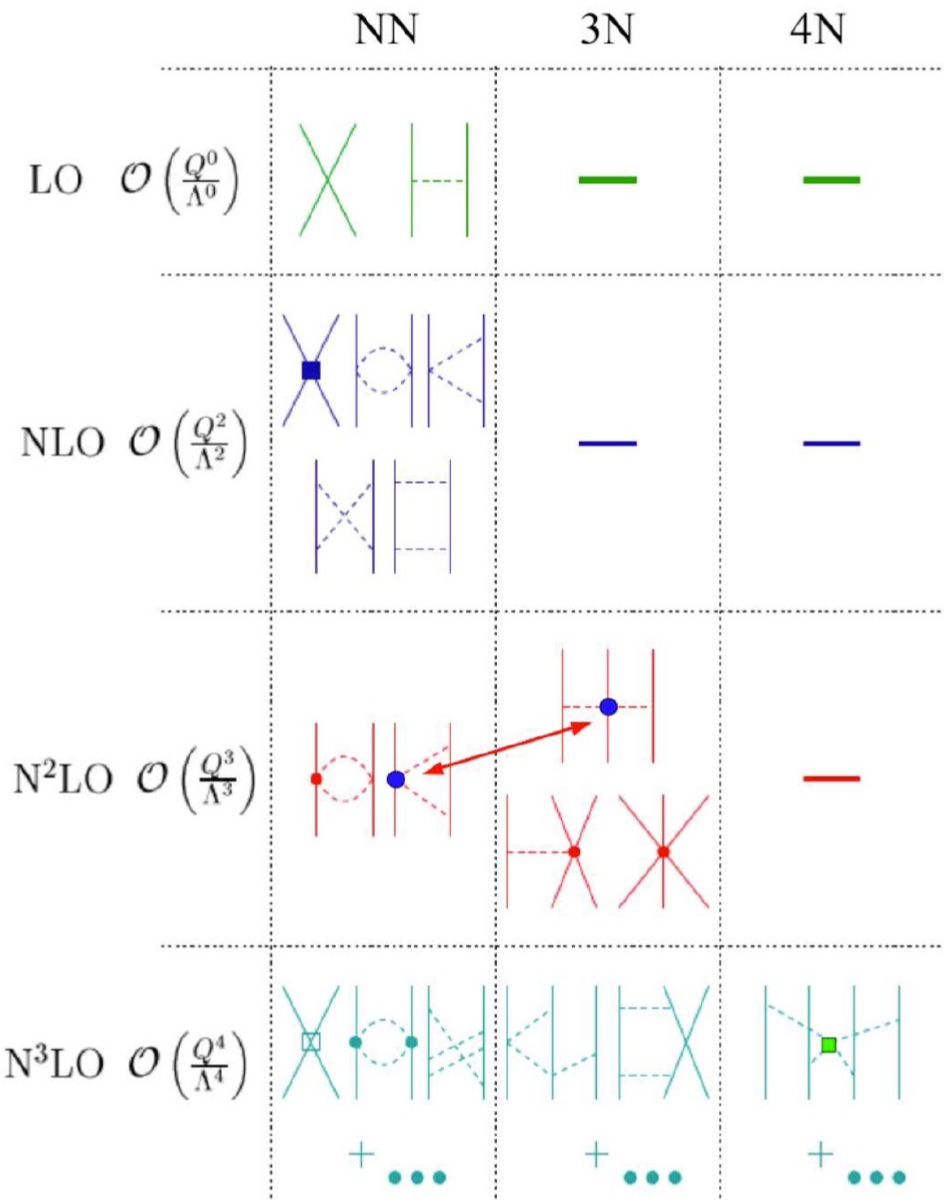
- The pion is the Nambu-Goldstone boson of the spontaneously broken chiral symmetry
  - Severely constrains the form of the nucleon-pion interaction ☺
  - Interactions between Nambu-Goldstone bosons are weak ☺
  - Provides the connection to QCD via chiral perturbation theory
- Pion exchange constitutes 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: $V(q) = -\frac{g_A^2}{4f_\pi^2}\frac{(\sigma_1 \cdot q)\,(\sigma_2 \cdot q)}{m_\pi^2 + q^2}\tau_1 \cdot \tau_2$

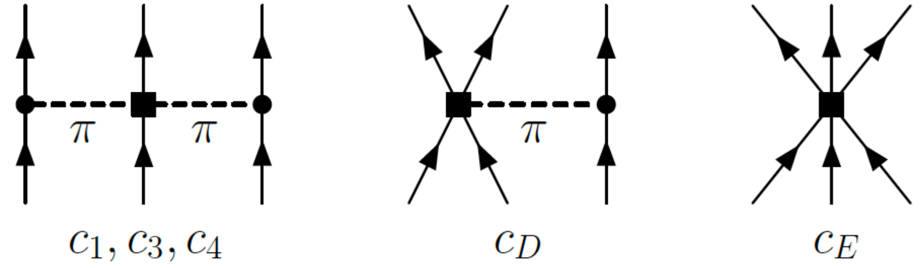
There are clouds in paradise (e.g. questions regarding the power counting), but these lectures will not dwell on them

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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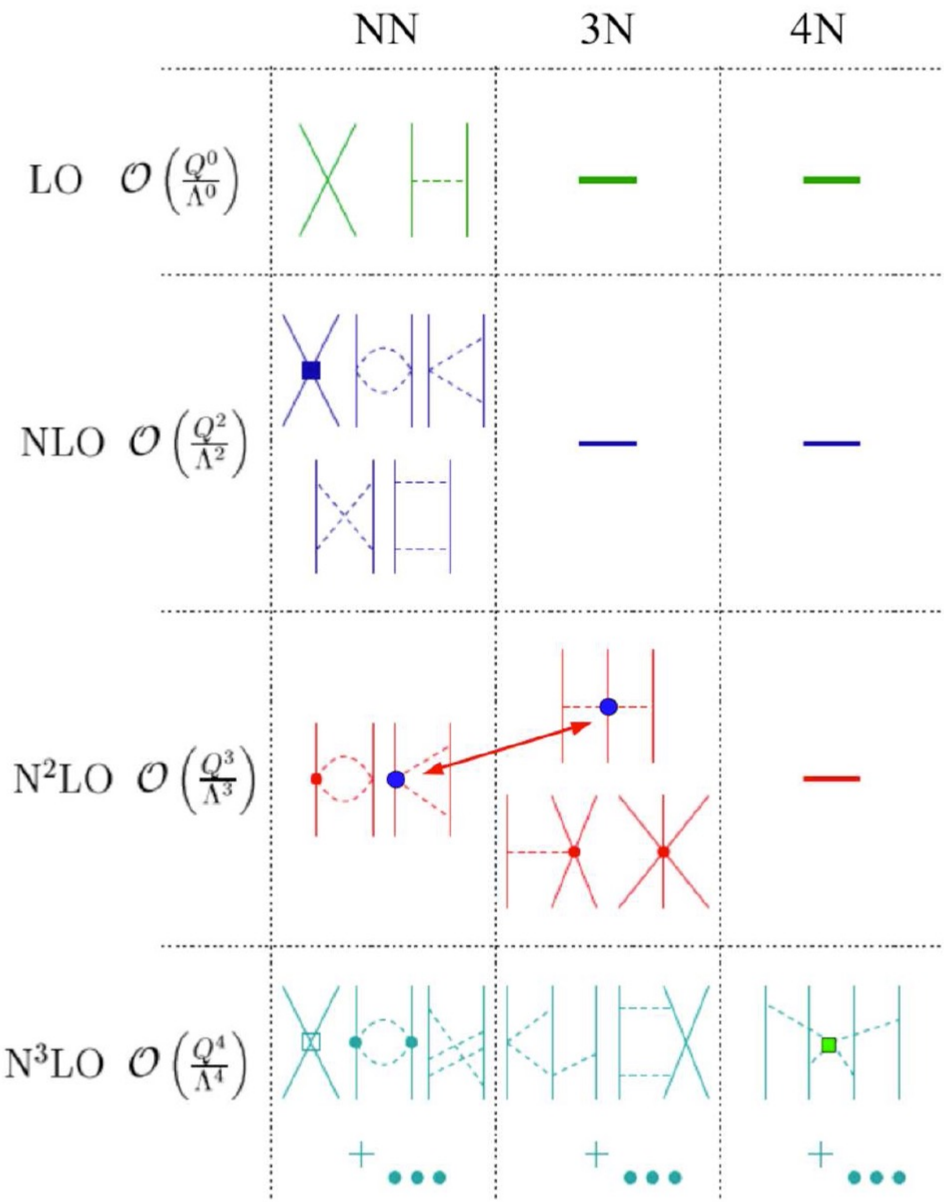

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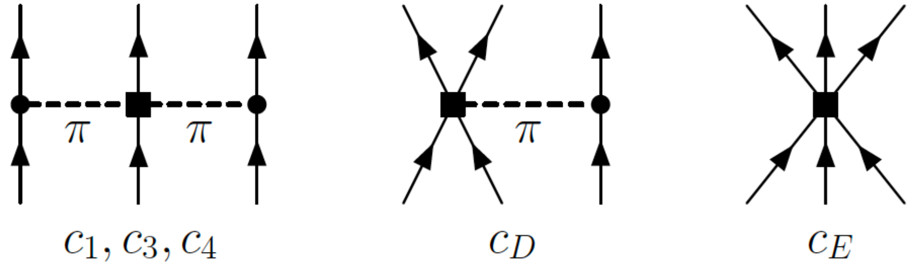

A1: In an EFT, one writes down everything that is allowed by symmetries and then orders according to a power counting

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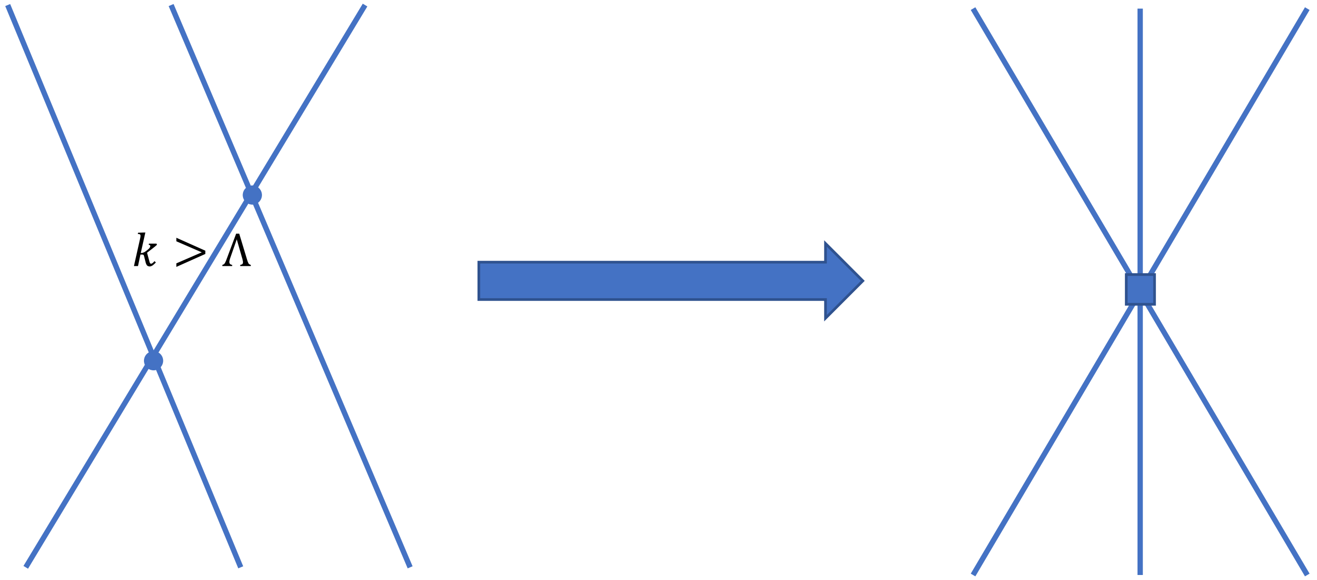
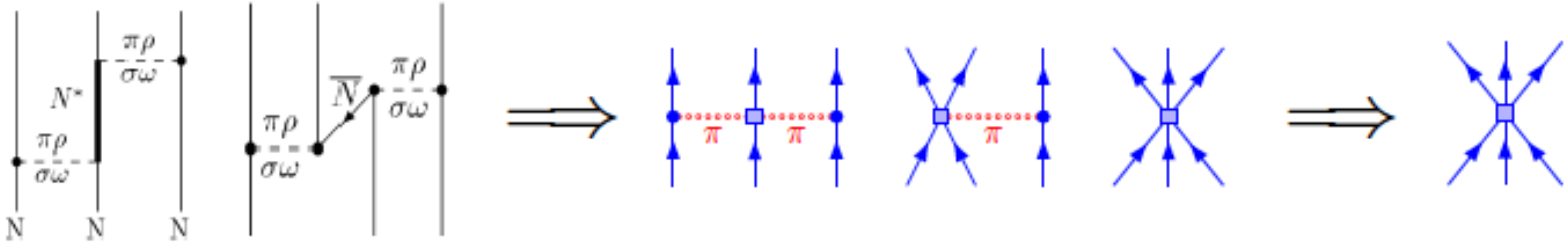
- What are omitted degrees of freedom? Can you draw diagrams that explain the origin of three nucleon forces?



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

3NFs in a theory with pions

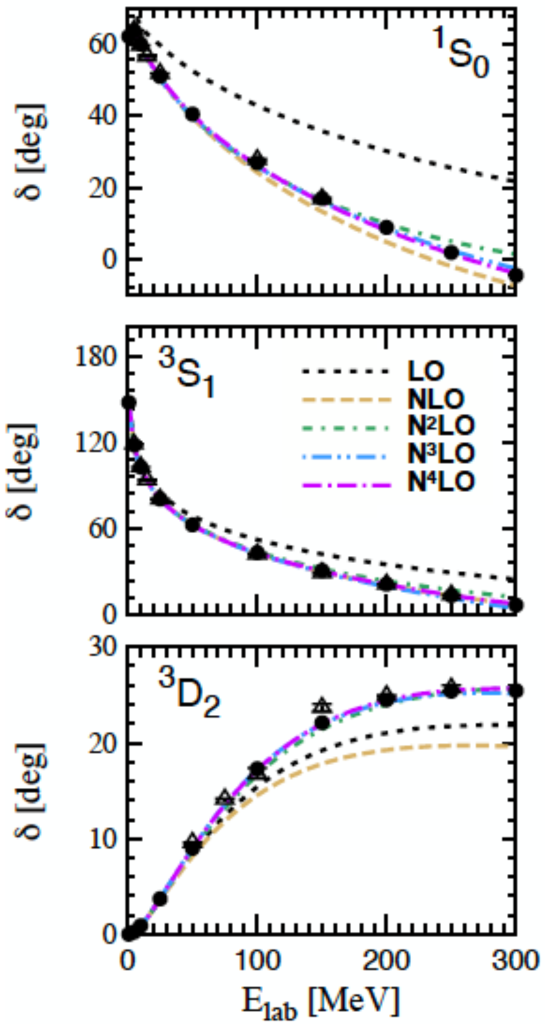


The essential rationale is:
Nuclei are extended objects, i.e. they have intrinsic degrees of freedom. They have excited states, can be deformed etc.
We treat nuclei as point particles, i.e. we neglect their intrinsic structure. While this is justified at low energies (low resolution), it comes with a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

Summary EFT Intro / three-nucleon forces

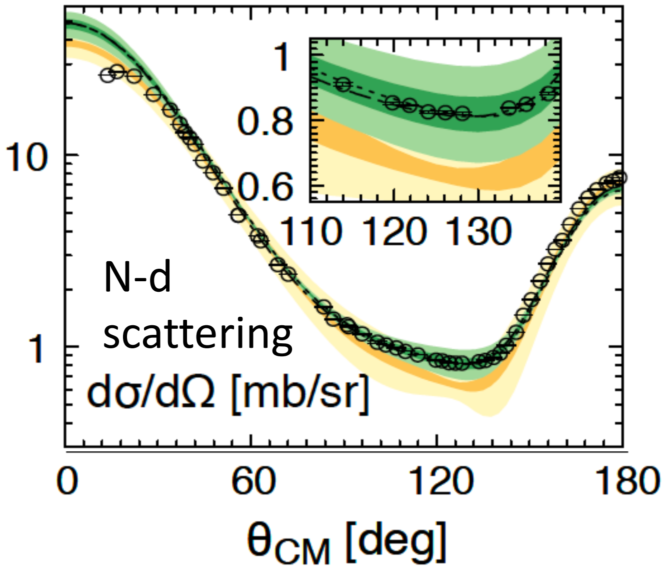
- Lattice QCD not yet there to compute nuclei
  - Even when that day arrives, the physical degrees of freedom are colorless hadrons
- Effective field theories can, in principle, be matched to QCD input
  - Meanwhile, we use data from nuclei
- Three-nucleon forces naturally arise as high-energy degrees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

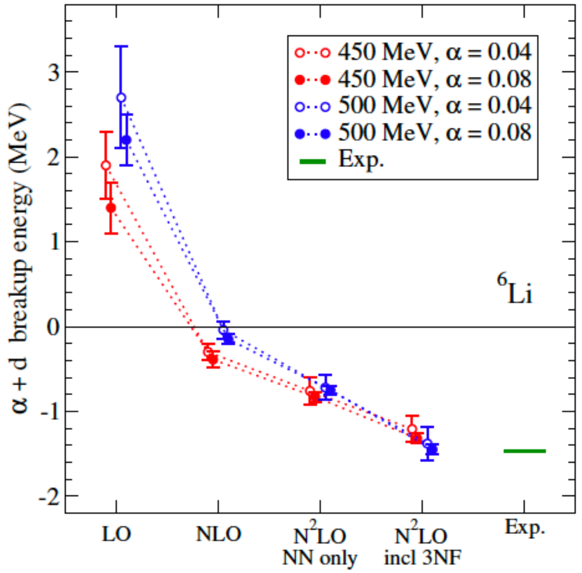
Chiral effective field theory: state of the art



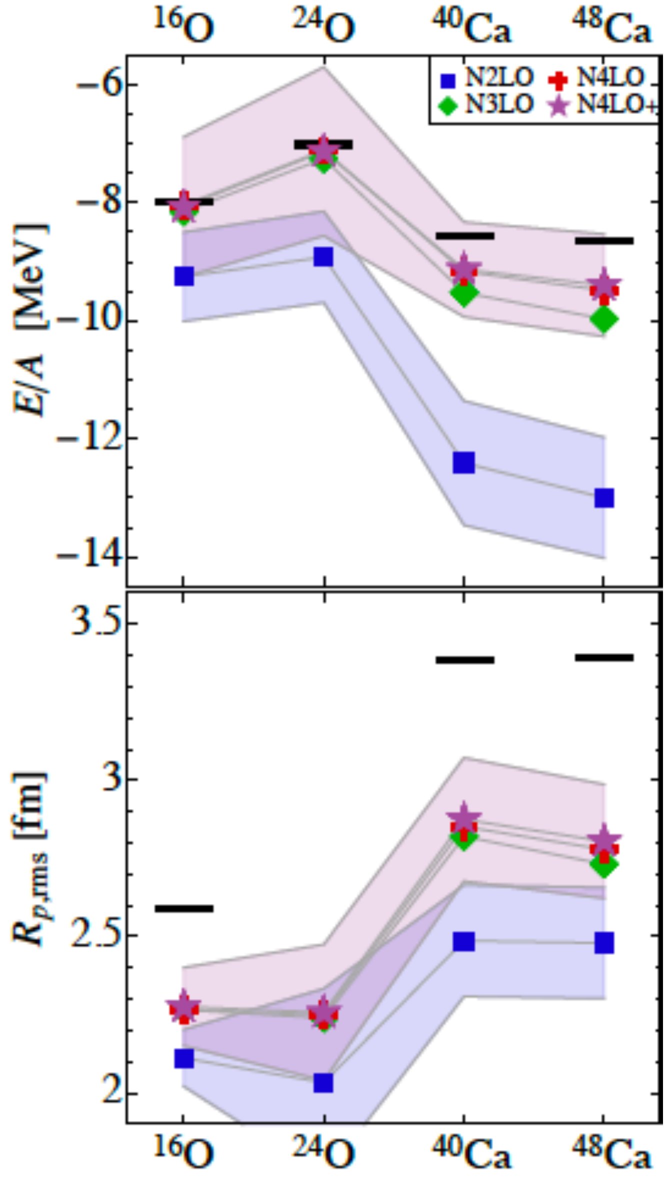
Reinert, Krebs, Epelbaum, Eur. Phys. J. A 54, 86 (2018)

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

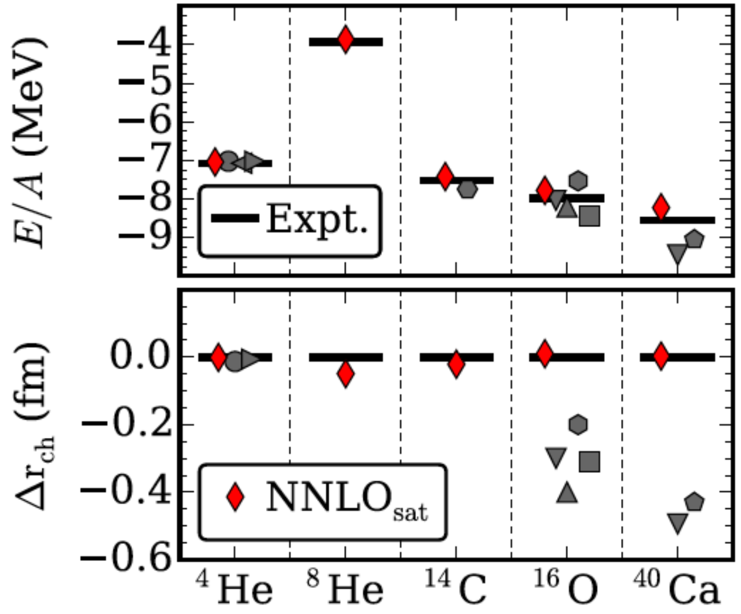
Problems:

- 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

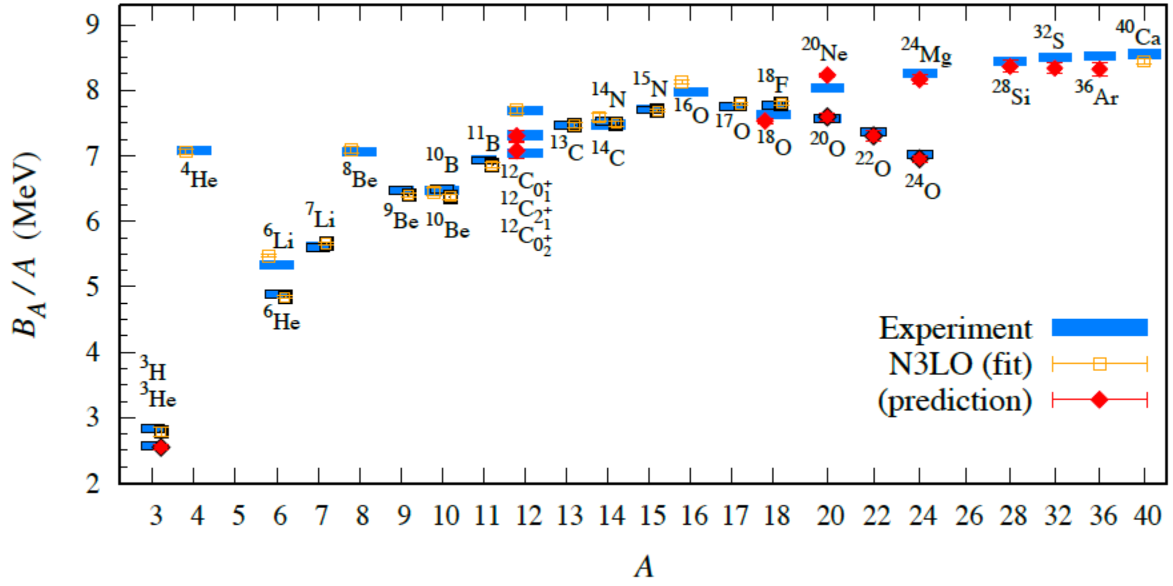
TABLE I. Binding energies (in MeV) and charge radii (in fm) for ^{3}H, ^{3,4}He, ^{14}C, and ^{16,22,23,24,25}O employed in the optimization of NNLO$_{sat}$.

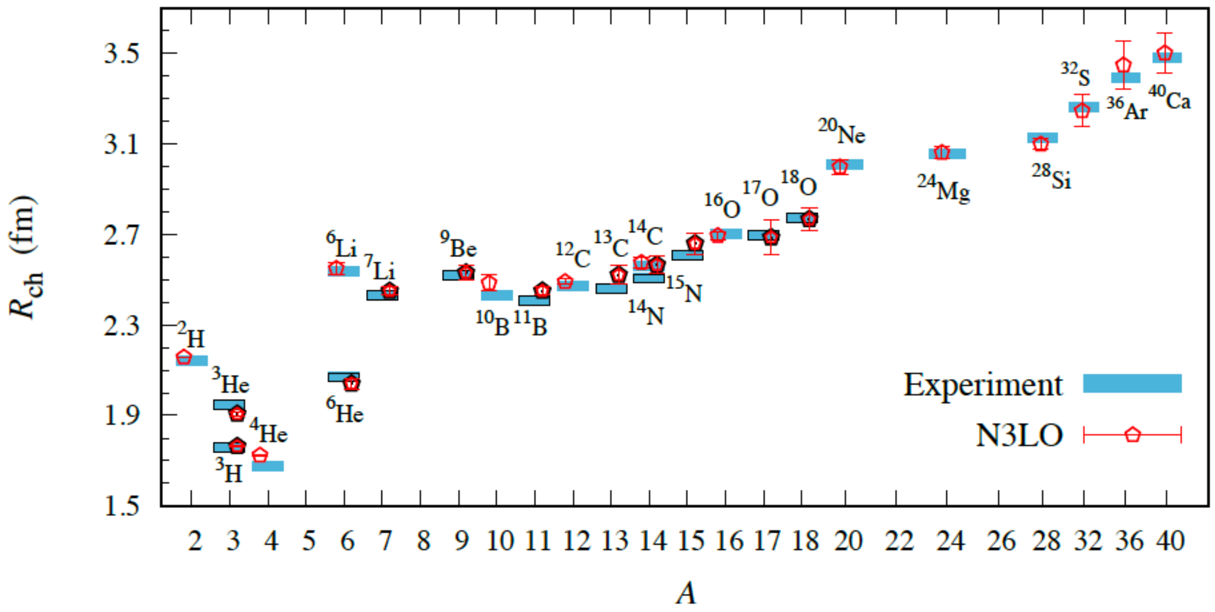
	$E_{g.s.}$	Expt. [69]	r_{ch}	Expt. [65,66]
^{3}H	8.52	8.482	1.78	1.7591(363)
^{3}He	7.76	7.718	1.99	1.9661(30)
^{4}He	28.43	28.296	1.70	1.6755(28)
^{14}C	103.6	105.285	2.48	2.5025(87)
^{16}O	124.4	127.619	2.71	2.6991(52)
^{22}O	160.8	162.028(57)		
^{24}O	168.1	168.96(12)		
^{25}O	167.4	168.18(10)		



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)

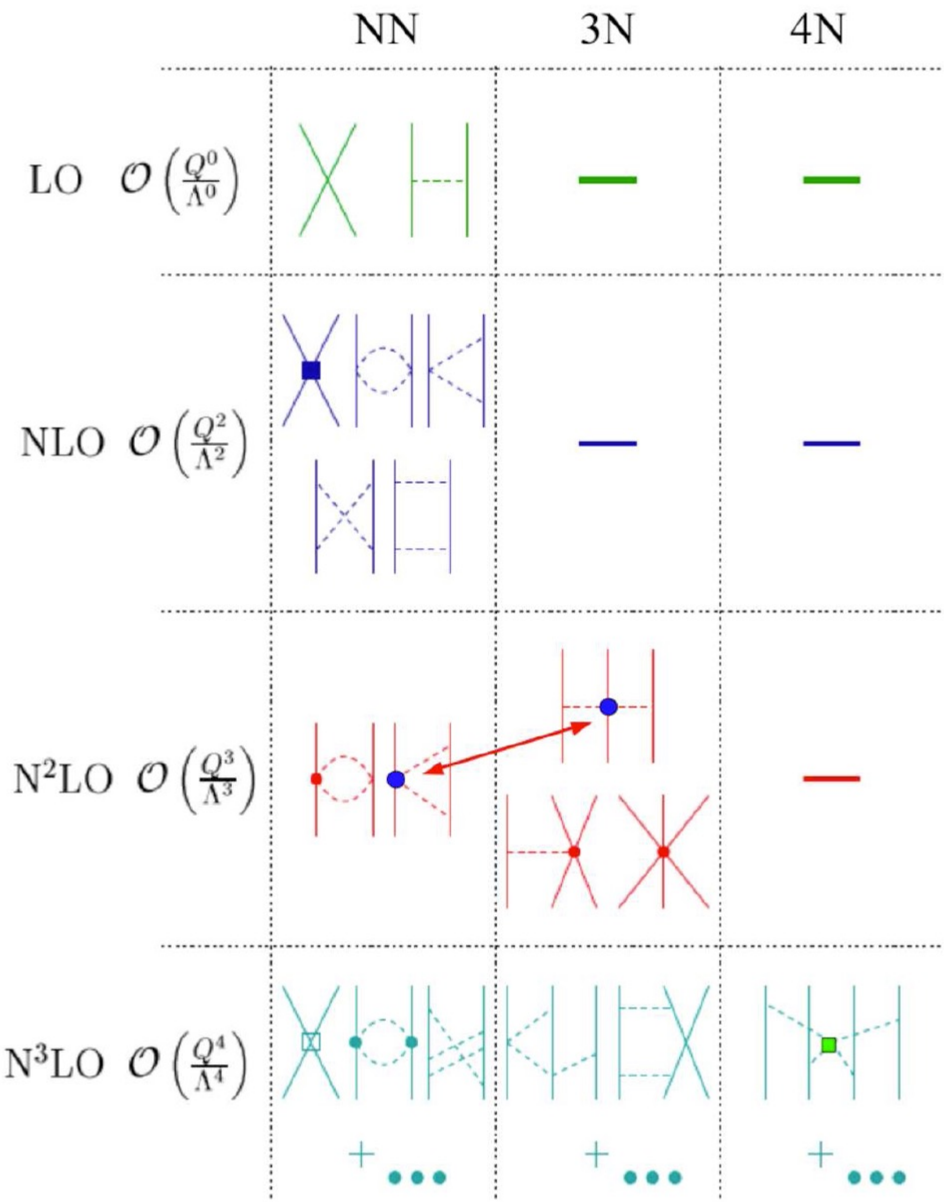
Adjusted energies of cluster states
(e.g. ^{8}Be = ^{4}He + ^{4}He, Hoyle state in ^{12}C = ^{4}He + ^{4}He + ^{4}He)

Result: accurate charge radii come out

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

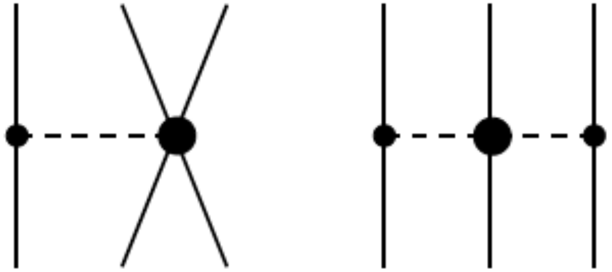
Chiral effective field theory: consistency of currents and interactions

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



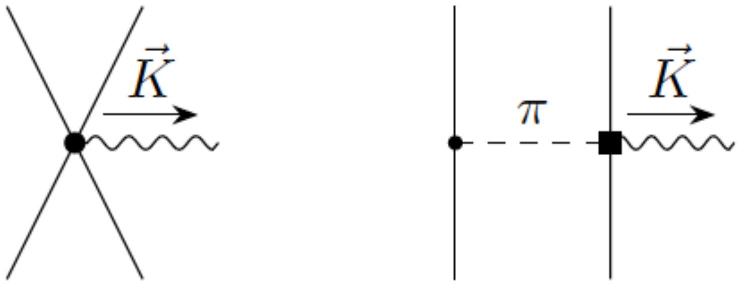
Effective field theories provide us with a consist formulation of

interactions



and

currents:



Heavy meson exchange c_D

Pion exchange $c_3,\ c_4$

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

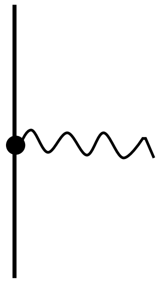
Consistency between Hamiltonians and currents
example: electromagnetic interactions

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

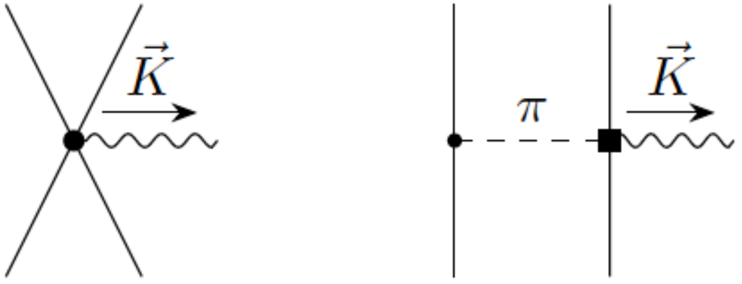
Continuity equation $\frac{d\rho}{dt} = -\nabla \cdot j$

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



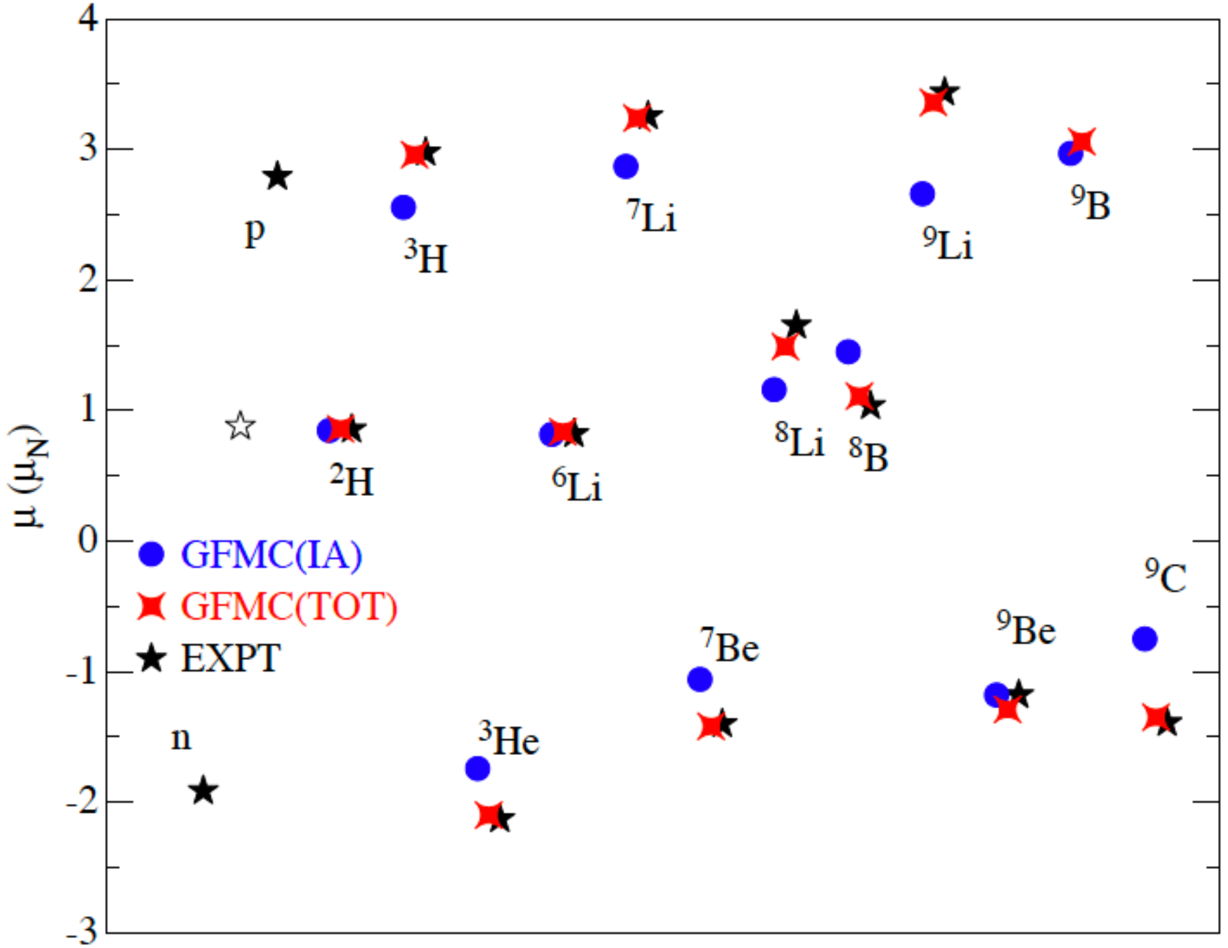
Subleading corrections: 2-body currents
a.k.a. “meson-exchange currents”



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

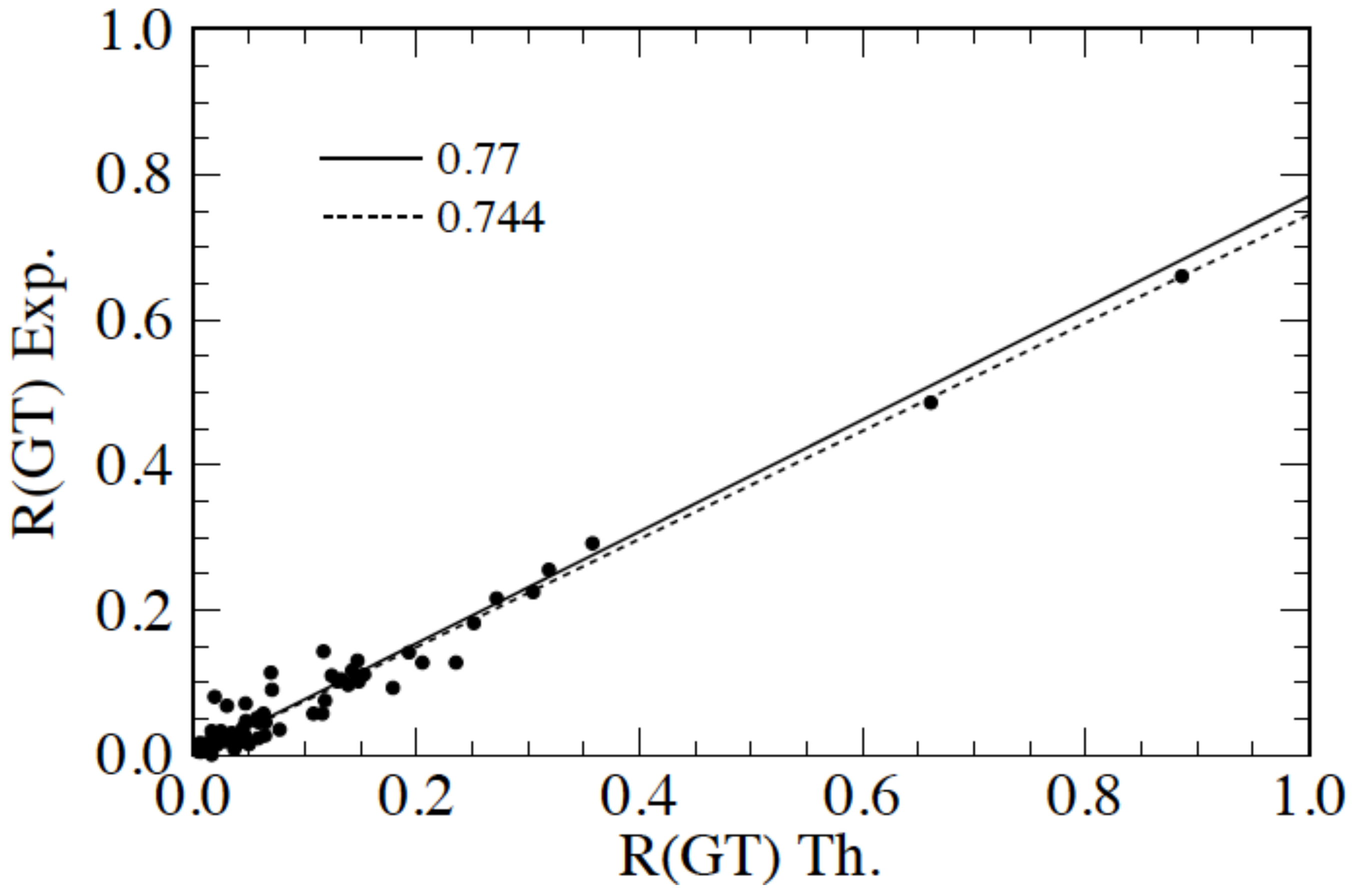


S. Pastore, Steven C. Pieper, R. Schiavilla, R. B. Wiringa, Phys. Rev. C 87, 035503 (2013); arXiv:1212.3375

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

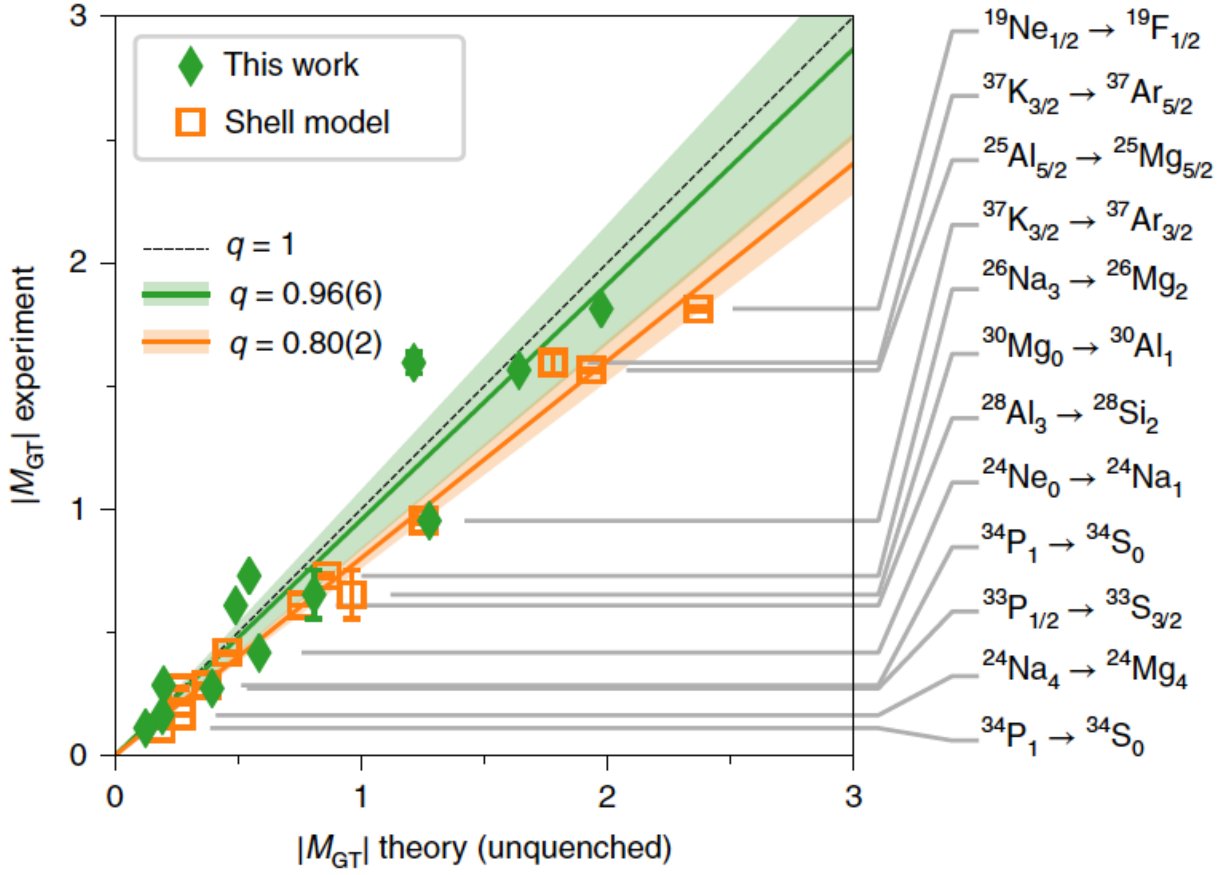
Puzzle: The strengths of Gamow-Teller transitions (operator $\propto g_A\vec{\sigma}\tau^{\pm}$) in nuclei are smaller ("quenched") than what is expected from the β-decay of the free neutron.

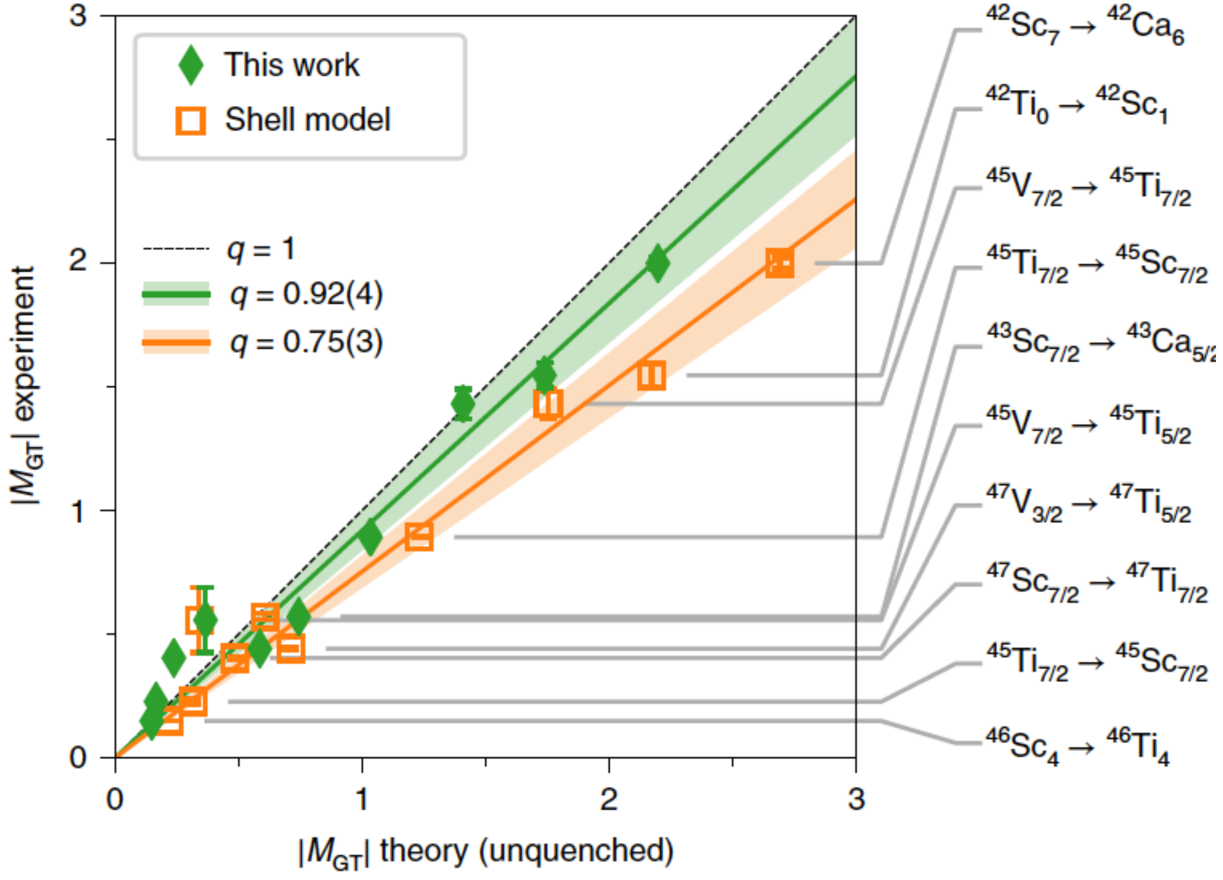
- Wilkinson (1973): quenching factor $q^2 \approx 0.90$ for nuclei with $A = 17 \ldots 21$
- Brown & Wildenthal (1985): quenching factor $q^2 \approx 0.77$ for nuclei with $A = 17 \ldots 40$
- Martinez-Pinedo et al. (1996): quenching factor $q^2 \approx 0.74$ for nuclei with $A = 40 \ldots 60$



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

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

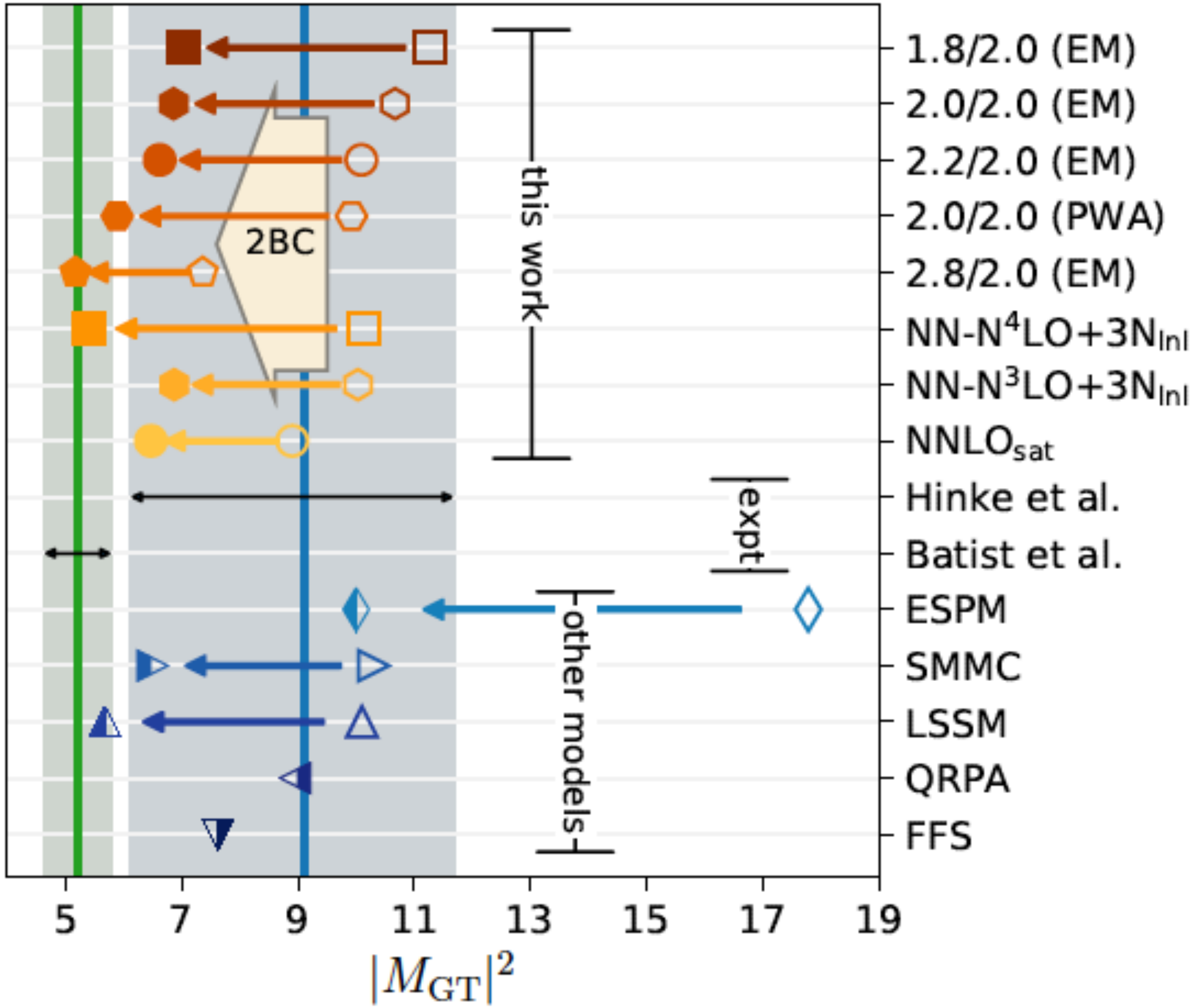




IMSRG computations with NN-N^{4}LO + 3Nlnl interaction

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.

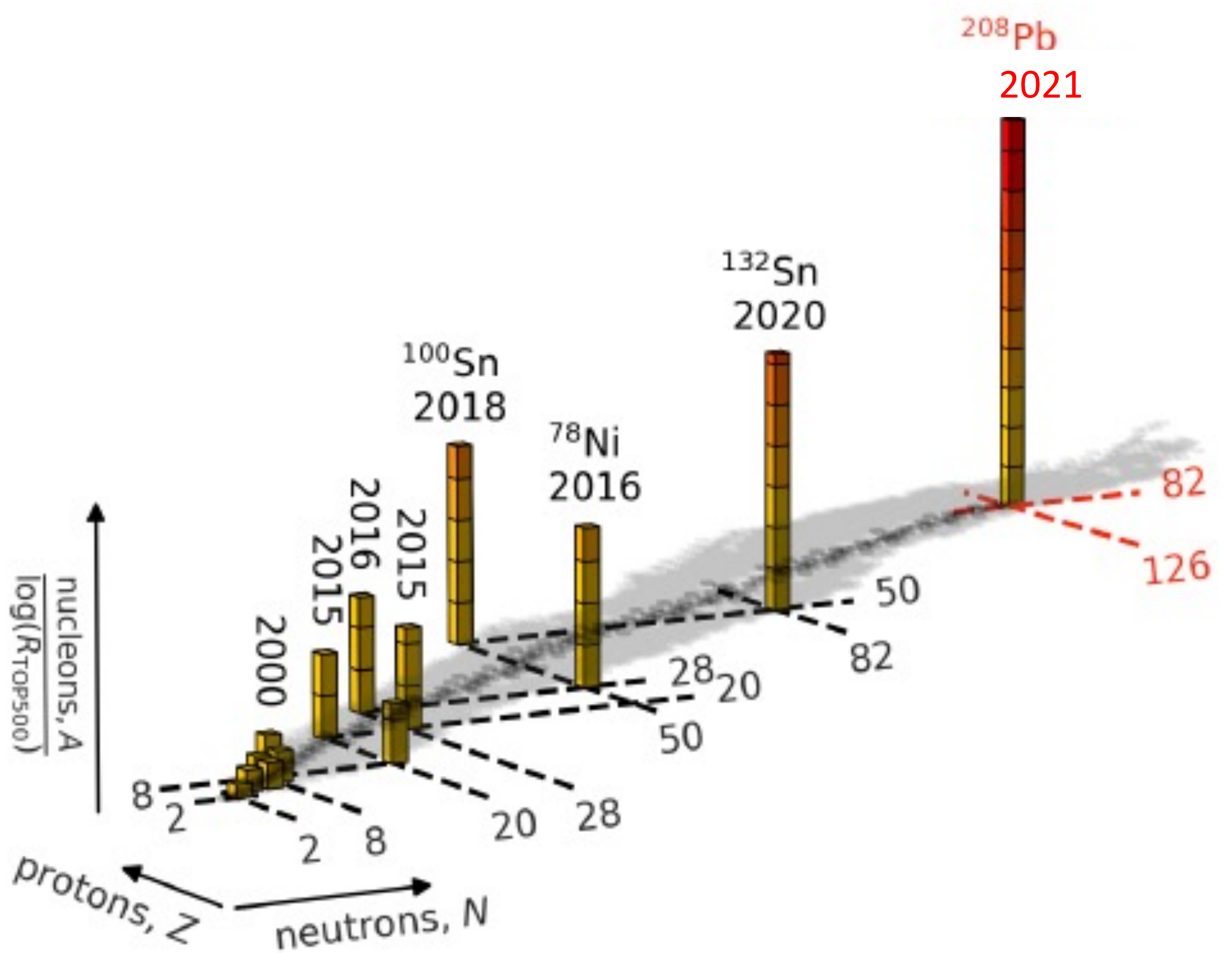
Traditional models need quenching factors to describe data.
(open symbols: no quenching).

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:
2. Spherical harmonic oscillator with maximum energy $\left(N+\frac{3}{2}\right)\hbar\omega$ and oscillator length $b=\left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}$
    - Conserved quantities:
    - Lacking/not conserved:
    - IR/UV cutoffs:

Symmetries of the single-particle basis

Bases:

1. Lattice in position space with periodic boundary conditions (L^3 sites, lattice spacing a)
   - Conserved quantities: momentum, parity
   - Lacking/not conserved:
   - IR/UV cutoffs:
2. Spherical harmonic oscillator with maximum energy $\left(N + \frac{3}{2}\right)\hbar\omega$ and oscillator length $b = \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}$
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Symmetries of the single-particle basis

Bases:

1. Lattice in position space with periodic boundary conditions (L^3 sites, lattice spacing a)
   - Conserved quantities: momentum, parity
   - Lacking/not conserved: angular momentum
   - IR/UV cutoffs:
2. Spherical harmonic oscillator with maximum energy $\left(N + \frac{3}{2}\right) \hbar\omega$ and oscillator length $b = \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}$
   - Conserved quantities:
   - Lacking/not conserved:
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Symmetries of the single-particle basis

Bases:

1. Lattice in position space with periodic boundary conditions (L^3 sites, lattice spacing a)
   - Conserved quantities: momentum, parity
   - Lacking/not conserved: angular momentum
   - IR/UV cutoffs: $\Lambda_{IR} = \frac{\pi}{La}, \Lambda_{UV} = \frac{\pi}{a}$
2. Spherical harmonic oscillator with maximum energy $\left(N + \frac{3}{2}\right)\hbar\omega$ and oscillator length $b = \left(\frac{\hbar}{m\omega}\right)^{\frac{1}{2}}$
   - Conserved quantities:
   - Lacking/not conserved:
   - IR/UV cutoffs:

Symmetries of the single-particle basis

Bases:

1. Lattice in position space with periodic boundary conditions (L^3 sites, lattice spacing a)
   - Conserved quantities: momentum, parity
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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.

Efficient computations of atomic nuclei

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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 (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!

Efficient computations of atomic nuclei

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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

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

SRG evolution of a chiral potential

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

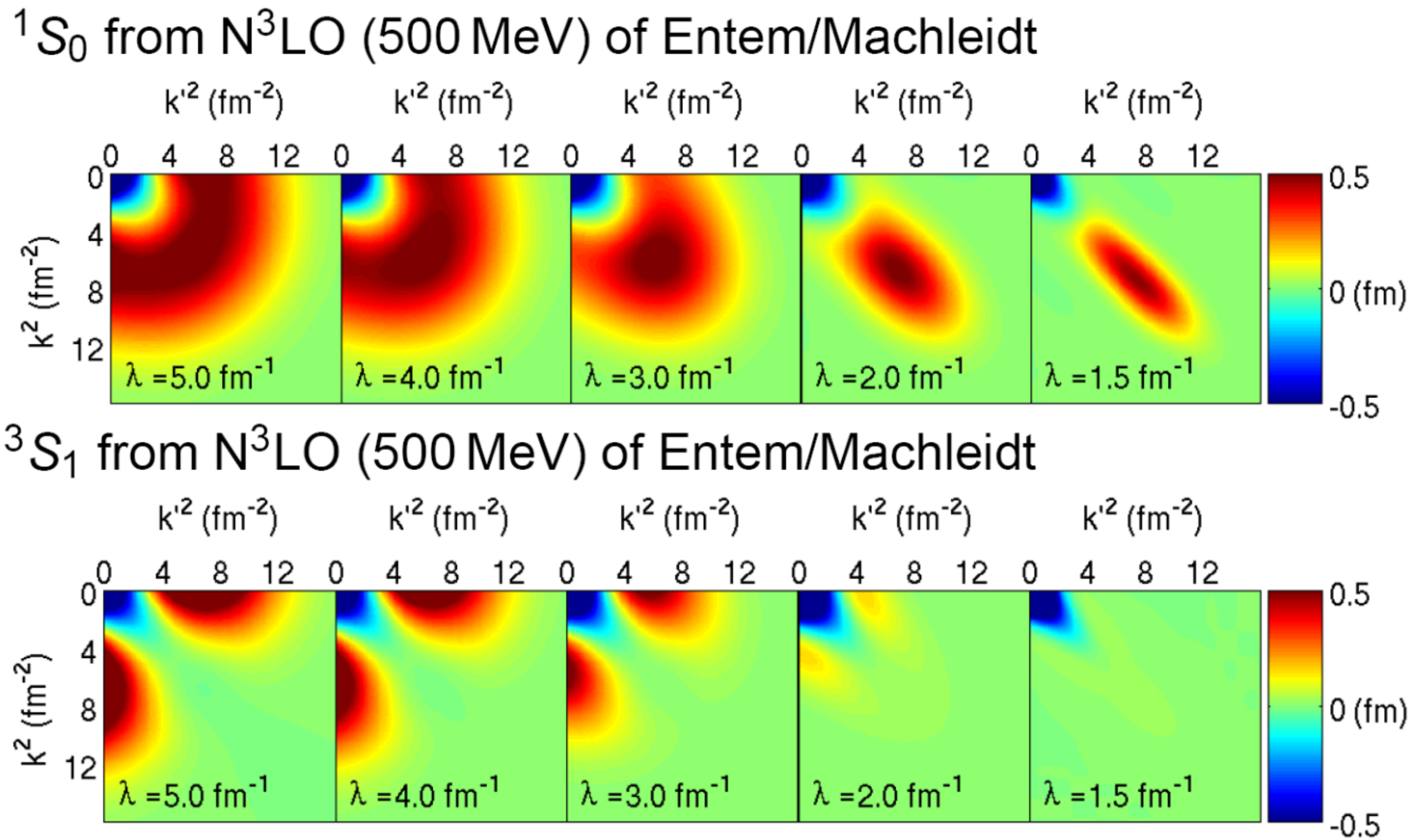
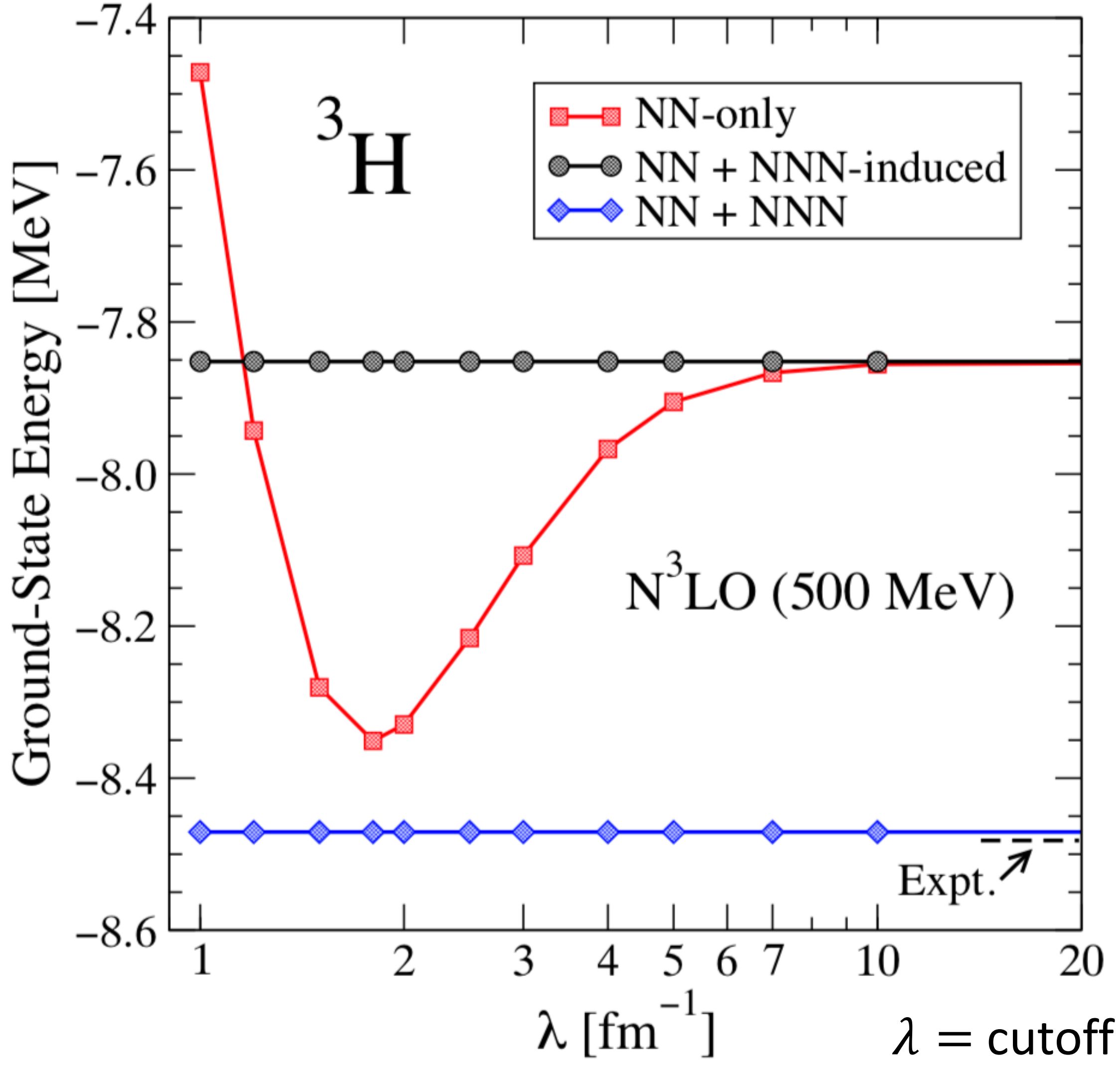
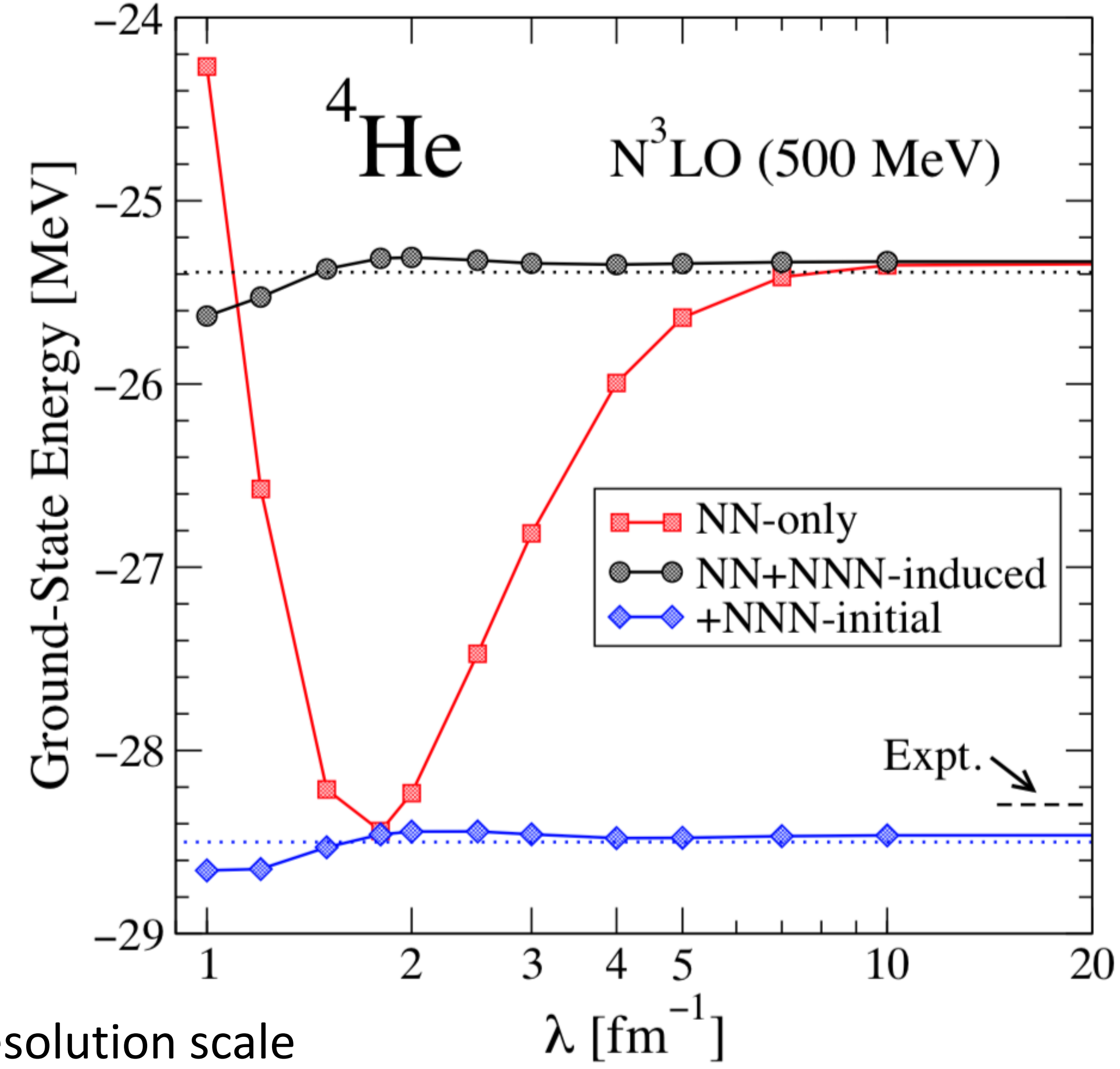


Fig.: Bogner & Furnstahl. See http://www.physics.ohio-state.edu/~ntg/srg

RG Evolution of Nuclear Many-Body Forces

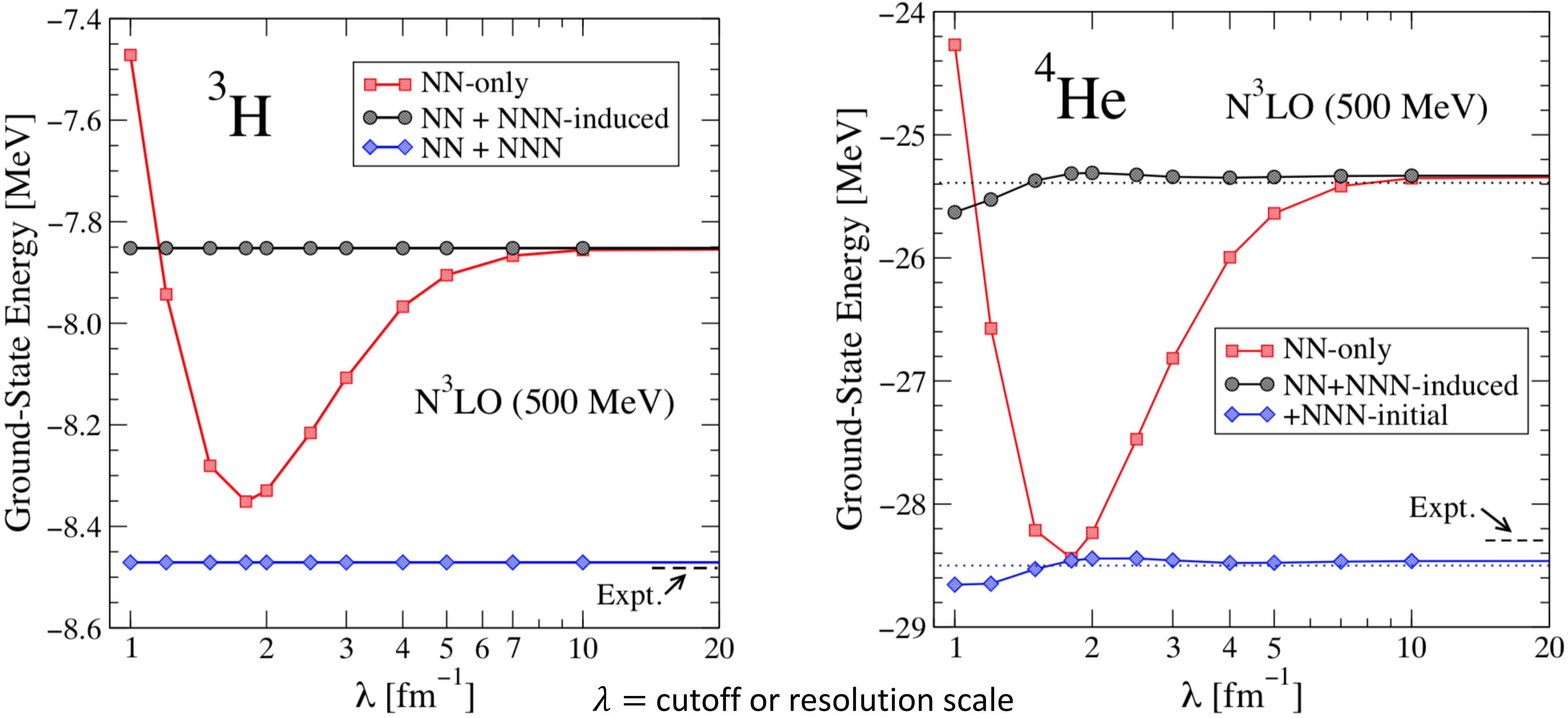




λ = cutoff or resolution scale

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

RG Evolution of Nuclear Many-Body Forces



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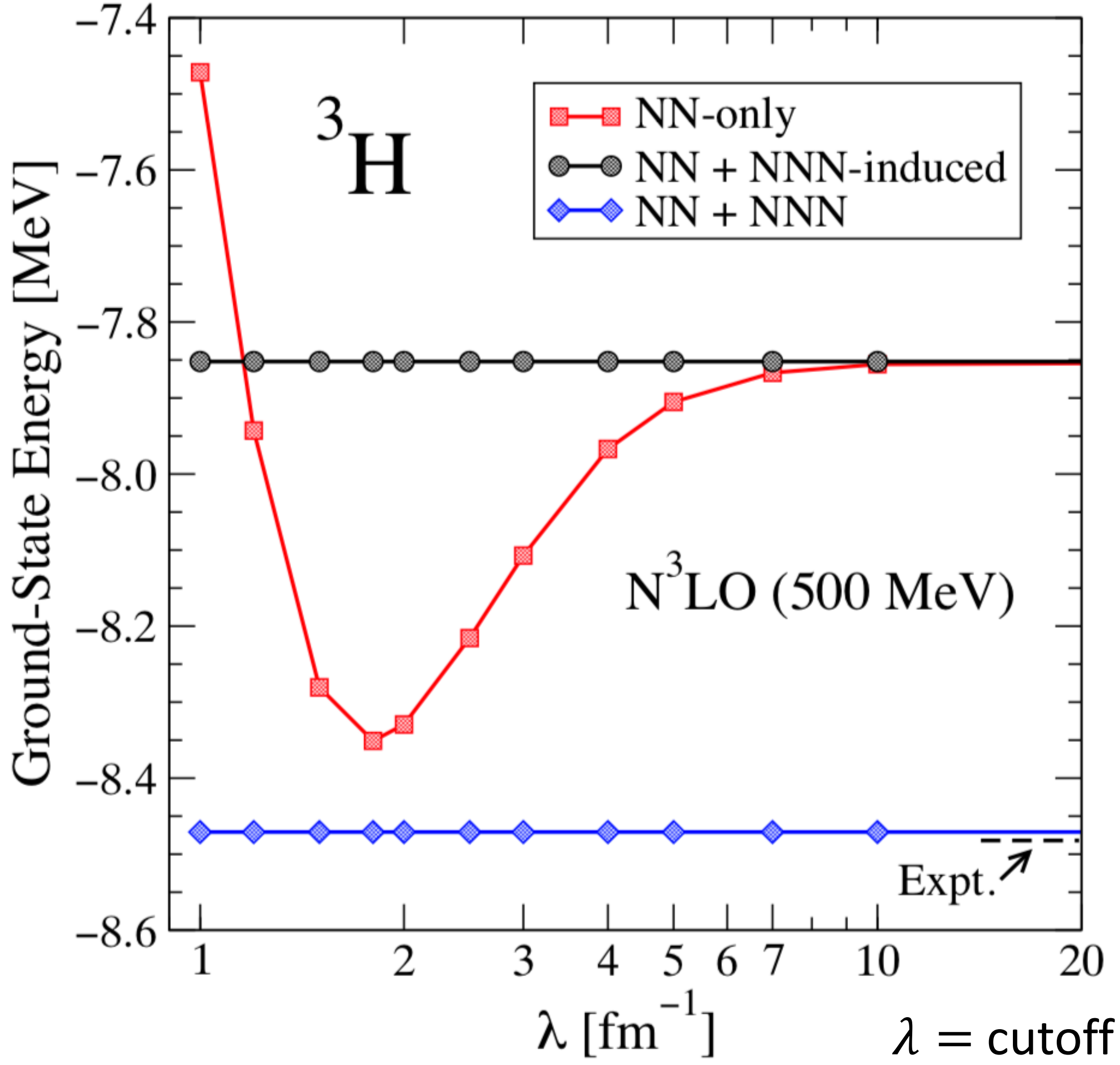
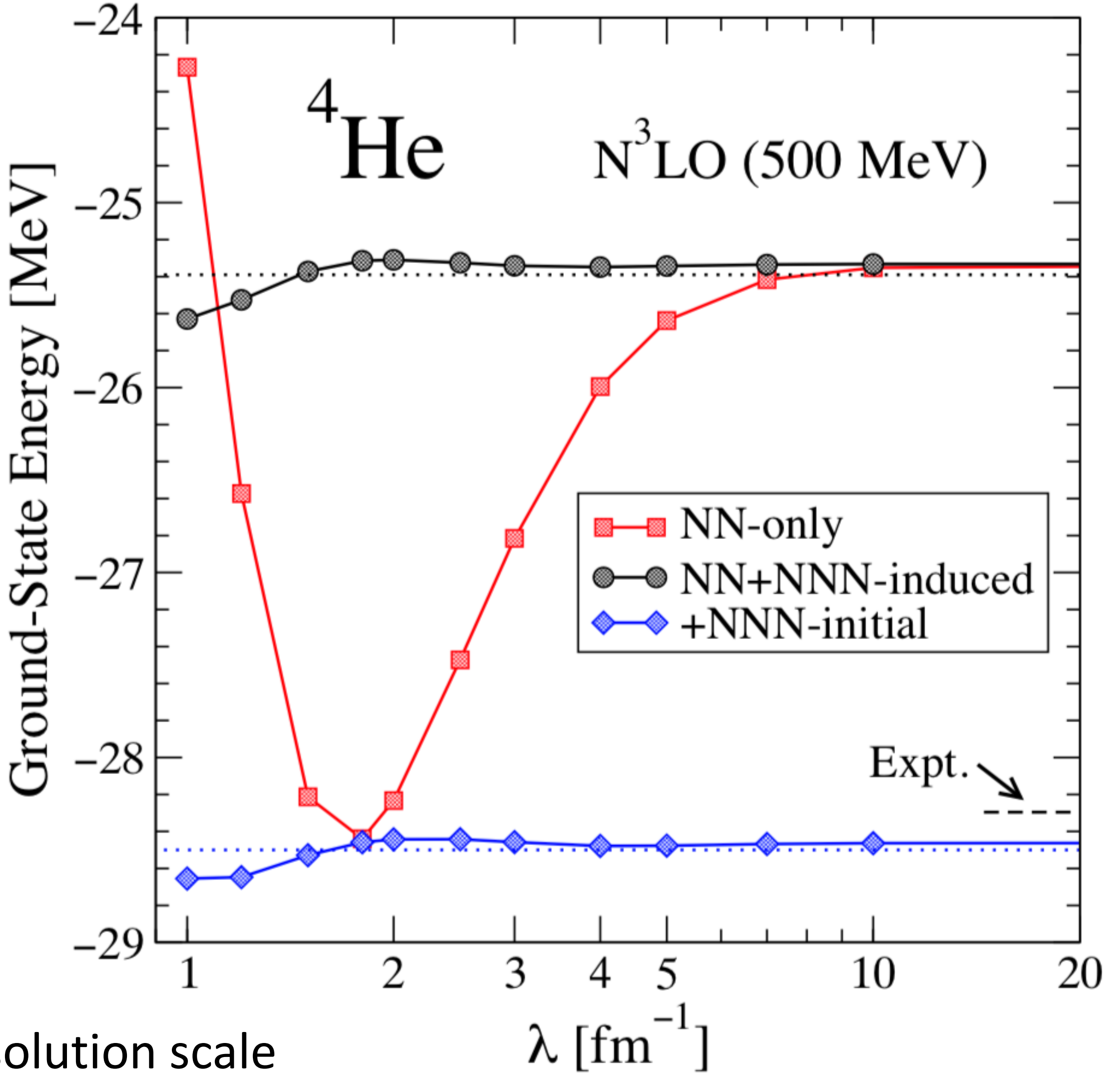
Q: For ^{4}He, why are the calculations including NNN cutoff-dependent at small λ?

RG Evolution of Nuclear Many-Body Forces





λ = cutoff or resolution scale

Q: For ^{4}He, why are the calculations including NNN cutoff-dependent at small λ?

A: Renormalization also introduces 4-body forces, and these were neglected.

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 $n_s \approx (3 \ldots 6)A$]

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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

Mean field

Possibly the most important computation one performs

- Provides us with a new single-particle basis
- Sets the stage for more sophisticated approximations
- Informs us about low-energy excitations

Have: single-particle basis $|q\rangle = c_q^+|0\rangle$ with $|q\rangle \equiv |n, l, j, j_z, \tau_z\rangle$ and $\{c_p, c_q^+\} = \delta_p^q$

n radial quantum number
l orbital angular momentum
j total angular momentum
j_z total angular momentum projection
τ_z isospin projection

Have: Hamiltonian $H = \sum_{pq}\langle p|H|q\rangle c_p^+ c_q + \frac{1}{4}\sum_{pqrs}\langle pq|H|rs\rangle c_p^+ c_q^+ c_s c_r + \frac{1}{36}\sum_{pqrstu}\langle pqr|H|stu\rangle c_p^+ c_q^+ c_r^+ c_u c_t c_s$

Want: new single-particle basis created by fermionic creation operator $a_q = \sum_q U_{pq} c_q$ with $\{a_p, a_q^+\} = \delta_p^q$ such that $\langle\psi_0|H|\psi_0\rangle = E_{ref}$ minimizes the energy.

Mean field

Equivalent statements

- $\langle\psi_0|H|\psi_0\rangle = E_{min}$ minimizes the energy
- Hartree-Fock state $|\psi_0\rangle \equiv \prod_{i=1}^{A} a_i^+|0\rangle$ fulfills $\langle\psi_0|a_i a_a^+ H|\psi_0\rangle = 0$. In the Hartree-Fock basis, the Hamiltonian exhibits no one-particle—one-hole excitations.

Convention: labels $i, j, k, \ldots$ refer to occupied single-particle states (hole states), $a, b, c, \ldots$ refer to unoccupied single-particle states (particle states), $p, q, r, \ldots$ refer to any single-particle state

The Hartree-Fock Hamiltonian $$H_{\rm HF} \equiv \sum_{pq} f_p^q \hat{a}_q^\dagger \hat{a}_p$$

has matrix elements $$f_p^q \equiv \langle q|H|p\rangle + \sum_i \langle qi|H|pi\rangle + \sum_{ij} \langle qij|H|pij\rangle$$

Question: $f_i^a = ?$

Mean field

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Question: $f_i^a = ?$

Answer: $f_i^a = 0$. (Because the Hamiltonian does not exhibit particle-hole excitations.)

Mean field

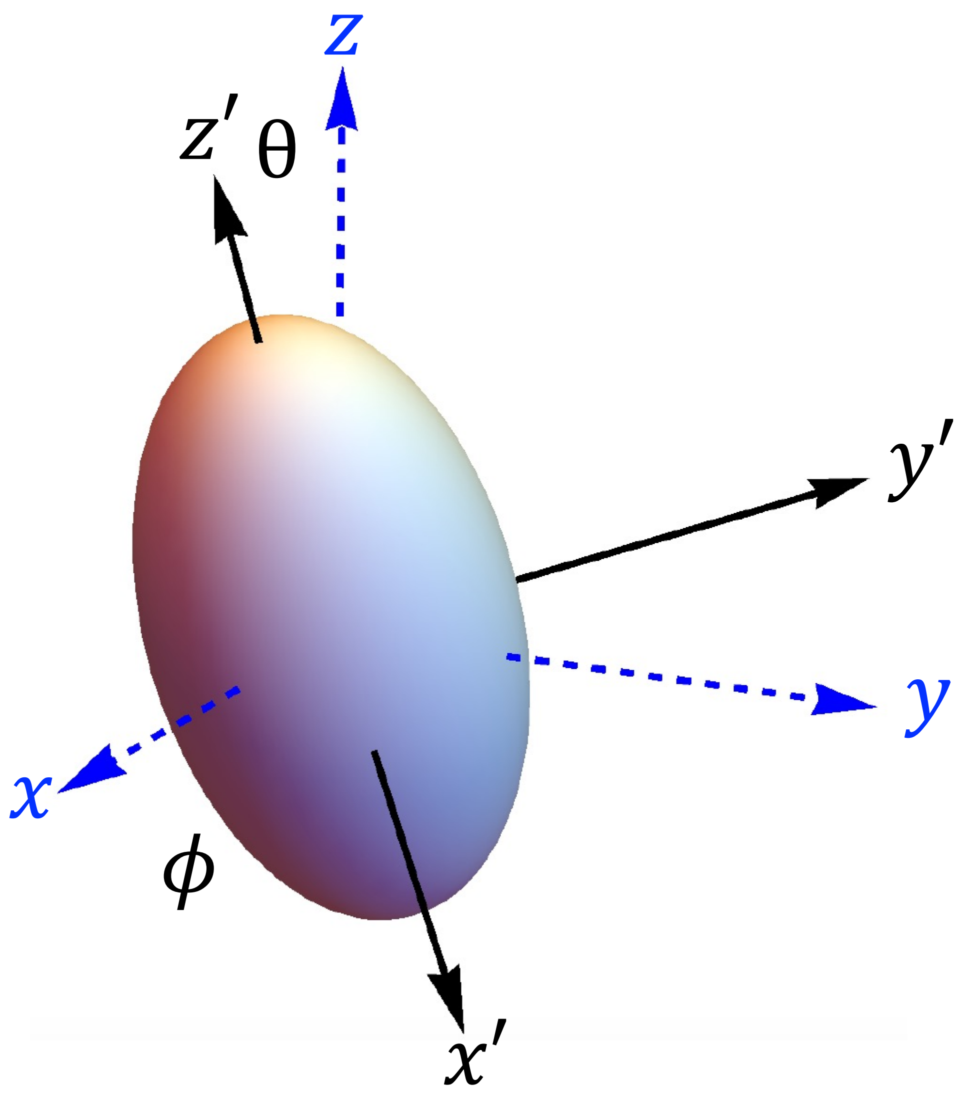
Comments:

1. The Hartree-Fock state is not unique. One can perform a unitary transformation between the hole states and another one between the particle states without changing the Hartree-Fock energy. However, one often chooses the Fock matrix f_p^q to be diagonal, i.e. $f_p^q = \varepsilon_p \delta_p^q$ are single-particle energies.
2. The Hartree-Fock state does not need to exhibit the symmetries of the Hamiltonian H. This is emergent symmetry breaking

Q: Why can symmetries be broken?

Hint: Take a look at $f_p^q \equiv \langle q|H|p\rangle + \sum_i \langle qi|H|pi\rangle + \sum_{ij} \langle qij|H|pij\rangle$

Symmetry breaking



Example: Hartree Fock state only axially symmetric (broken spherical symmetry); choose z axis as symmetry axis

- Rotated state $|\psi(\Omega)\rangle \equiv |\psi(\phi,\theta)\rangle \equiv e^{-i\phi J_z} e^{-i\theta J_y}|\psi_0\rangle$ has the same energy as $|\psi_0\rangle$, i.e.

$$\langle\psi(\Omega)|H|\psi(\Omega)\rangle = \langle\psi_0|H|\psi_0\rangle$$

- Compute norm kernel $N_{\Omega'\Omega} \equiv \langle\psi(\Omega')|\psi(\Omega)\rangle$ and Hamiltonian kernel $H_{\Omega'\Omega} \equiv \langle\psi(\Omega')|H|\psi(\Omega)\rangle$
- Generalized eigenvalue problem $H|\Psi\rangle = EN|\Psi\rangle$
- Diagonalize $H_{eff} = N^{-\frac{1}{2}} H N^{-\frac{1}{2}}$ and find states with good angular momentum
- Q: What will this give?

Symmetry breaking

Compute $N_{\Omega'\Omega} \equiv \langle\psi(\Omega')|\psi(\Omega)\rangle$ and $H_{\Omega'\Omega} \equiv \langle\psi(\Omega')|H|\psi(\Omega)\rangle$

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Diagonalize $H_{eff} = N^{-\frac{1}{2}} H N^{-\frac{1}{2}}$ and find states with good angular momentum

Q: What will this give?

A: Symmetry breaking implies universal low-energy physics (Nambu-Goldstone modes)

We can develop an effective theory $H_{eff} \to H_{EFT} = E_0 - a\nabla_\Omega^2 + \cdots$

with $\nabla_\Omega \equiv e_\theta \partial_\theta + e_\phi \frac{1}{\sin\theta}\partial_\phi$

Rationale: $\Omega = (\phi, \theta)$ is the collective coordinate; rotational invariance implies that only derivatives can enter. (Nambu-Goldstone modes only couple via derivatives)

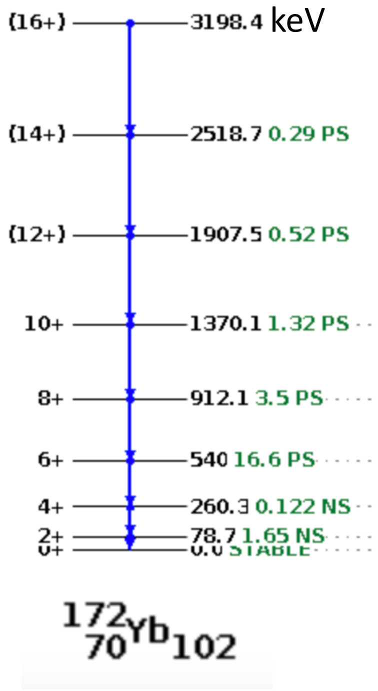
Eigenfunctions are spherical harmonics $Y_{IM}(\Omega)$

Eigenvalues are $E_I = E_0 + aI(I+1)$; rotational bands are the result

Symmetry breaking

Understanding symmetry breaking:

- The axially symmetric state $|\psi_0\rangle$ is a superposition of states that belong to a rotational band, i.e. $|\psi_0\rangle = \sum_I c_I |I, M = 0\rangle$
- Solution of the effective collective Hamiltonian $H_{eff} = N^{-\frac{1}{2}} H N^{-\frac{1}{2}}$, or symmetry projection via $E_I = \frac{\int d\Omega D^I_{00}(\Omega,0) H(0,\Omega)}{\int d\Omega D^I_{00}(\Omega,0) N(0,\Omega)}$ yield states with good angular momentum.



Superposition of these states makes a deformed state. As rotational excitations are low in energy, the symmetry breaking only has a small impact on the total binding energy.

Symmetry breaking

Feature or Bug?

Symmetry breaking

Feature!

Points out the existence of universal long-range physics ("Nambu-Goldstone modes")

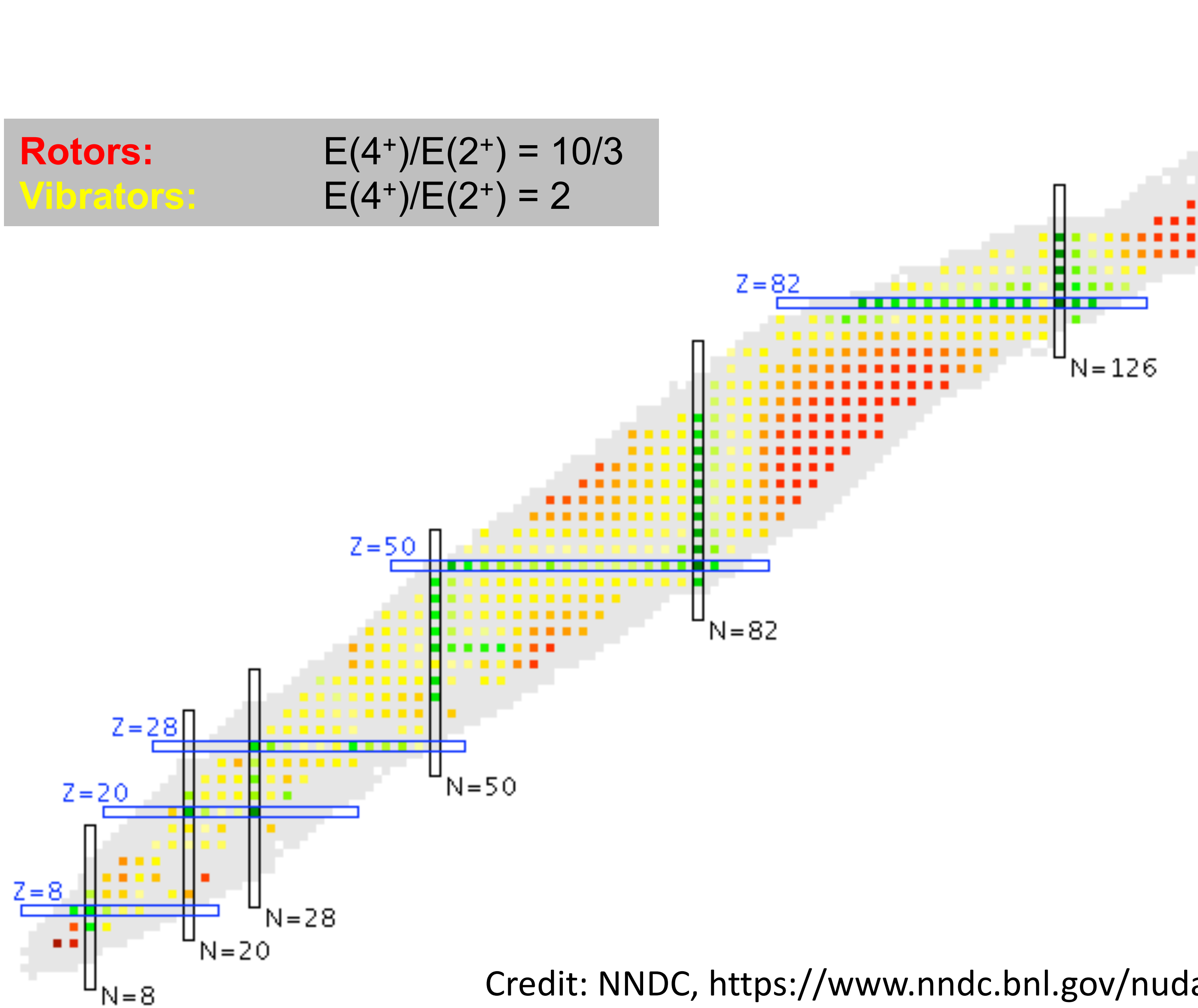
1. Deformation (HF) → rotational bands
2. Broken phases (HFB) → pairing rotational bands
3. Broken parity → bands with opposite parities close in energy

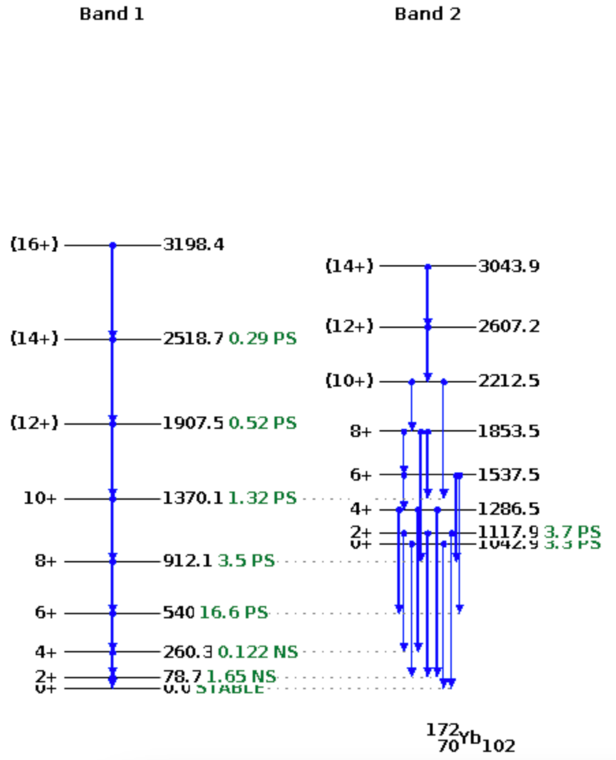
Separation of scales enable construction of effective theories

Broken symmetry	Tool	Phenomenon	Low-lying excitations	Energy gain from symmetry projection	Energy scale (rare earth region)	Number of participating nucleons
SO(3)	HF	Deformation Rotational bands	$\frac{1}{2a}I(I+1)$	$\frac{1}{2a}\langle I^2\rangle$	$\frac{1}{2a} \sim 13\text{keV}$	A
U(1)	HFB	Superfluidity Pairing rotational bands	$\frac{1}{2a}(n-n_0)^2$	$\frac{1}{2a}\langle \Delta n^2\rangle$	$\frac{1}{2a} \sim 0.2\text{ MeV}$	$A^{1/3} \dots A^{2/3}$

Symmetry breaking: nuclear deformation

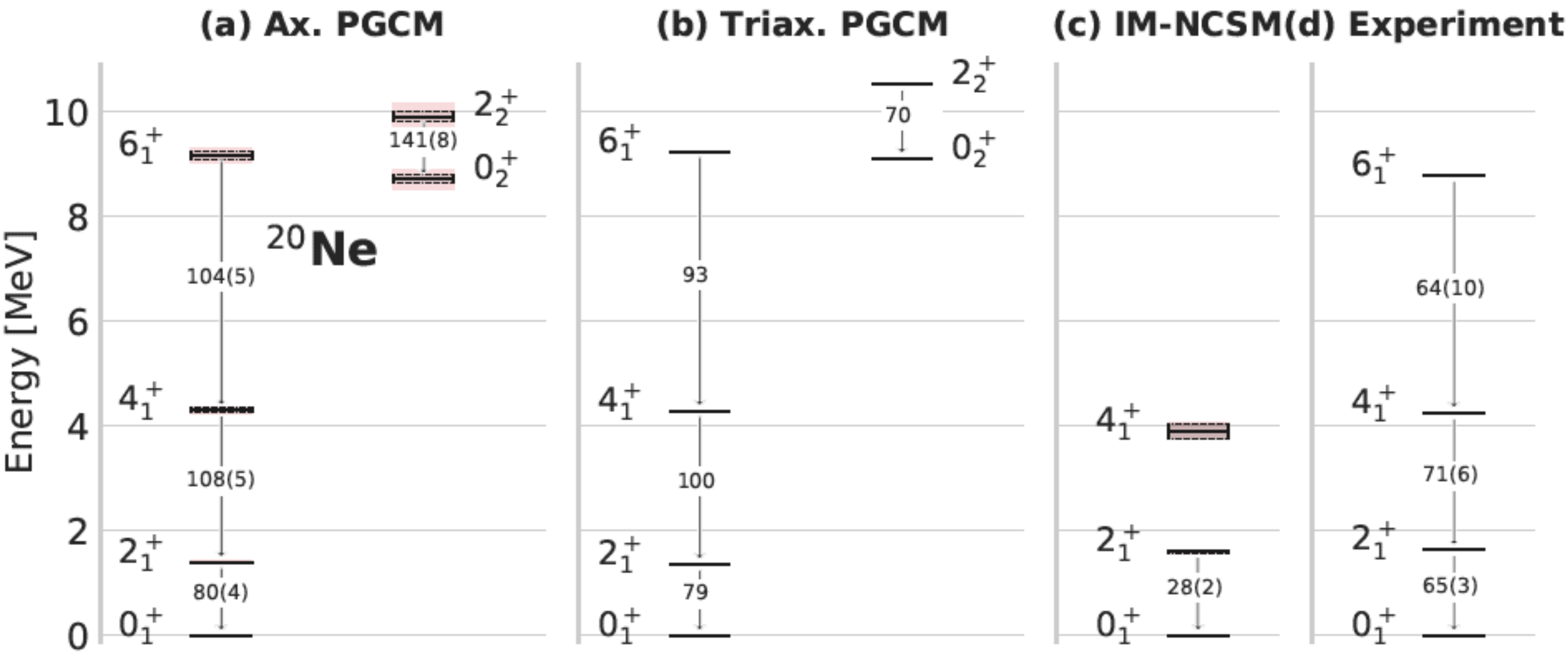
Rotors: E(4⁺)/E(2⁺) = 10/3
Vibrators: E(4⁺)/E(2⁺) = 2





Credit: NNDC, https://www.nndc.bnl.gov/nudat3/

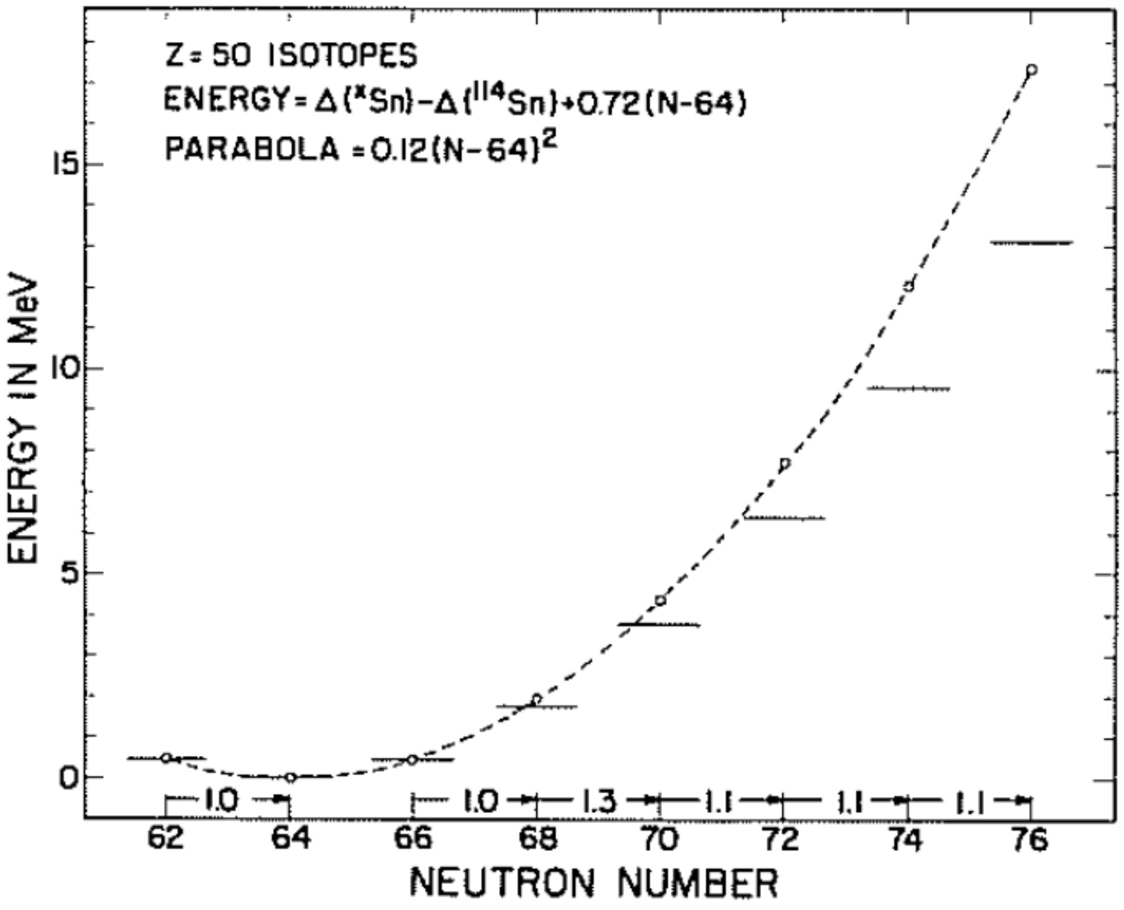
Projected Hartree-Fock-Bogoliubov calculations yield rotational bands



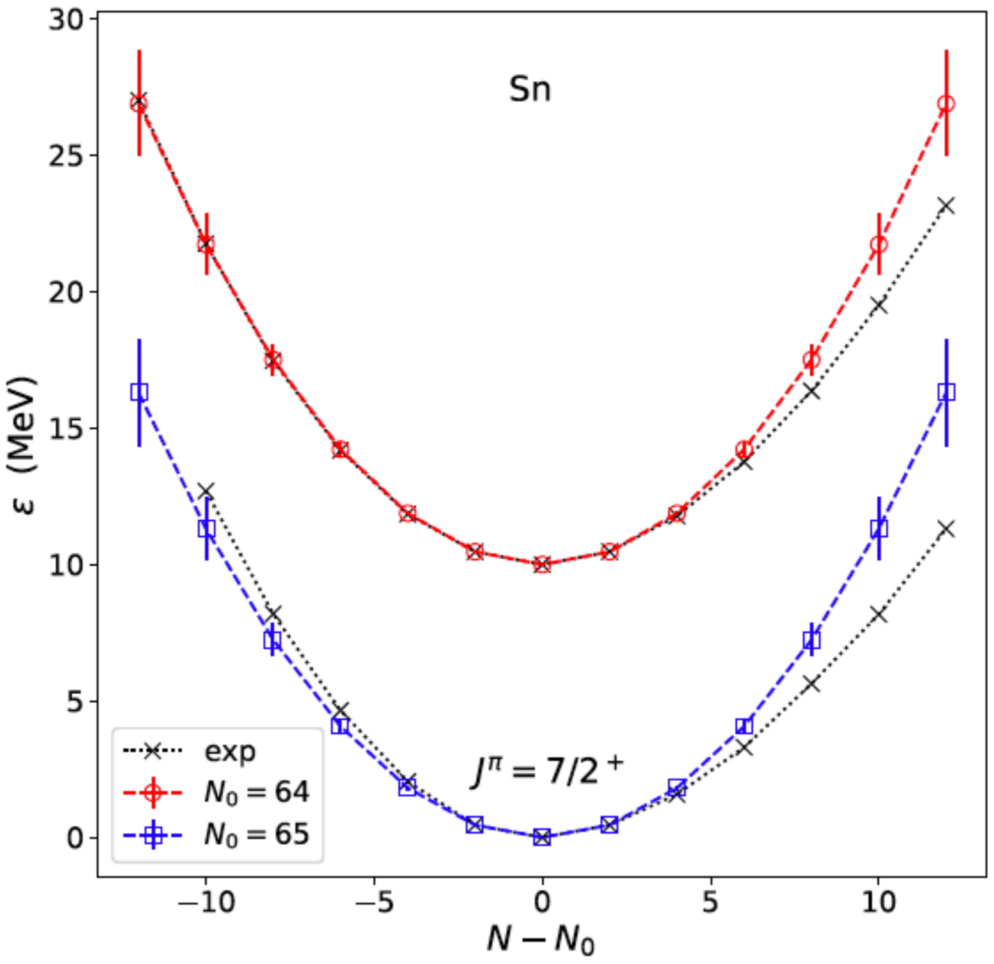
Frosini et al., Eur. Phys. J. A 58, 63 (2022); arxiv:2111.00797

One does not need to include dynamical correlations to compute rotational bands

Symmetry breaking: nuclear superfluidity



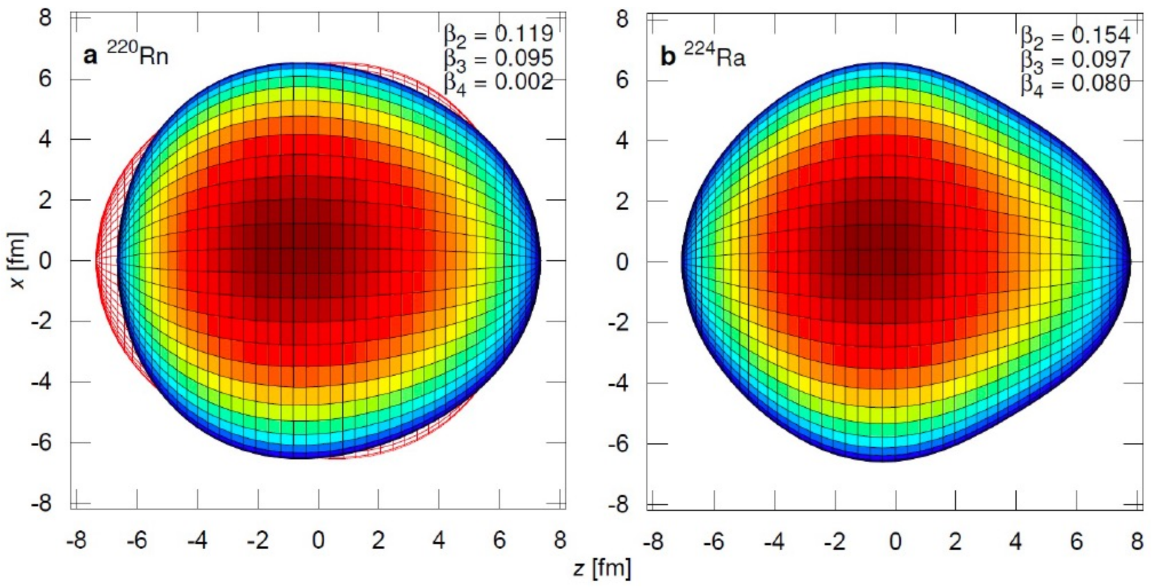
Broglia, Hansen, Riedel, Adv. Nucl. Phys. (1973)



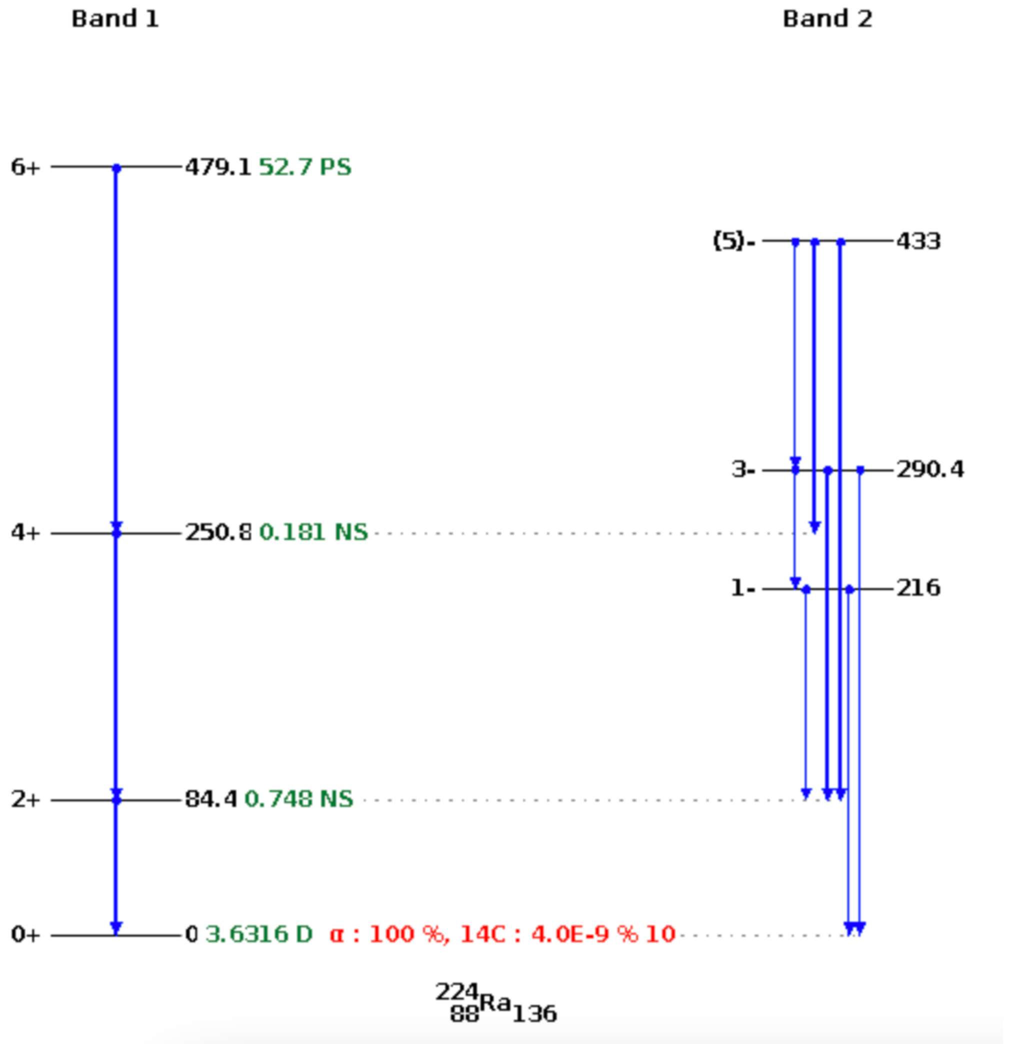
TP, Phys. Rev. C 105, 044322 (2022)

Potel, Idini, Barranco, Vigezzi, Broglia, Rep. Prog. Phys. 76, 106301 (2013)
Potel, Idini, Barranco, Vigezzi, Broglia, Phys. Rev. C 96, 034606 (2017).

Symmetry breaking: octupole deformation

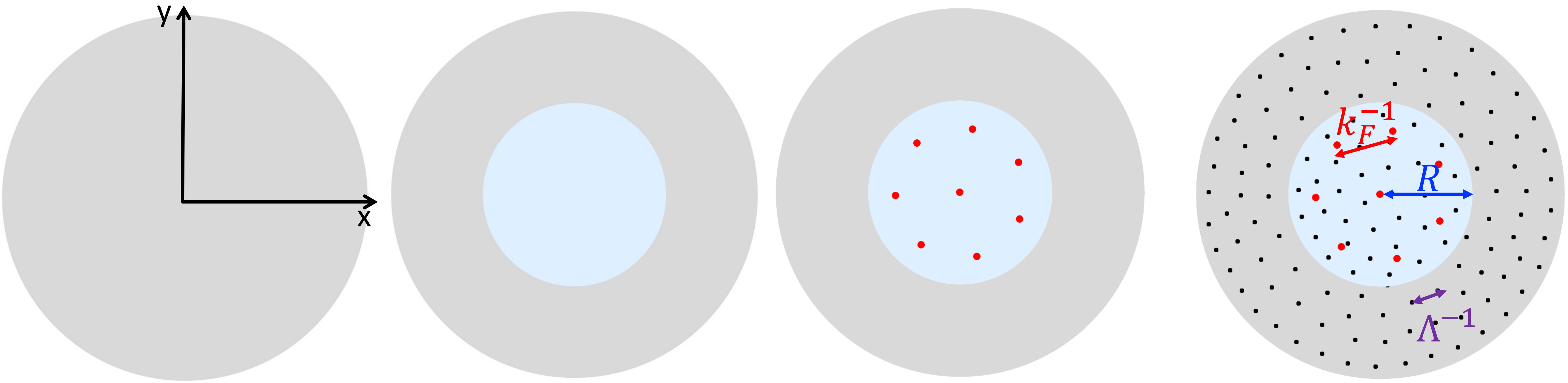


Gaffney et al. Nature 497, 199 (2013)



Credit: NNDC, https://www.nndc.bnl.gov/nudat3/

A picture of the mean-field basis in position space



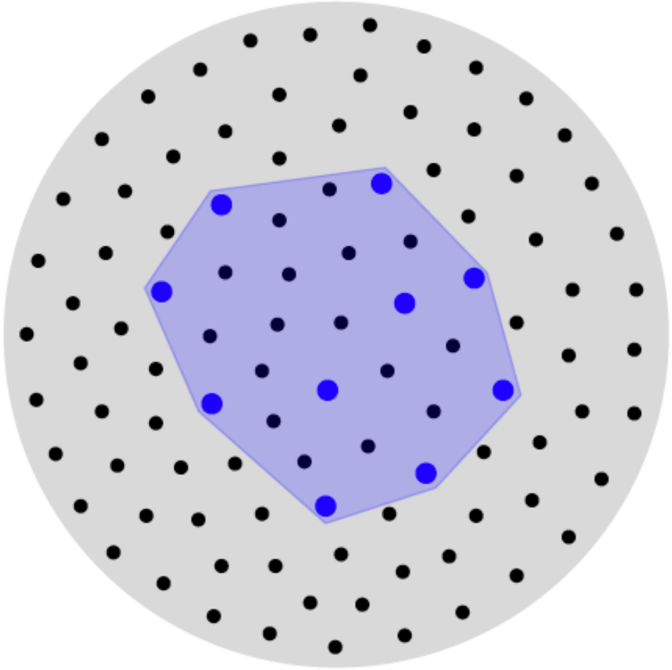
Fock space: Single-particle states fill part of position space.

HF calculation: Divides Hilbert space into hole space (blue area with nuclear radius R) and particle space (grey remainder)

Hole space: Introduce localized basis functions (centered at red points) via unitary transformation; distance of points $\sim k_F^{-1}$.
Edmiston & Ruedenberg, RMP 1963; Høyvik et al, JCP 2012

Particle space: Introduce localized basis functions (centered at black points); distance of points $\sim \Lambda^{-1}$.

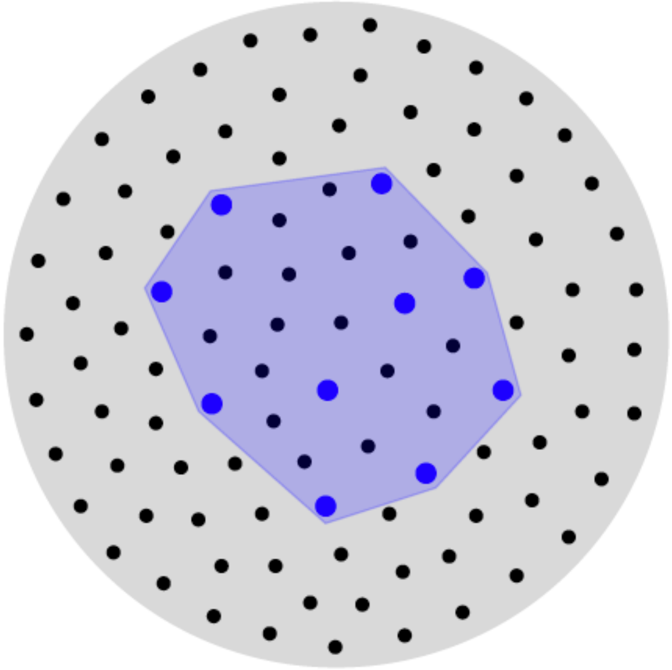
The binding energy is proportional to the mass number



$$
\begin{aligned}
E_{\mathrm{ref}} &\equiv \langle\psi_0|H|\psi_0\rangle \\
&= \sum_i \langle i|H|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|H|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|H|ijk\rangle
\end{aligned}
$$

Q: We have sums $\sum_{ij=1}^{A}\cdots$, $\sum_{ijk=1}^{A}\cdots$. How can the result be $\propto A$ (and not $\propto A^2$ and $\propto A^3$)?

The binding energy is proportional to the mass number



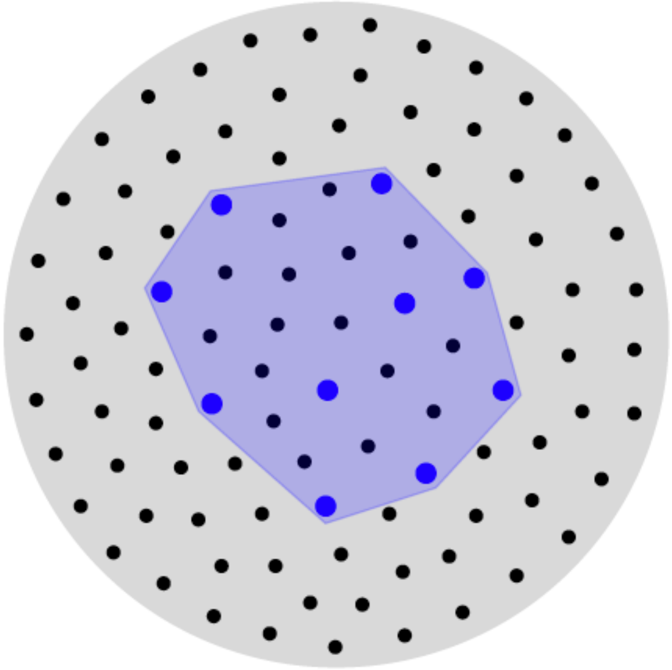
$$E_{\text{ref}} \equiv \langle \psi_0 | H | \psi_0 \rangle$$
$$= \sum_i \langle i|H|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|H|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|H|ijk\rangle$$

$\propto \delta_{x_i}^{x_j}$ (short range)

$\propto \delta_{x_i}^{x_j}\delta_{x_i}^{x_k}$ (short range, short range)

A: The nuclear force is short ranged!

The binding energy is proportional to the mass number



$$E_{\text{ref}} \equiv \langle \psi_0 | H | \psi_0 \rangle$$
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$\propto \delta_{x_i}^{x_j}$ — short range

$\propto \delta_{x_i}^{x_j} \delta_{x_i}^{x_k}$ — short range

effectively $\sum_{i=1}^{A} \cdots$ effectively $\sum_{i=1}^{A} \cdots$

$\propto A$

A: The nuclear force is short ranged!

Summary mean field

- The most important computation
    - Provides us with a single-particle basis
- Symmetry breaking is a virtue and identifies relevant physics and low-lying excitations
- The resulting mean-field (reference) state is the non-trivial vacuum

Task: Rewrite Hamiltonian with respect to this non-trivial vacuum state!

The mean-field state is the nontrivial vacuum

The mean-field state (or ‘’reference’’ state) provides us with a non-trivial vacuum.

- Symmetry breaking exhibits essential physics and makes low-energy excitations obvious (this is infrared or long-range physics; we deal with it later in detail)
- Want to include short-range physics (so-called “dynamical correlations”) first.
- Profitable to rewrite Hamiltonian with respect to the non-trivial vacuum

Normal ordering: Rewrite Hamiltonian such that all operators that annihilate the reference state $|\psi_0\rangle = \Pi_i a_i^+ |0\rangle$ are to the right.

Q: $a_i^+ |\psi_0\rangle = ?$

$a_a |\psi_0\rangle = ?$

The mean-field state is the nontrivial vacuum

The mean-field state (or ‘’reference’’ state) provides us with a non-trivial vacuum.

- Symmetry breaking exhibits essential physics and makes low-energy excitations obvious (this is infrared or long-range physics; we deal with it later in detail)
- Want to include short-range physics (so-called “dynamical correlations”) first.
- Profitable to rewrite Hamiltonian with respect to the non-trivial vacuum

Normal ordering: Rewrite Hamiltonian such that all operators that annihilate the reference state $|\psi_0\rangle = \Pi_i a_i^+|0\rangle$ are to the right.

Q: $a_i^+|\psi_0\rangle = 0$

$a_a\,|\psi_0\rangle = 0$

The normal-ordered Hamiltonian

We rewrite

$$H = E_{\rm ref} + H_{\rm no}$$

with

$$E_{\rm ref} = \sum_i \langle i|H|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|H|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|H|ijk\rangle$$

Brackets {…} indicate normal ordering

$$H_{\rm no} \equiv \sum_{pq}\langle q|H_{\rm no}|p\rangle \left\{\hat{a}_q^\dagger \hat{a}_p\right\} + \frac{1}{4}\sum_{pqrs}\langle pq|H_{\rm no}|rs\rangle \left\{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\right\} + \frac{1}{36}\sum_{pqrsuv}\langle pqu|H|rsv\rangle \left\{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_u^\dagger \hat{a}_v \hat{a}_s \hat{a}_r\right\}$$

and matrix elements

$$\langle q|H_{\rm no}|p\rangle = \langle q|H|p\rangle + \sum_i \langle qi|H|pi\rangle + \sum_{ij}\langle qij|H|pij\rangle \ ,$$

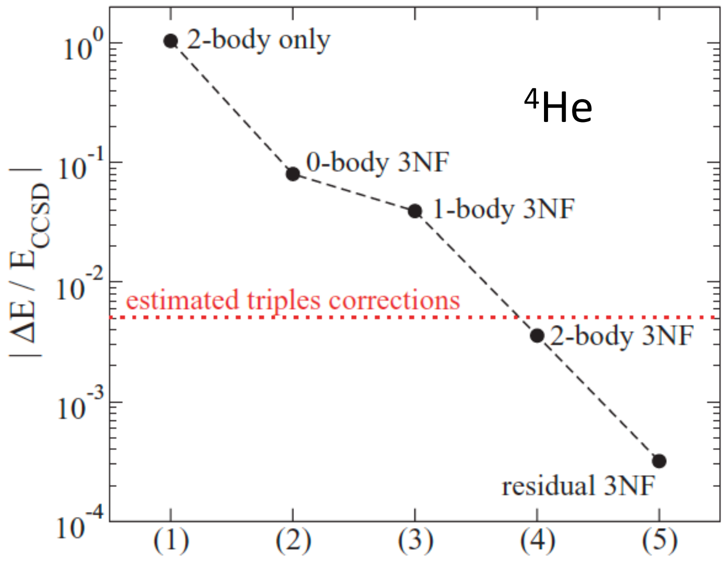
$$\langle pq|H_{\rm no}|rs\rangle = \langle pq|H|rs\rangle + \sum_i \langle pqi|H|rsi\rangle \ .$$

Note where the three-body force enters in all matrix elements!

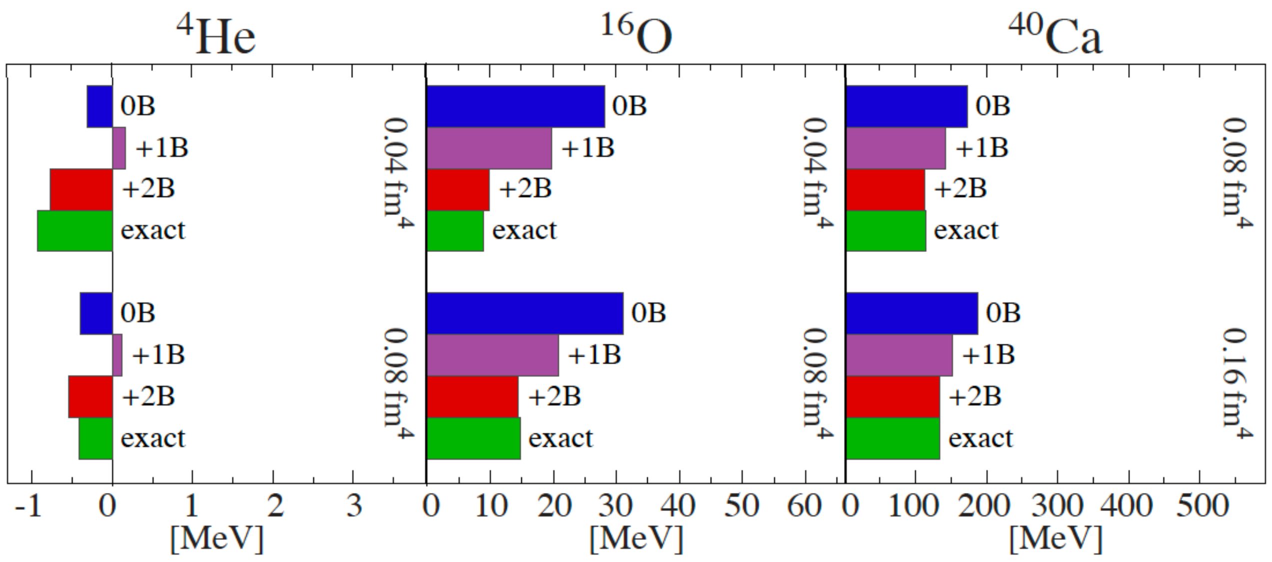
Normal-ordered two-body approximation

Neglect ``residual'' three-body forces:

$$H_{\rm no} \equiv \sum_{pq} \langle q|H_{\rm no}|p\rangle \, \{\hat{a}_q^\dagger \hat{a}_p\} + \frac{1}{4}\sum_{pqrs}\langle pq|H_{\rm no}|rs\rangle \, \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_s \hat{a}_r\} + \frac{1}{36}\sum_{pqrsuv}\langle pqu|H|rsv\rangle \, \{\hat{a}_p^\dagger \hat{a}_q^\dagger \hat{a}_u^\dagger \hat{a}_v \hat{a}_s \hat{a}_r\}$$



Hagen et al., Phys. Rev. C 76, 034302 (2007)



Roth et al., Phys. Rev. Lett. 109, 052501 (2012)

Where we stand

- Lecture 1
  - What is ab initio
  - Ideas from effective field theory / the renormalization group
  - Interactions from chiral effective field theory
  - Three body forces come with two-body currents
    - Explain magnetic moments and reduced beta-decay strengths
- Lecture 2
  - Number of single-particle states increases with mass number and with the cube of the cutoff
    - Can use renormalization group transformations to lower the cutoff
    - Exact solutions impossible for all but the lightest nuclei
  - The mean field is so useful
    - Selects single-particle basis and the non-trivial vacuum state
    - Broken symmetries imply physics (deformation, superfluidity) and low-lying excitations (rotational bands, pairing rotational bands)
    - Take mean-field state as the nontrivial vacuum; normal-order Hamiltonian; apply normal-ordered two-body approximation

Including correlations in wave-function based approaches

Self consistent Green's functions

In-medium similarity renormalization group

Many-body perturbation theory

Coupled-cluster theory

•

•

•

Including correlations: couped-cluster theory

Ansatz $|\psi\rangle = e^T|\psi_0\rangle$

Cluster operator
$$T \equiv T_1 + T_2 + T_3 + \ldots$$
$$= \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i + \frac{1}{4}\sum_{ijab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i + \frac{1}{36}\sum_{ijkabc} t_{ijk}^{abc} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_c^\dagger \hat{a}_k \hat{a}_j \hat{a}_i + \ldots$$

Note: the cluster operator only contains excitations, but no de-excitations!
Q: Is e^T unitary?

Key: similarity transformed Hamiltonian $\overline{H}_{\mathrm{no}} \equiv e^{-T} H_{\mathrm{no}} e^T$

Equations to solve
$$\langle\psi_i^a|\overline{H}_{\mathrm{no}}|\psi_0\rangle = 0 \,,$$
$$\langle\psi_{ij}^{ab}|\overline{H}_{\mathrm{no}}|\psi_0\rangle = 0 \,,$$
$$\langle\psi_{ijk}^{abc}|\overline{H}_{\mathrm{no}}|\psi_0\rangle = 0 \,,$$
$$\vdots$$
$$\langle\psi_{i_1\cdots i_A}^{a_1\cdots a_A}|\overline{H}_{\mathrm{no}}|\psi_0\rangle = 0 \,.$$

Interpretation: The similarity-transformed Hamiltonian has no 1p-1h, no 2p-2h, no 3p-3h, … excitations.

Thus, the reference state becomes an eigenstate, i.e. it becomes decoupled from many-particle—many-hole excitations

using the expressions
$$|\psi_i^a\rangle \equiv \hat{a}_a^\dagger \hat{a}_i|\psi_0\rangle \,,$$
$$|\psi_{ij}^{ab}\rangle \equiv \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i|\psi_0\rangle$$

The correlation energy is $E_{\mathrm{corr}} \equiv \langle\psi_0|\overline{H}_{\mathrm{no}}|\psi_0\rangle$

Key properties of coupled-cluster theory

🙂 The truncation of the cluster operator $e^T = e^{T_1+T_2}$ or $e^T = e^{T_1+T_2+T_3}$ is the only approximation

- The Baker-Campbell-Hausdorff expansion terminates at $k \times n$ nested commutators for k-body Hamiltonians and cluster operators with np-nh excitations.
- The numerical effort is $\propto n_s^4 A^2$ for $T = T_1 + T_2$ and $\propto n_s^5 A^3$ for $T = T_1 + T_2 + T_3$. This is expensive (supercomputers required) but affordable.
- Experience shows: $T = T_1 + T_2$ yields 90% of the correlation energy and $T = T_1 + T_2 + T_3$ yields 98-99% of the correlation energy

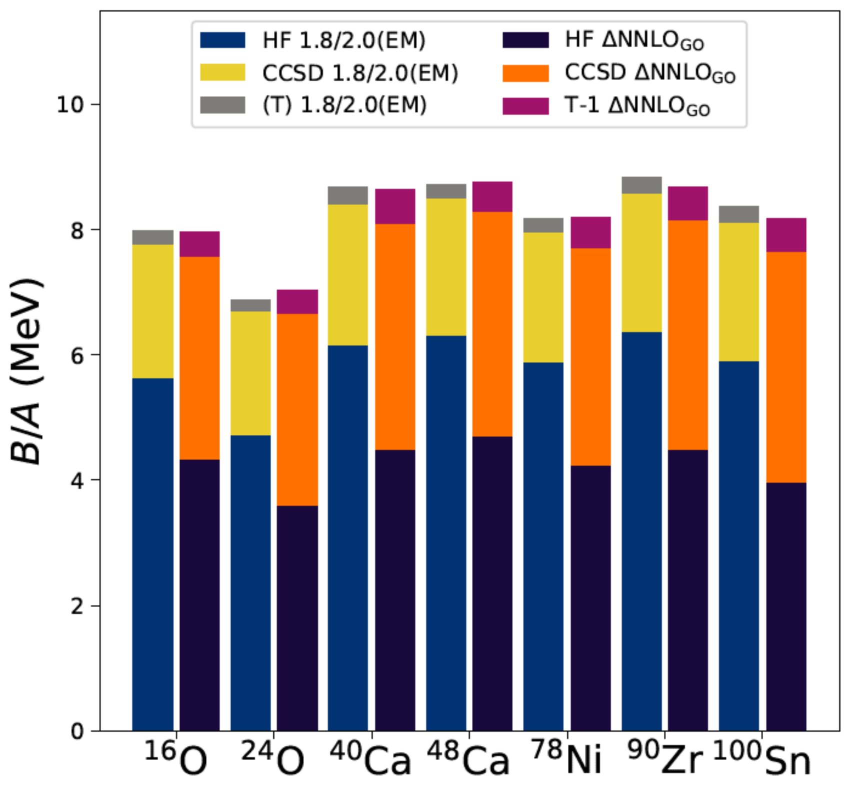
😕 The similarity-transformed Hamiltonian is not Hermitian: right and left eigenvectors are not adjoints of each other

- Expectation values are based on left and right eigenvectors of the similarity-transformed Hamiltonian
- Requires one to solve two (instead of one) large-scale eigenvalue problems

Note: Coupled-cluster method is orders of magnitude more efficient than unitary similarity transformations (IMSRG)

How much energy comes from T_1(Hartree Fock), T_2, and T_3?

Contributions to the binding energy

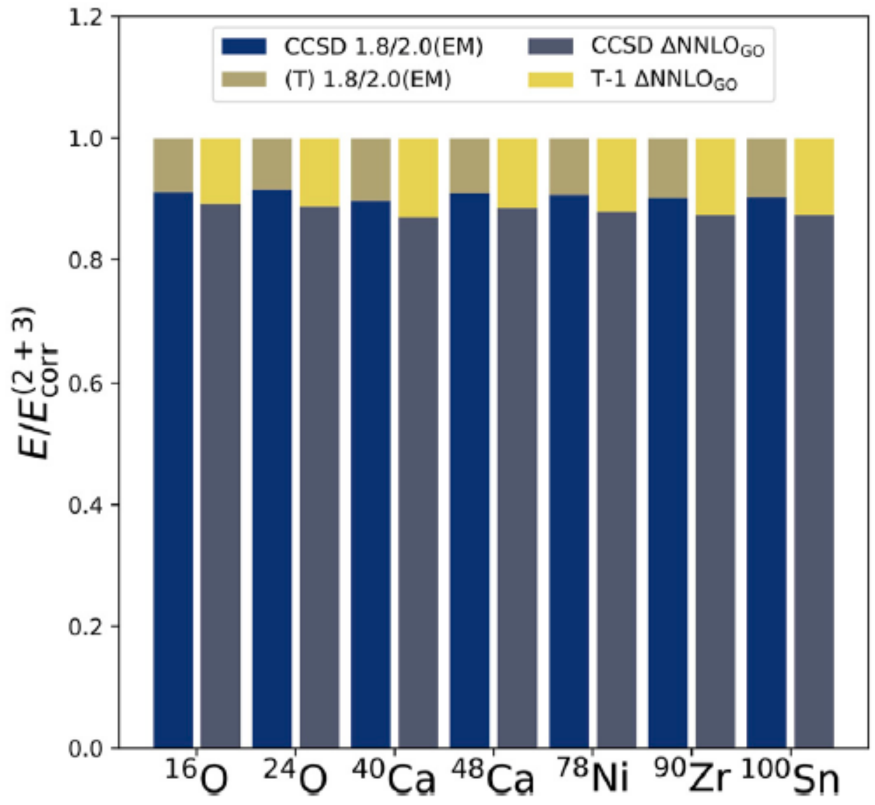


$$E_0 = E_{\text{ref}} + E_{\text{corr}}$$

Cutoffs of the interactions

1.8/2.0 (EM)	ΔNNLO$_{GO}$
1.8 fm^{-1} in NN	2.0 fm^{-1} in NN
2.0 fm^{-1} in NNN	2.0 fm^{-1} in NNN

Composition of the correlation energy



Left: Binding energy per nucleon from the 1.8/2.0(EM) and the ΔNNLO$_{GO}$ interactions using Hartree Fock (HF), $T = T_1 + T_2$ (CCSD), and triples approximation $T = T_1 + T_2 + T_3$ (T). Right: Composition of correlation energy.

Adapted from Sun et al, PRC 106, L061302 (2022); Ekström et al. *Front. Phys.* (2023)

Q Which interaction yields more correlation energy?

Q Why do you think that is so? What could be the reason for that?

Q What fraction of the correlation energy do the “triples” T_3, denoted as (T) or as T-1, contribute?

Contributions to the ground-state energy of deformed nuclei:

The bulk of the binding energy is from short-range correlations
Symmetry projection accounts for small details

Coester and Kümmel (1960), “Short-range correlations in nuclear wave functions”
Lipkin (1960): “Collective motion in many-particle systems: Part 1. the violation of conservation laws”

	E_{HF}	$E_{CCSD(T)}$	$E_{Proj.}$	$\langle J_{HF}\rangle$	$\langle J_{CCSD(T)}\rangle$
^{8}Be	−16.74	−50.24	−53.57	11.17	5.82
^{20}Ne	−59.62	−161.95	−164.21	21.26	12.09
^{34}Mg	−90.21	−264.34	−265.84	22.62	15.03

Data from Hagen et al., Phys. Rev. C 105, 064311 (2022)

Q: What gives the most of the ground-state energy?

Multiscale problem:

The bulk of the binding energy is from short-range correlations
Symmetry projection accounts for small details

Coester and Kümmel (1960), "Short-range correlations in nuclear wave functions"
Lipkin (1960): "Collective motion in many-particle systems: Part 1. the violation of conservation laws"

	E_{HF}	$E_{CCSD(T)}$	$E_{Proj.}$	$\langle J_{HF} \rangle$	$\langle J_{CCSD(T)} \rangle$
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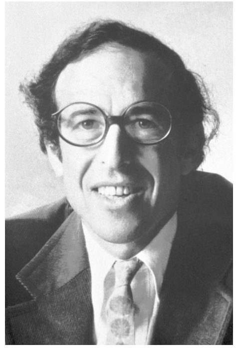
Data from Hagen et al., Phys. Rev. C 105, 064311 (2022)

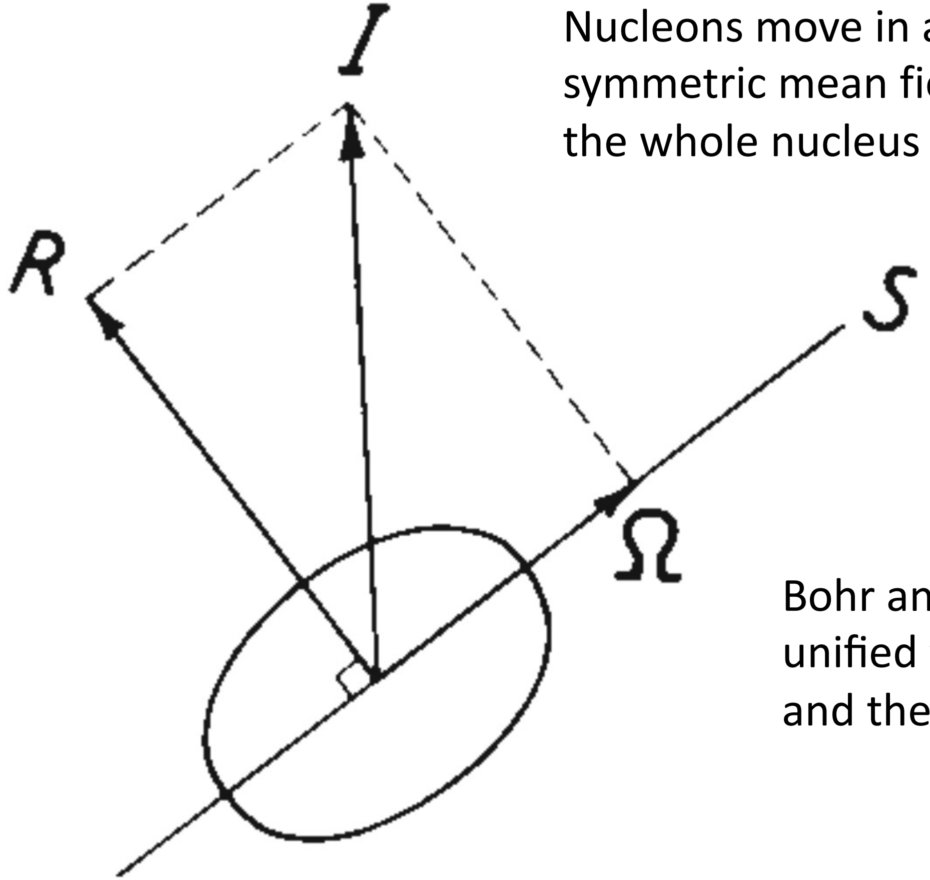
Q: What gives the most of the ground-state energy?
Q: Why does the energy contribution from symmetry projection decrease with increasing mass number?

Summary: Short and long-range correlations

- Short-range correlations
  - give the bulk of the ground-state energy
  - 2p-2h and 3p-3h excitations, relatively small number of them $A^2 n_s^2$, $A^3 n_s^3$
  - also known as "dynamical correlations"
- Long-range correlations
  - yield small contributions to the binding energy
  - Dominate low-lying excited states
  - Many-particle—many-hole excitations
  - Inclusion via symmetry projection of symmetry-breaking reference states
  - Inclusion via other collective coordinates, e.g. quadrupole deformation

1975 Nobel Prize in Physics:
Aage Bohr, Ben Mottelson,
Leo Rainwater

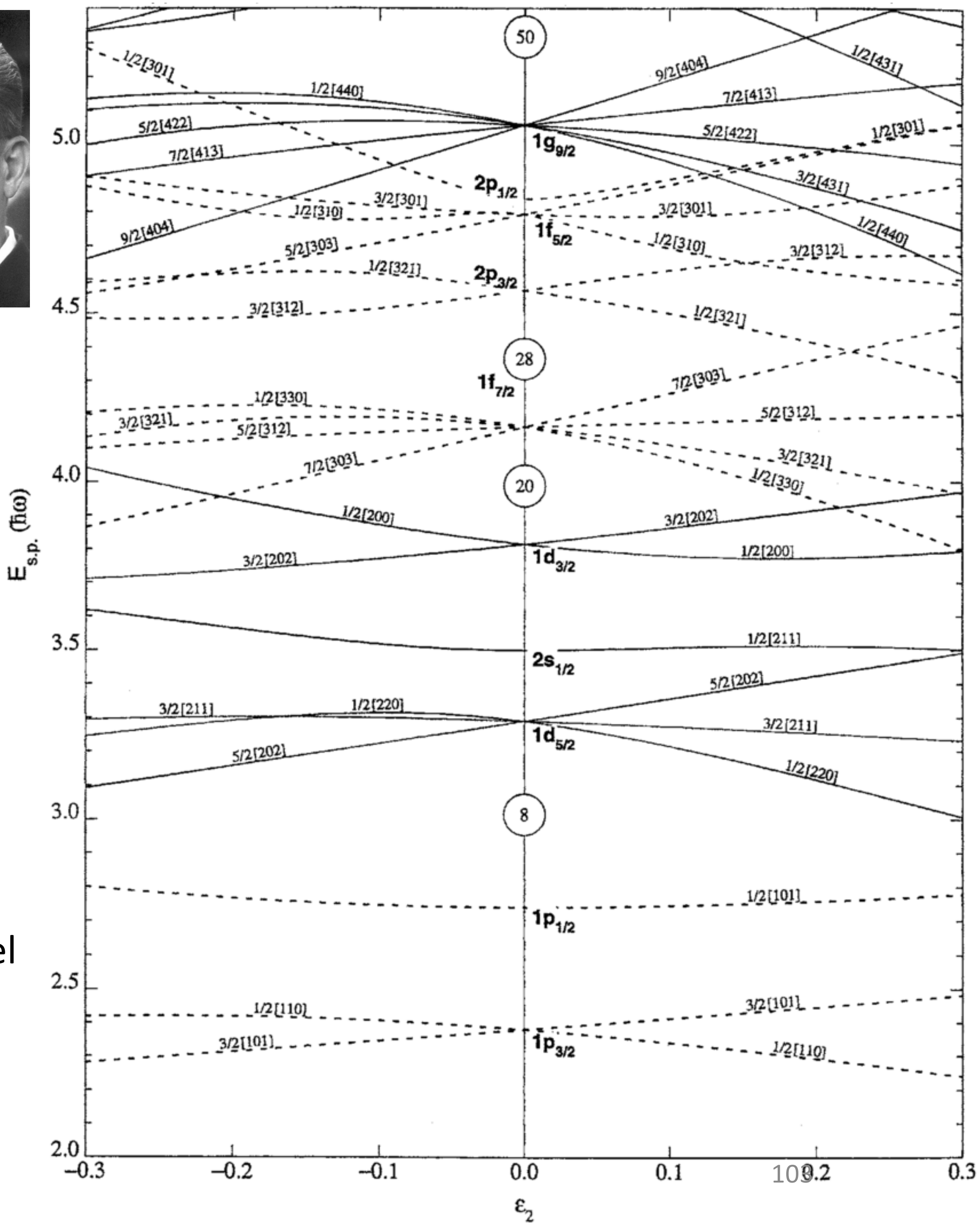




A. Bohr (1950s)

Nucleons move in an axially
symmetric mean field and
the whole nucleus rotates

Bohr and Mottelson’s model
unified the spherical shell model
and the liquid drop model



70 years later: High-resolution picture of Bohr and Mottelson's unified model

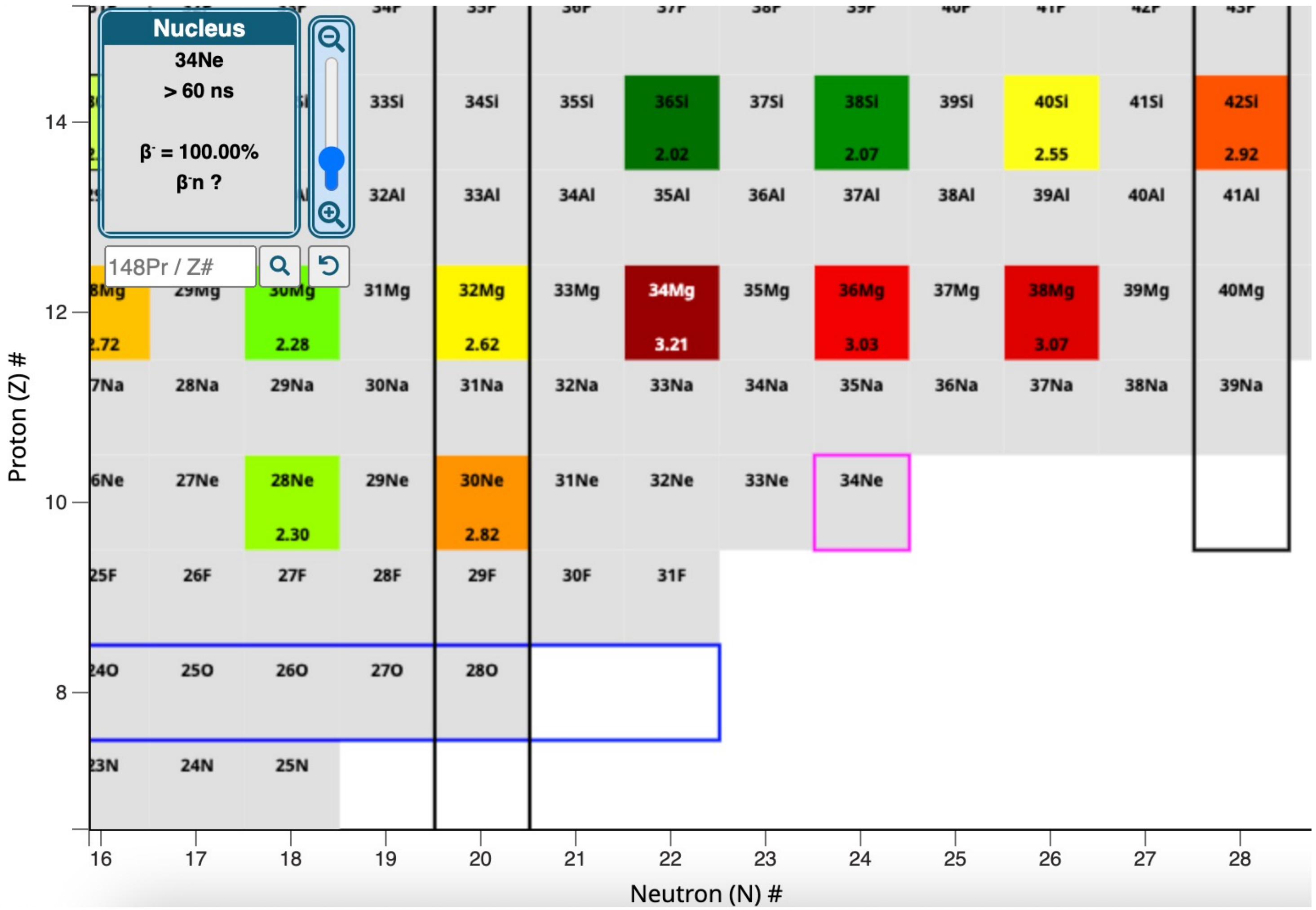
1. Take Hamiltonians from chiral effective field theory: $H = T + V_{NN} + V_{NNN}$
2. Perform Hartree-Fock or Hartree-Fock-Bogoliubov computation
   a. Yields non-trivial vacuum state $|\psi_0\rangle$
   b. Informs us about nuclear deformation and superfluidity
   c. Introduces Fermi momentum $k_F \approx 1.35$ fm^{-1} as the dividing scale between IR and UV physics
   d. Allows us to normal-order H w.r.t. $|\psi_0\rangle$
3. Include correlations / entanglement via your favorite method of choice (Coupled-cluster theory, Green's function method, IMSRG, …)
   a. 2-particle–2-hole (2p-2h) excitations and 3p-3h excitations (UV physics) dominate size-extensive contributions to the binding energy
   b. Symmetry restoration and collective (IR physics) yield smaller contributions that are not size extensive

Neutron-rich nuclei beyond $N \geq 20$ are deformed

$$R_{4/2} \equiv \frac{E_{4^+}}{E_{2^+}}$$

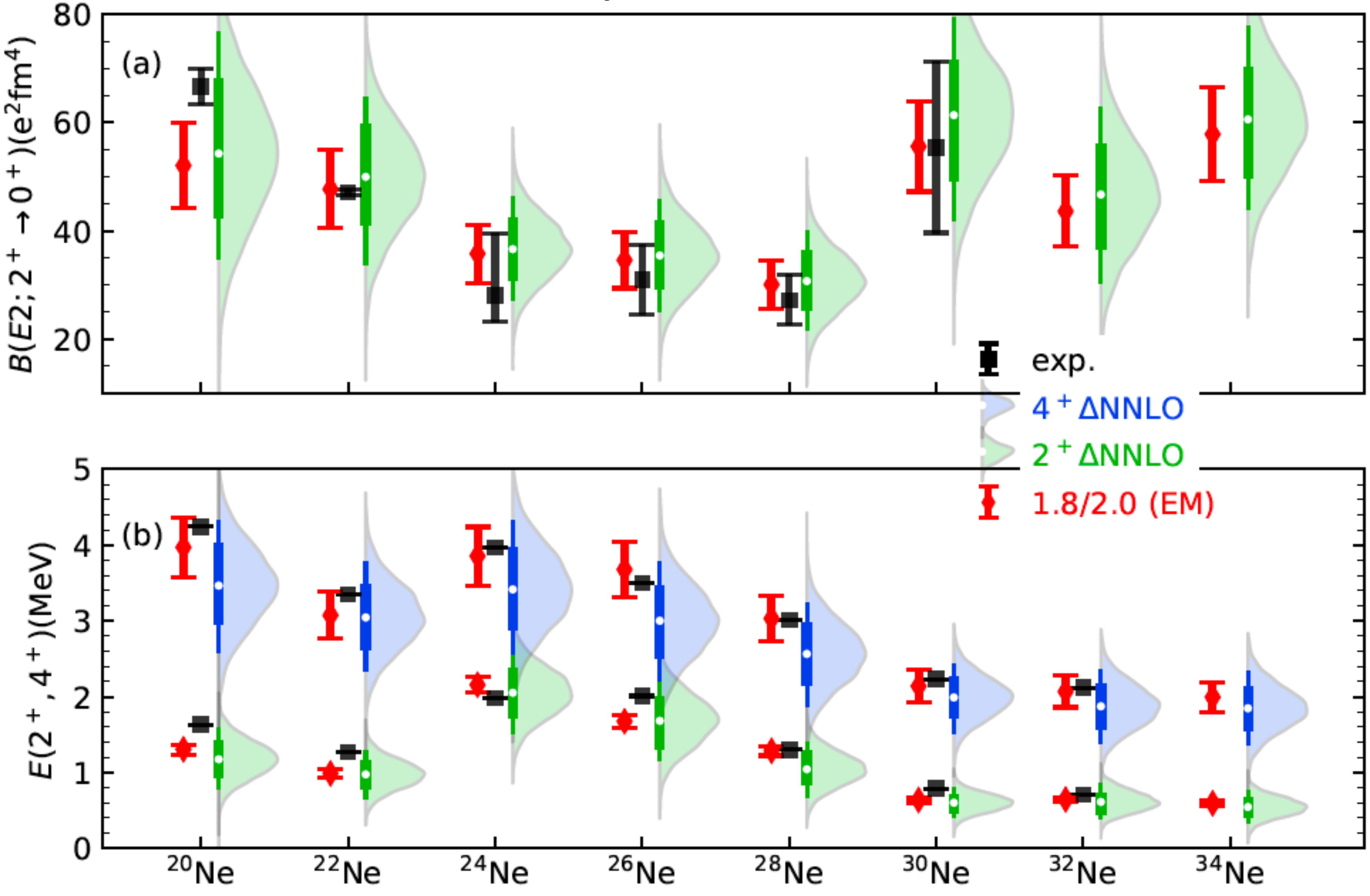
$R_{4/2} = 10/3$ for a rigid rotor

Simple picture: Spherical states (magic $N = 20$ number in the traditional shell model) coexist with deformed ground states



Poves & Retamosa (1987); Warburton, Becker, and Brown (1990); …

Collectivity of neon nuclei



Zhonghao Sun et al., arXiv:2404.00058

Shape coexistence

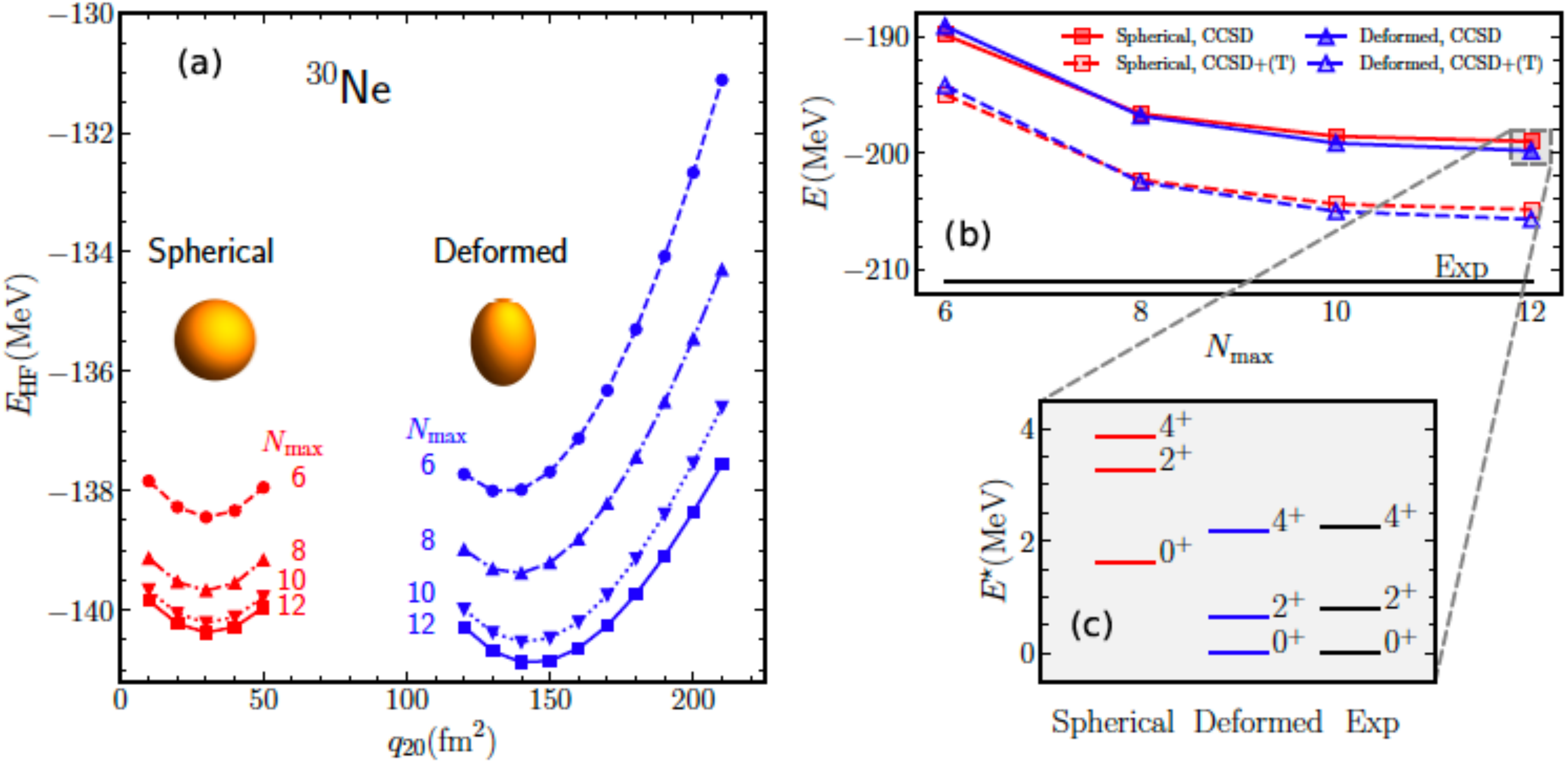
States with different shapes that are close in energy

Reviews: Heyde and Wood, Rev. Mod. Phys. 83, 1467 (2011); Gade and Liddick, J. Phys. G 43, 024001 (2016); Bonatsos, et al., Atoms 11, 117 (2023).

Observed in ^{30}Mg by Schwerdtfeger et al., Phys. Rev. Lett. 103, 012501 (2009) and in ^{32}Mg by Wimmer et al., Phys. Rev. Lett. 105, 252501 (2010).

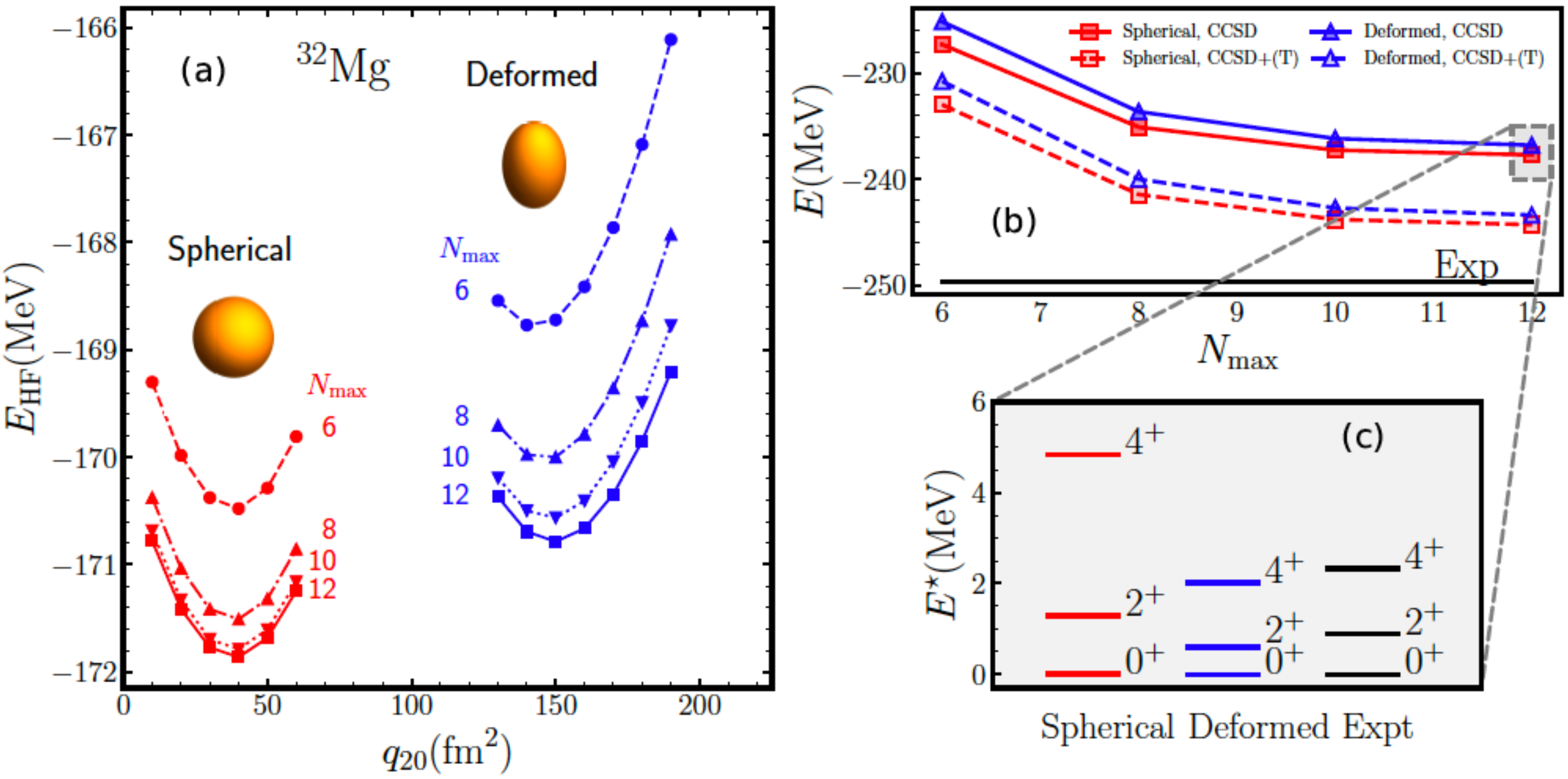
Theoretical descriptions: Reinhard et al., Phys. Rev. C 60, 014316 (1999); Rodríguez-Guzmán, Egido, and Robledo, Nucl. Phys. A 709, 201 (2002); Péru and Martini, Eur. Phys. J. A 50, 88 (2014); Caurier, Nowacki, and Poves, Phys. Rev. C 90, 014302 (2014); see also Tsunoda et al., Nature 587, 66 (2020).

Prediction: Shape coexistence in ^{30}Ne



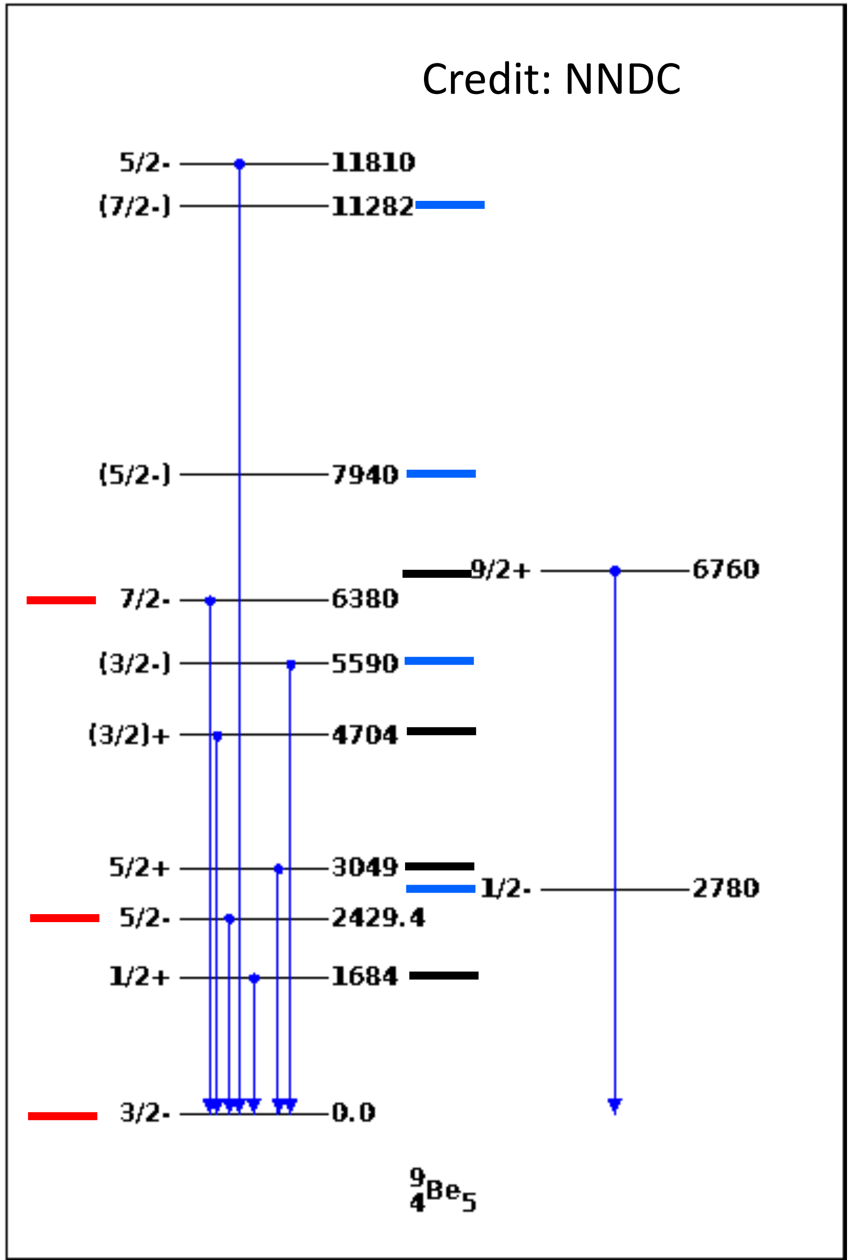
Zhonghao Sun et al., arXiv:2404.00058

Confirmation: Shape coexistence in ^{32}Mg



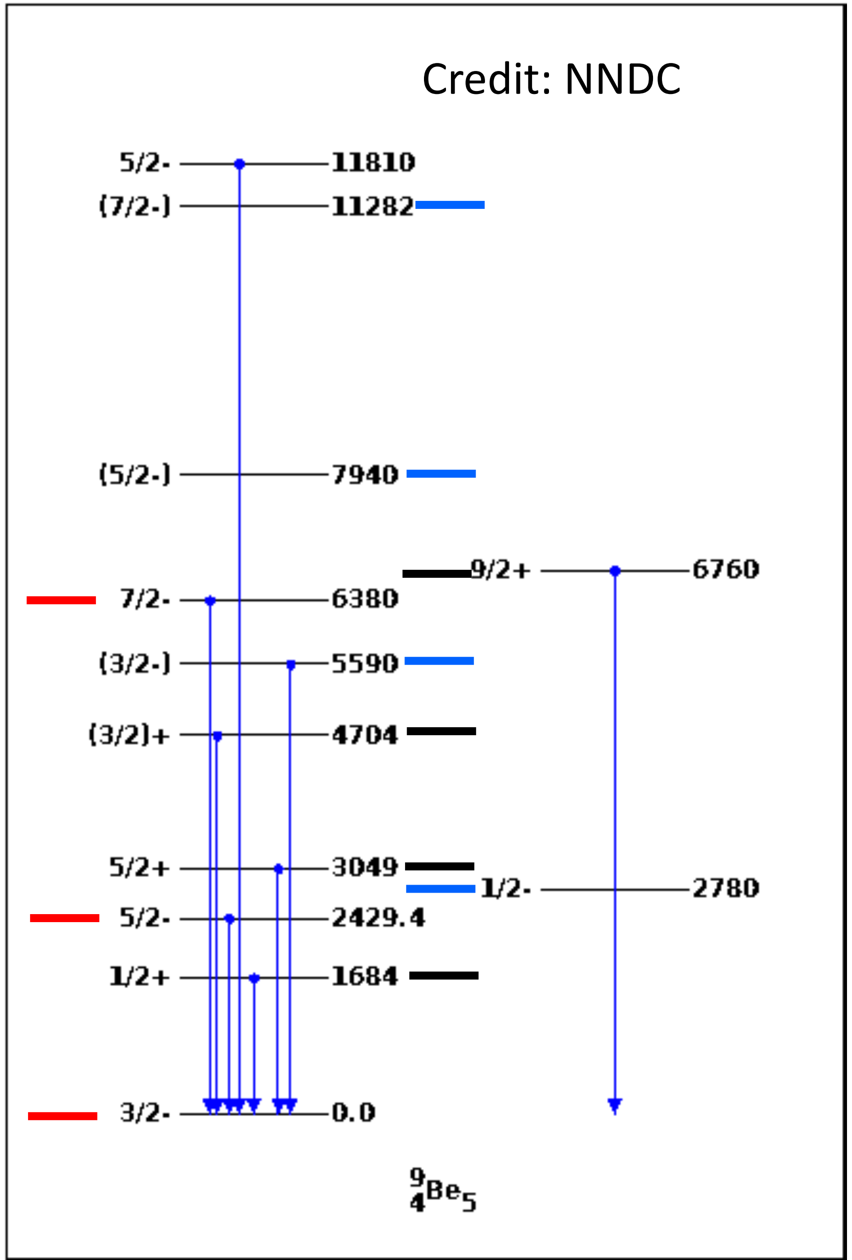
Zhonghao Sun et al., arXiv:2404.00058

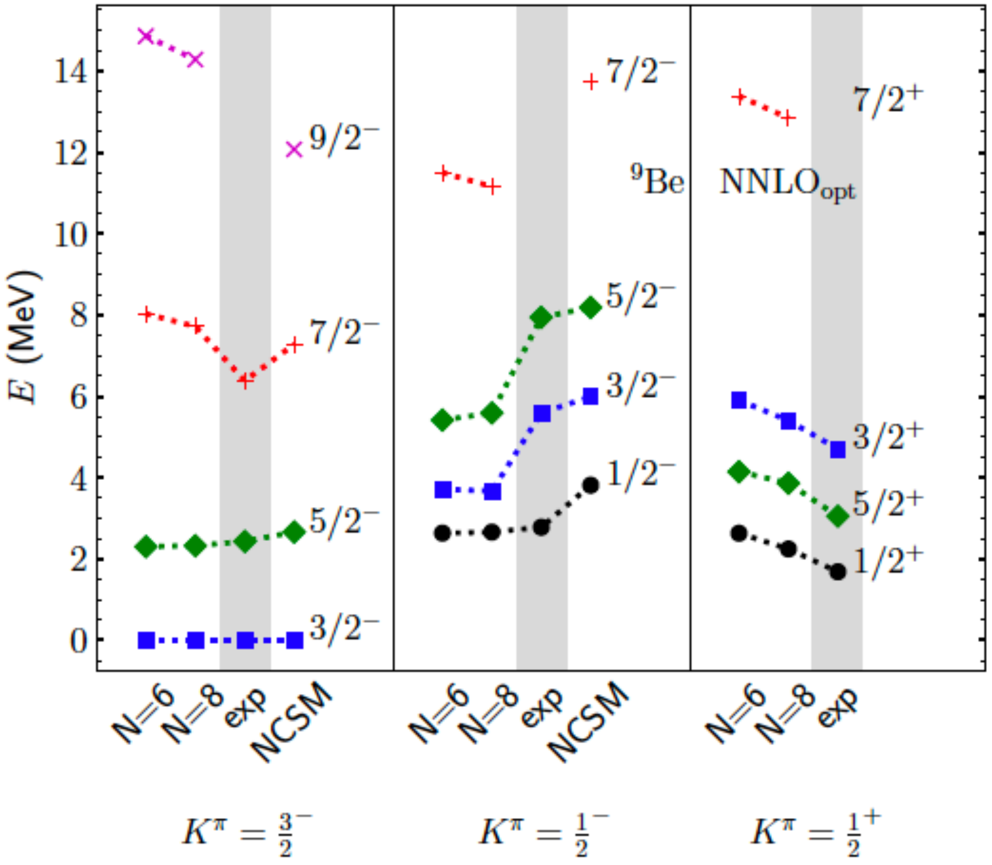
Odd-mass deformed nuclei



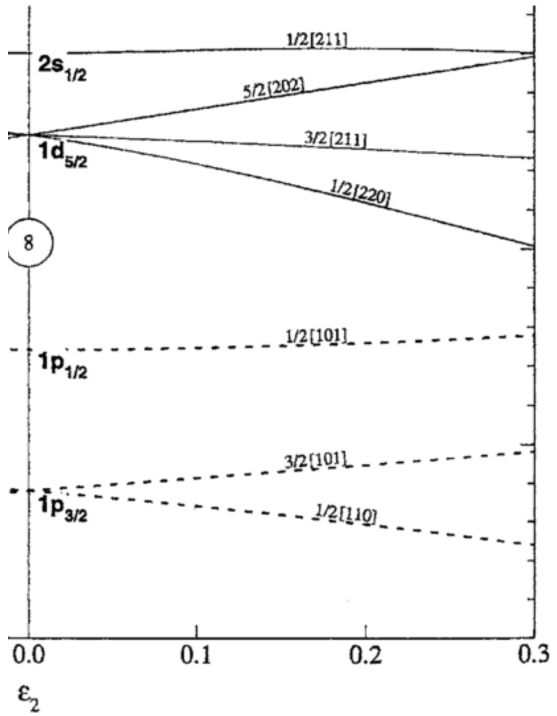
Rhetorical Q: Who sees patterns here?
Who sees a stamp collection?

Odd-mass deformed nuclei



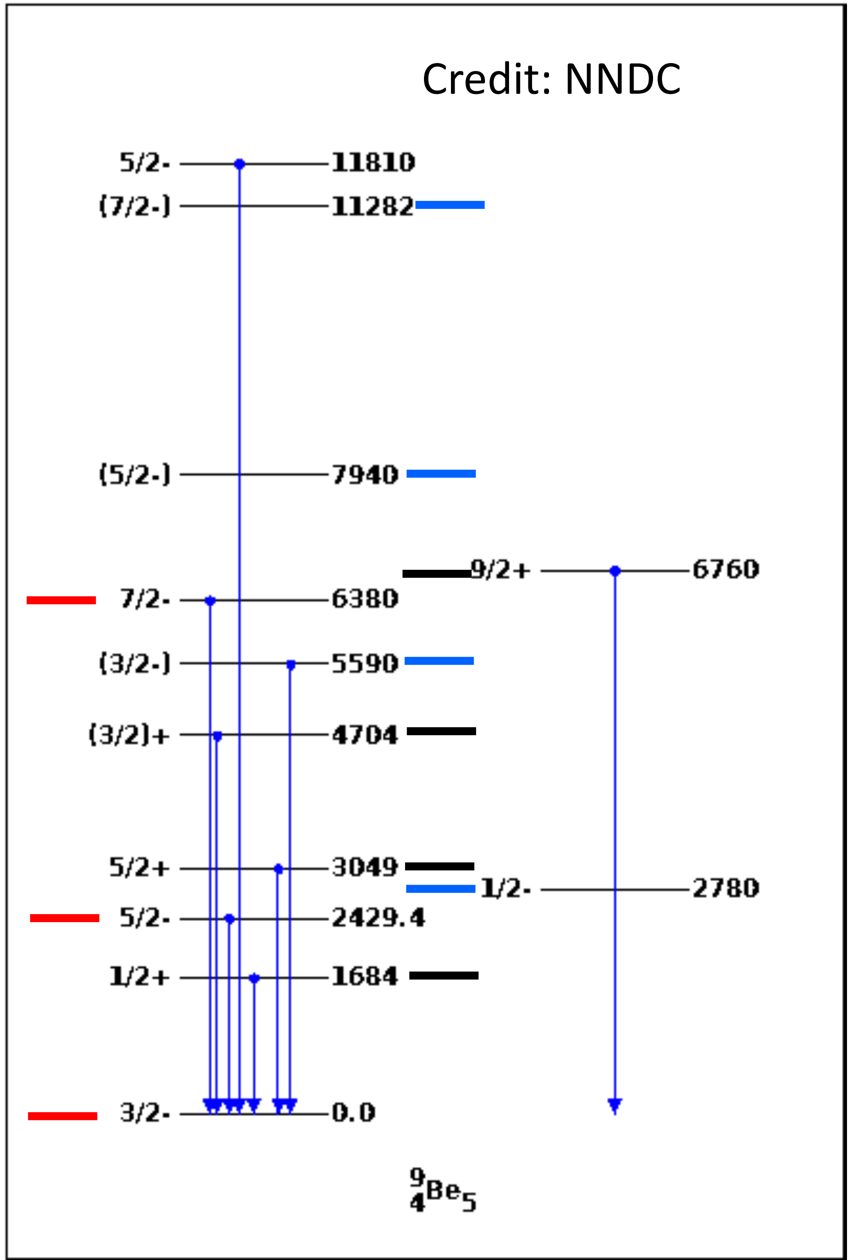


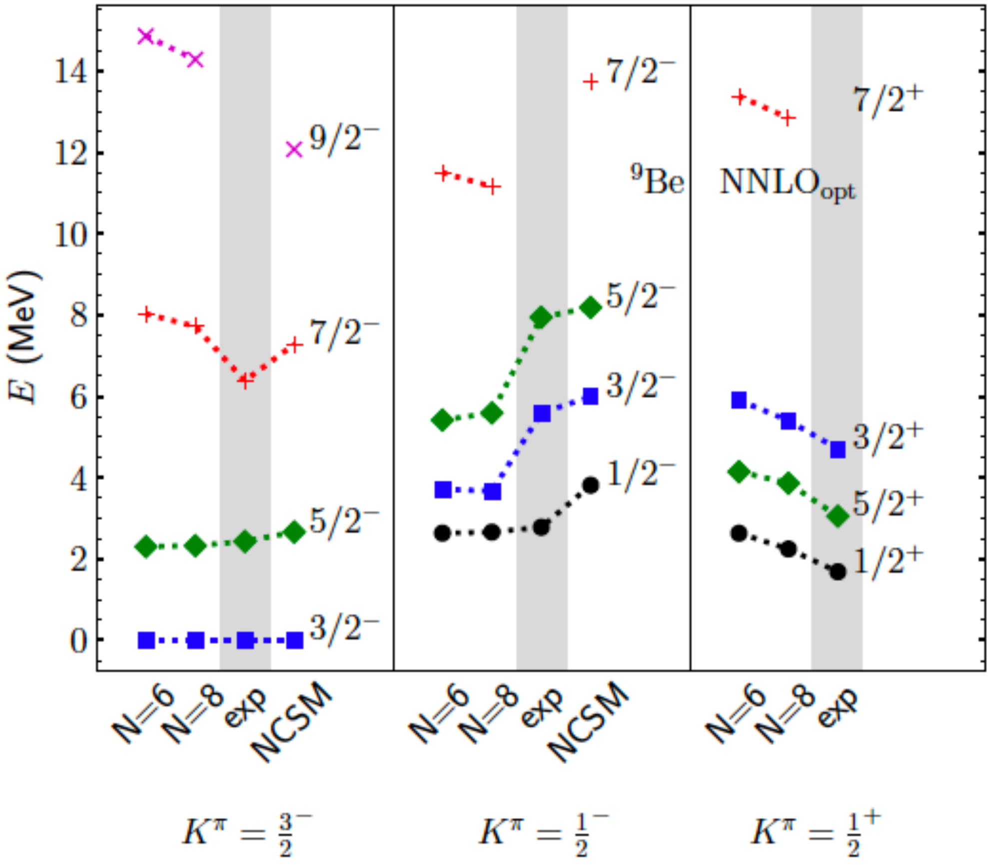
Zhonghao Sun et al., in preparation
NCSM: Caprio et al., Int. J. Mod. Phys. E 24, 1541002 (2015).



Q: For ^{9}Be (Z=4, N=5), can you place the odd neutron in the Nilsson diagram for each of the bands shown in the middle?

Odd-mass deformed nuclei





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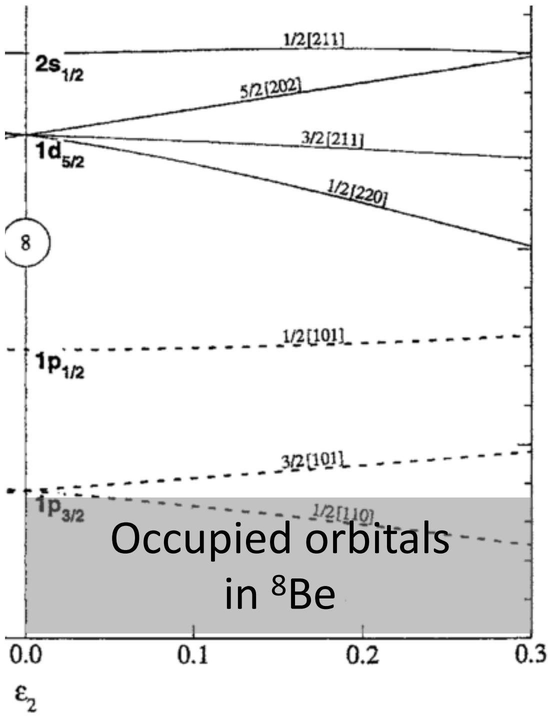

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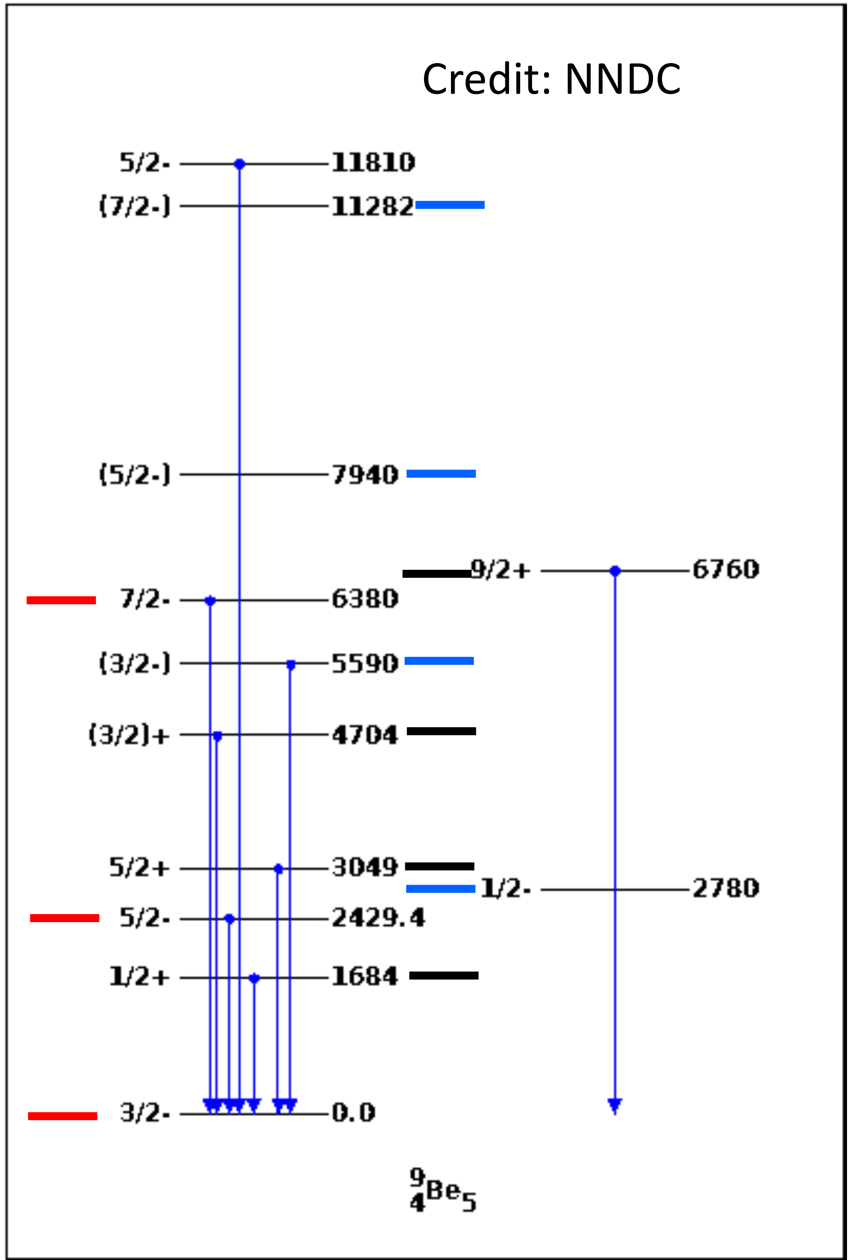
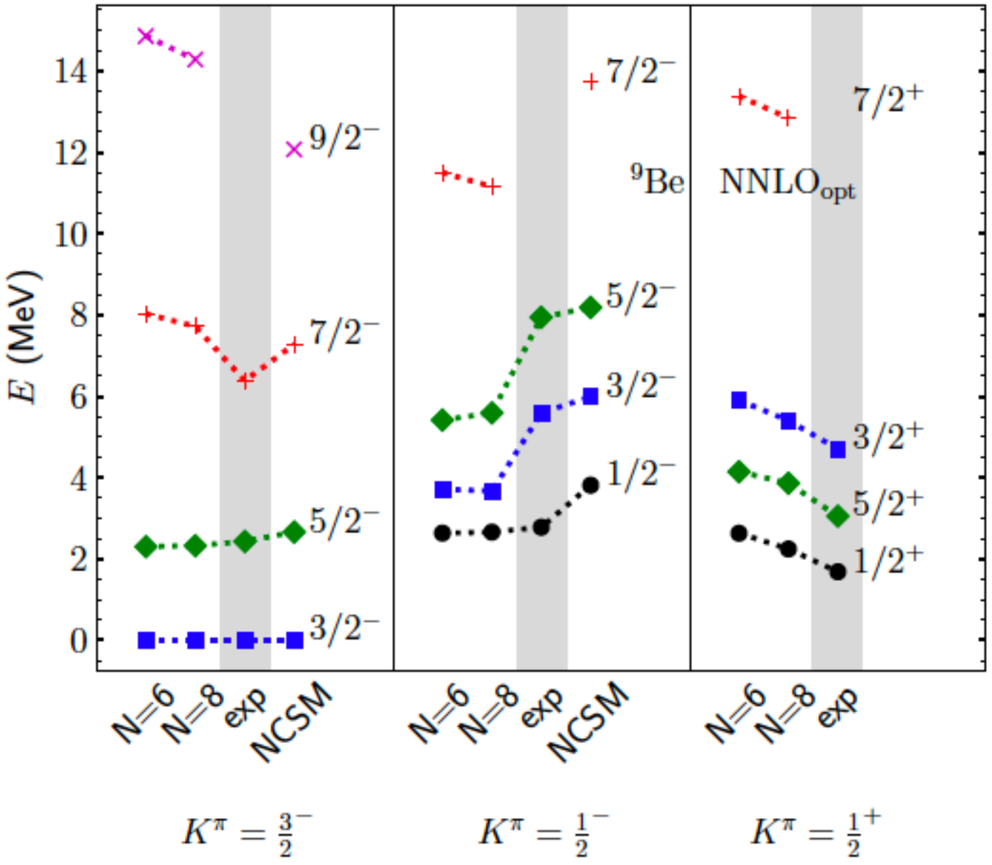
Odd-mass deformed nuclei





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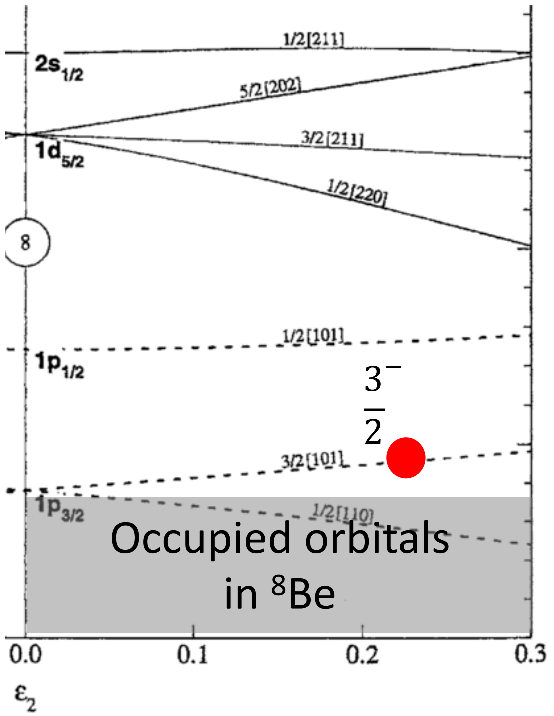

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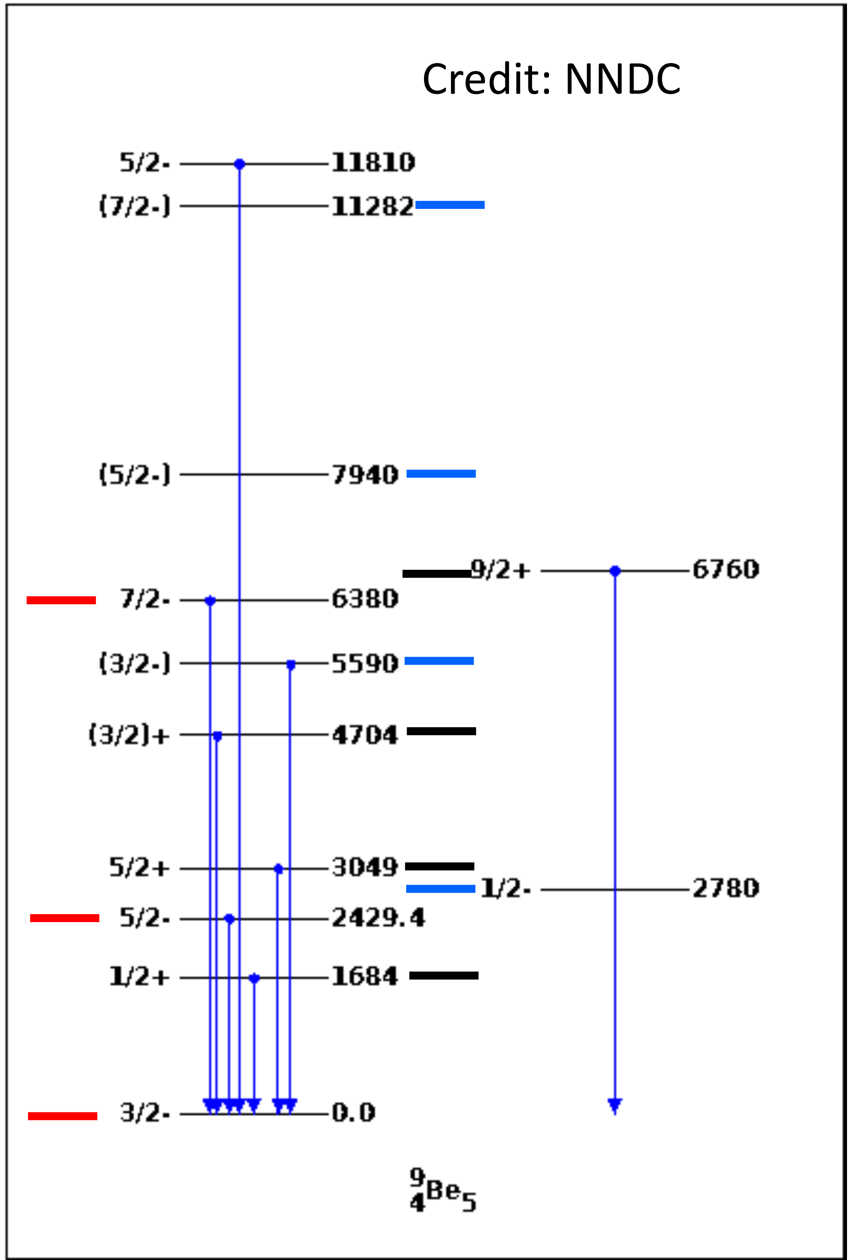
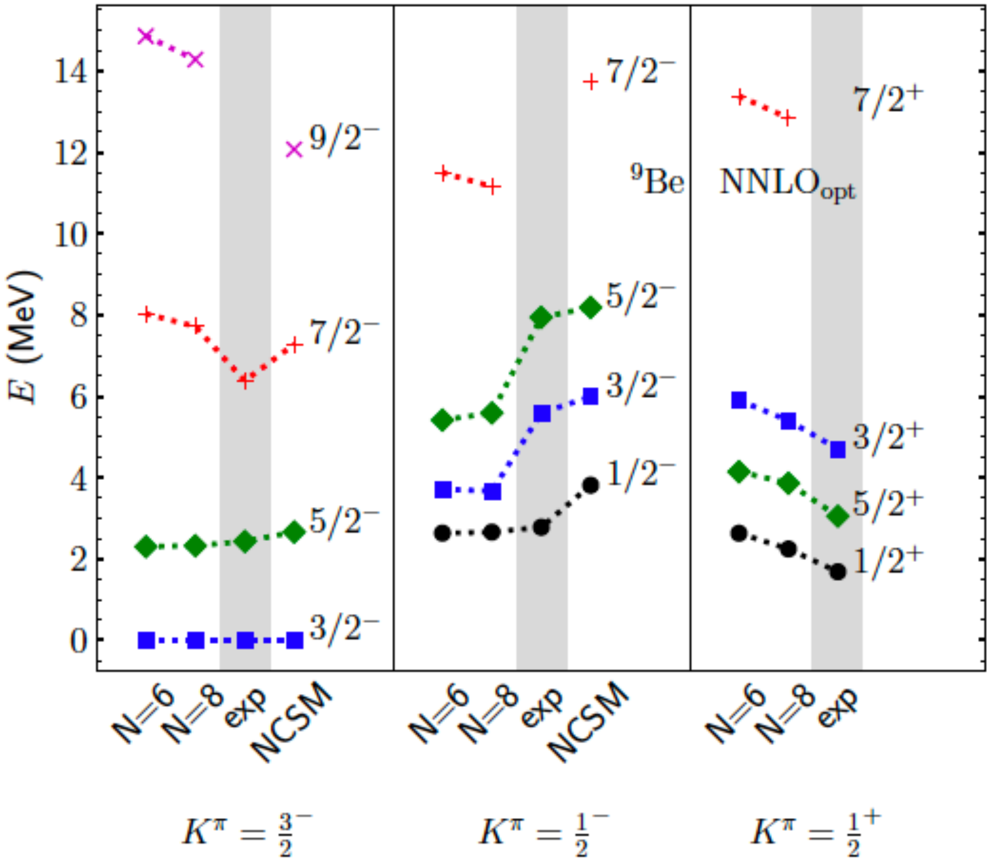
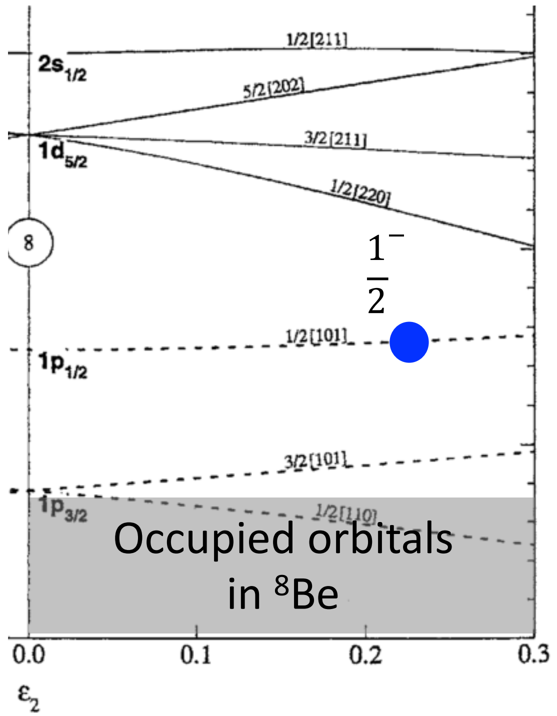




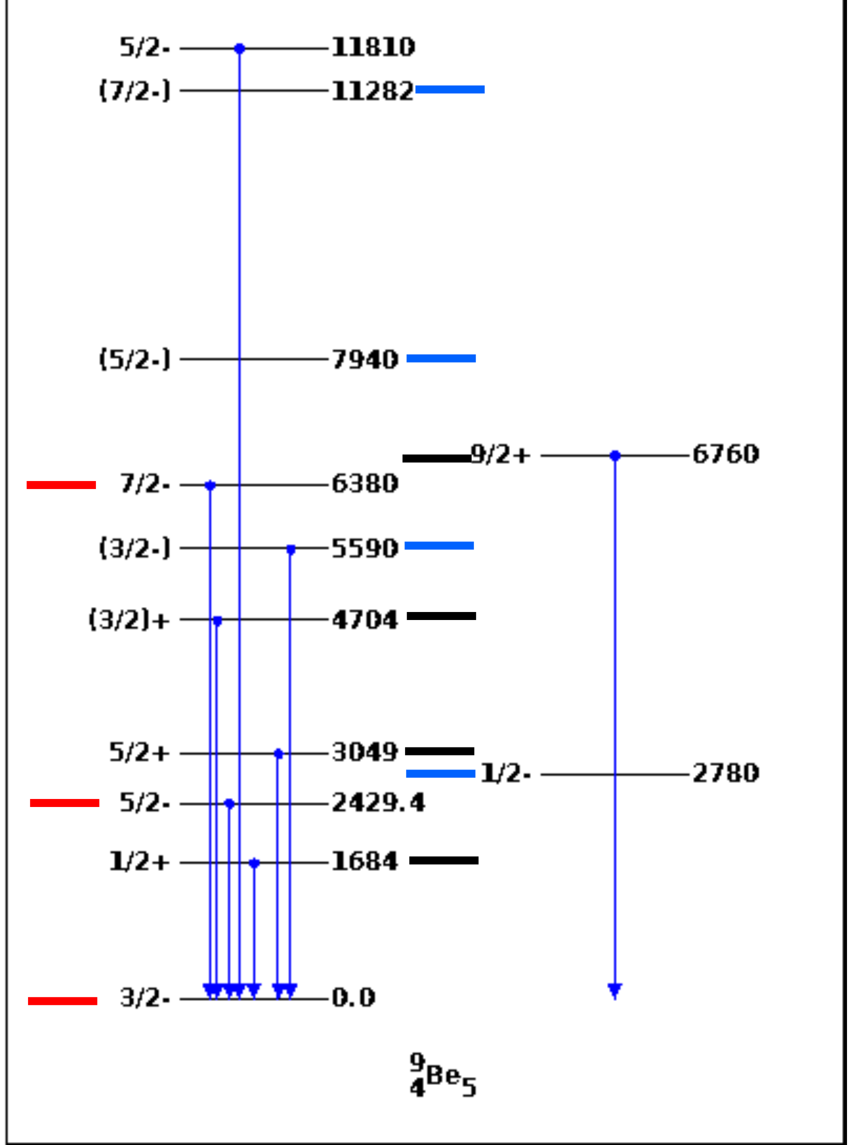
Zhonghao Sun et al., in preparation
NCSM: Caprio et al., Int. J. Mod. Phys. E 24, 1541002 (2015).

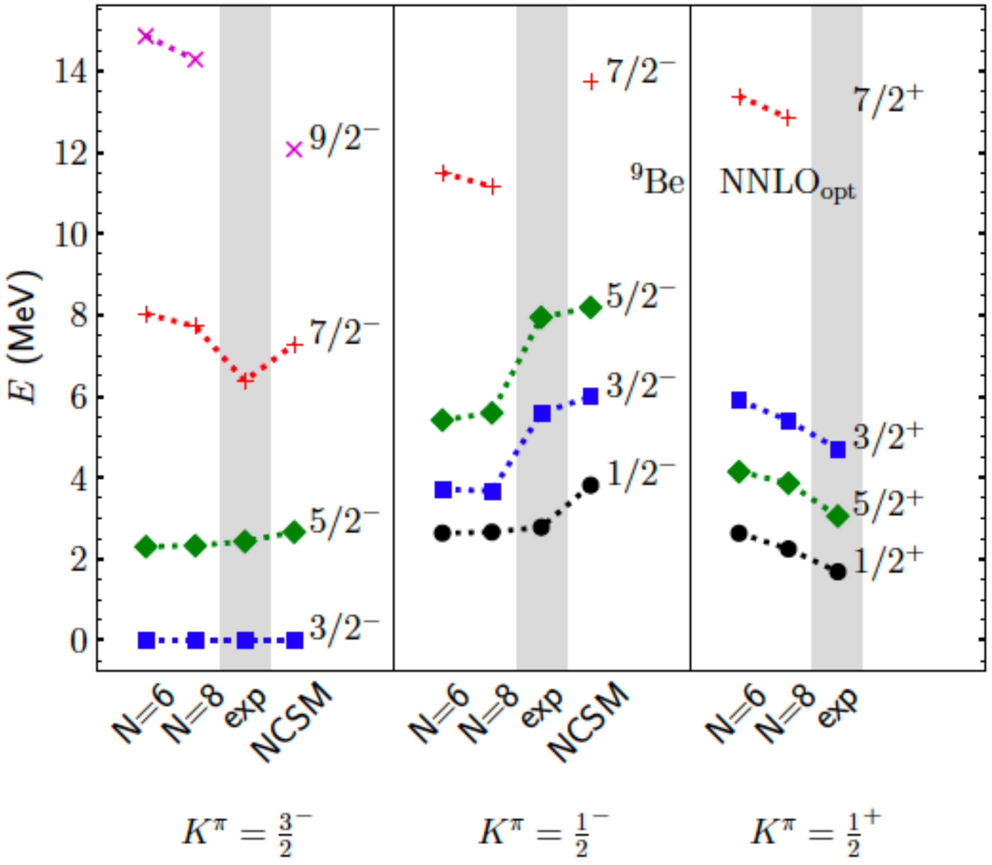


Q: For ^{9}Be (Z=4, N=5), can you place the odd neutron in the Nilsson diagram for each of the bands shown in the middle?

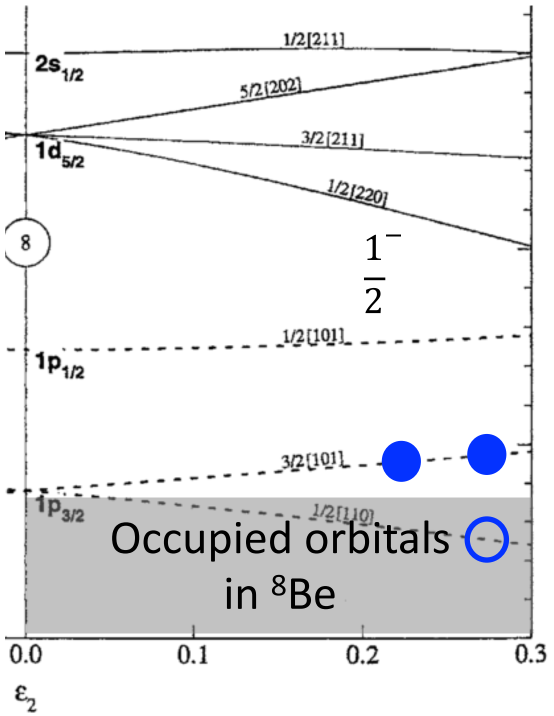
Odd-mass deformed nuclei

Credit: NNDC





Zhonghao Sun et al., in preparation
NCSM: Caprio et al., Int. J. Mod. Phys. E 24, 1541002 (2015).



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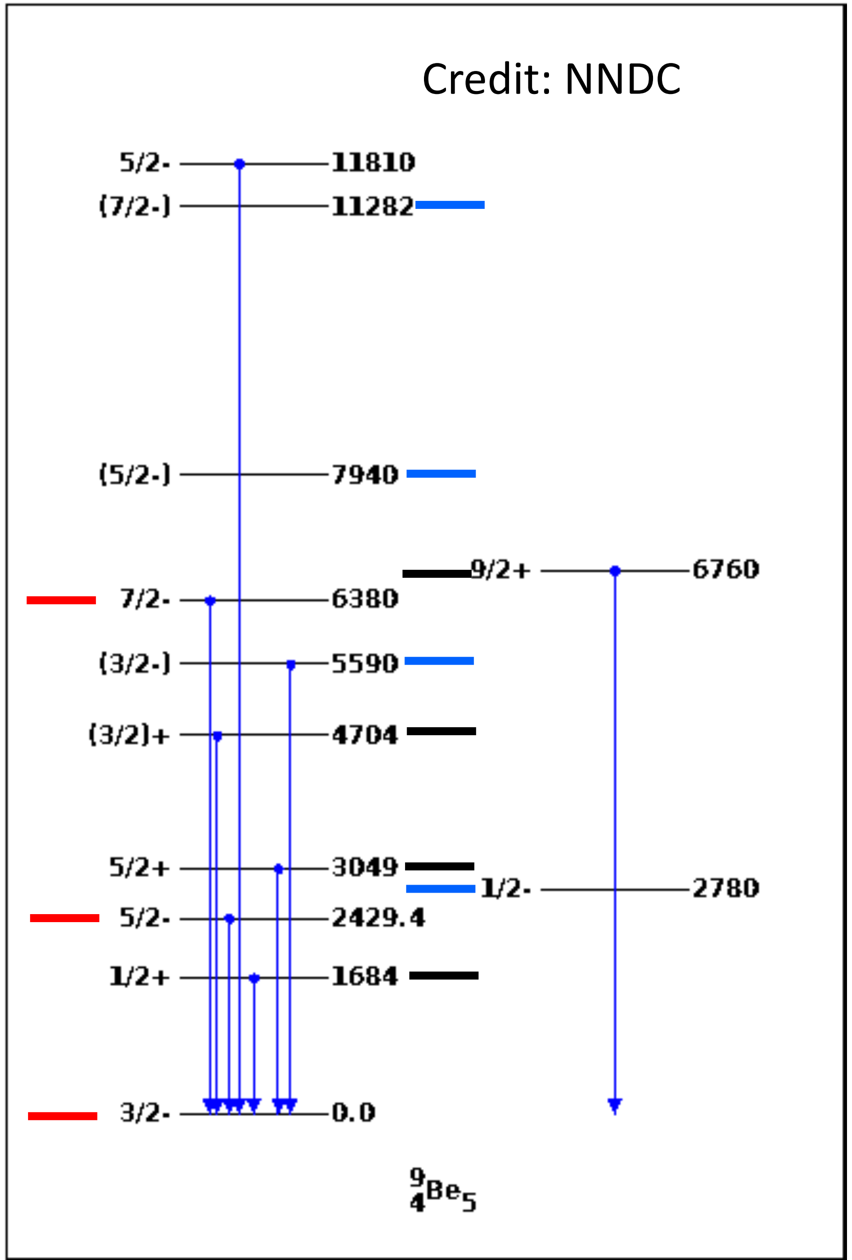
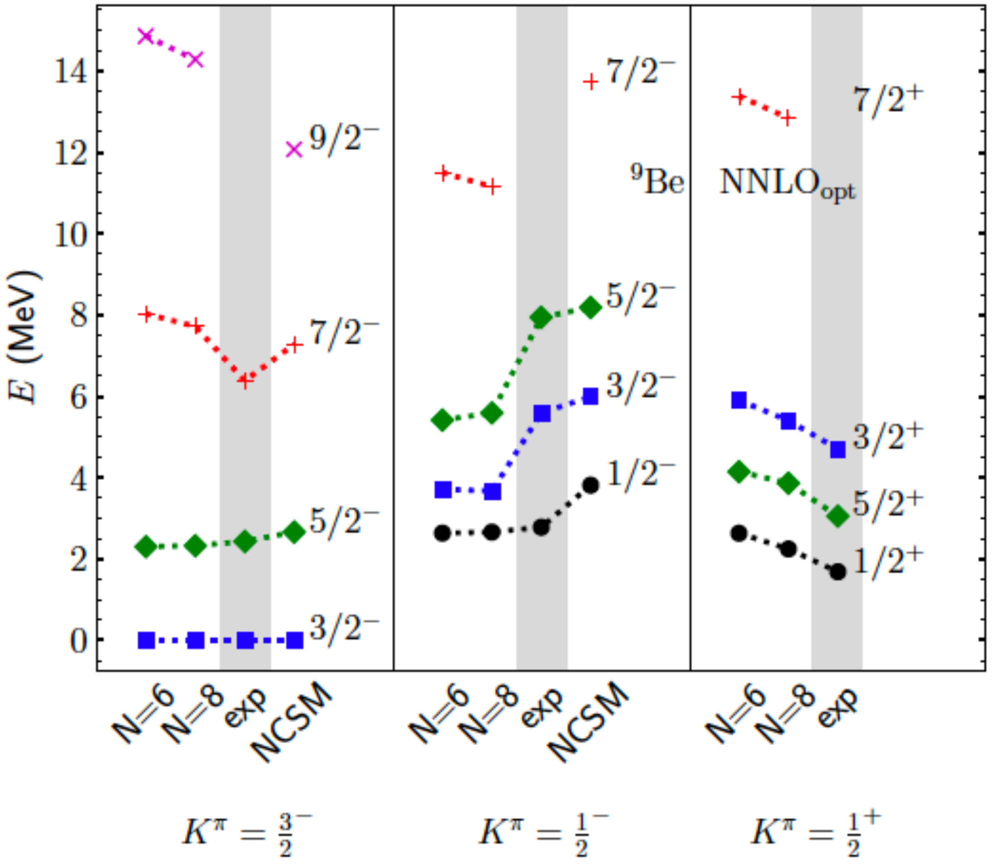
Odd-mass deformed nuclei





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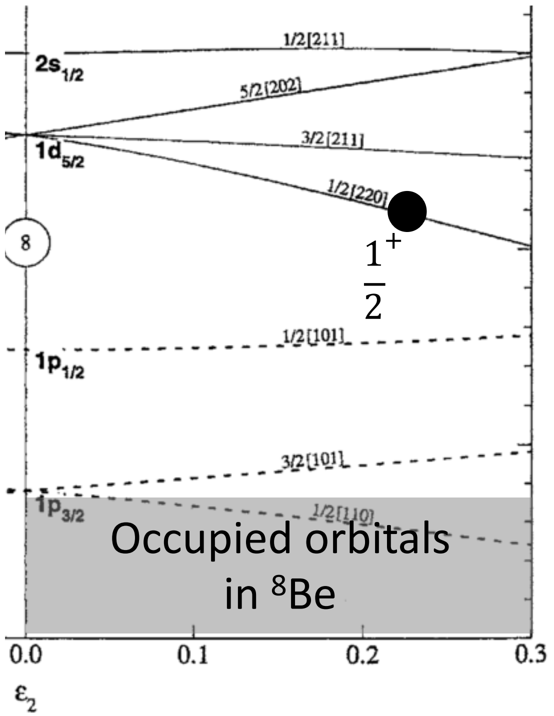


Q: For ^{9}Be (Z=4, N=5), can you place the odd neutron in the Nilsson diagram for each of the bands shown in the middle?

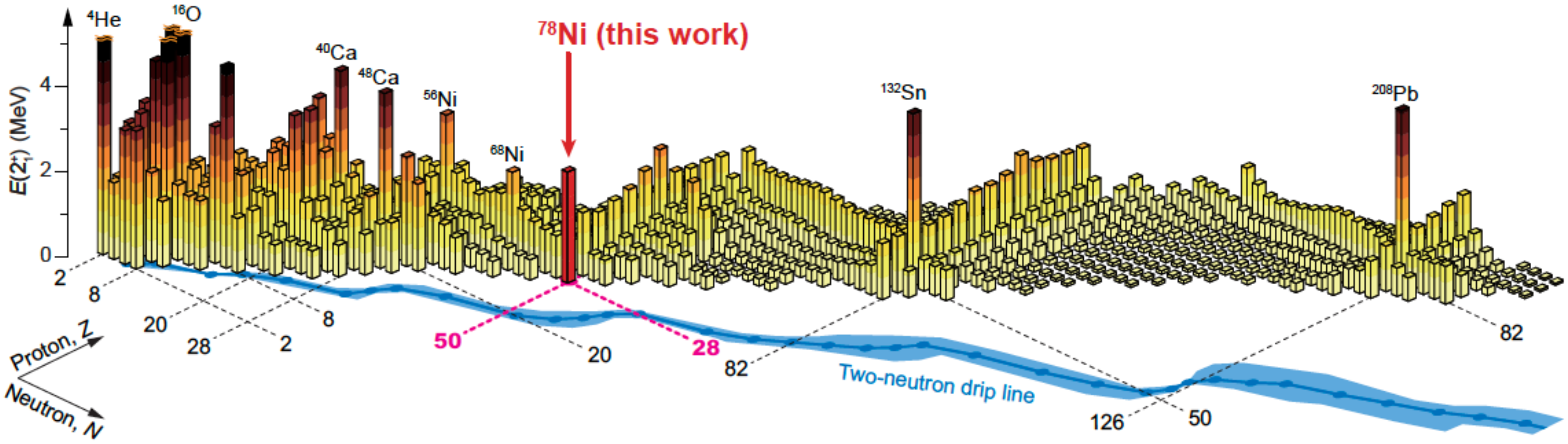
Summary: Ab initio computations

A conceptually simple picture emerges

- Start with a mean-field computation (and break symmetries)
  - This gives reference state that is useful for all what follows
- Include dynamical correlations via coupled-cluster theory (or IMSRG or Greens functions, or …)
  - This gives the bulk of the binding energy; dominantly from short-range correlations
- Include static correlations via symmetry restoration and/or using collective coordinates
  - This gives long-range correlations; contributes little to the binding but a lot to the structure

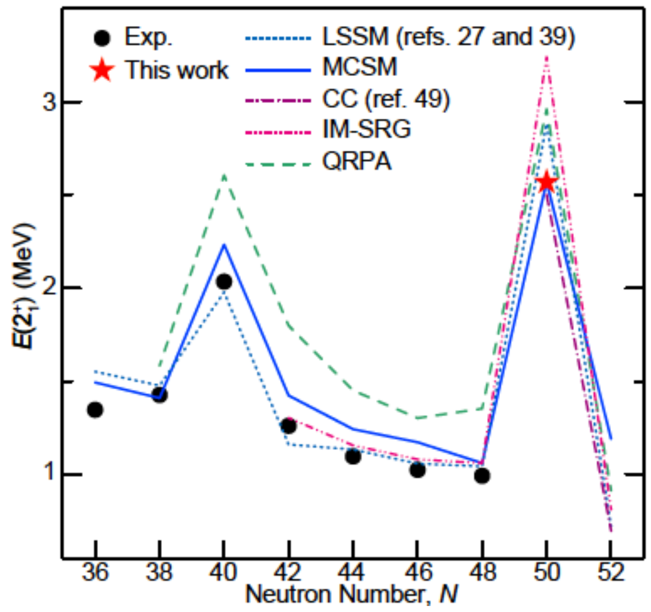
A few more success stories of ab initio computations of nuclei

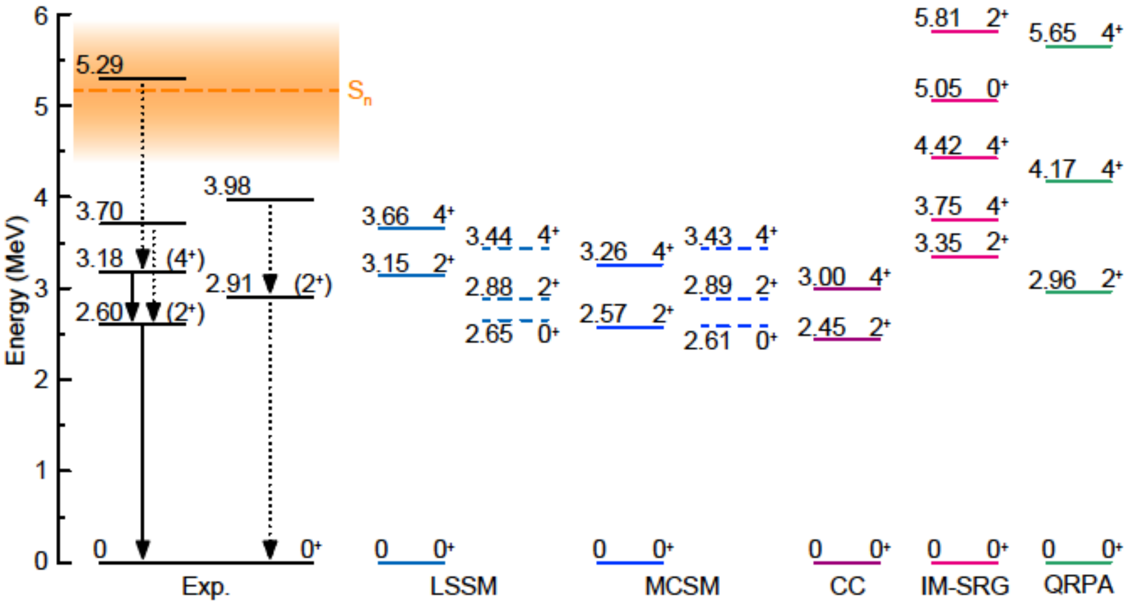
^{78}Ni (Z=28, N=50) is a neutron-rich doubly magic nucleus



Doubly magic nuclei are more strongly bound, and more difficult to excite, than their neighbors

They are the cornerstones for understanding entire regions of the nuclear chart





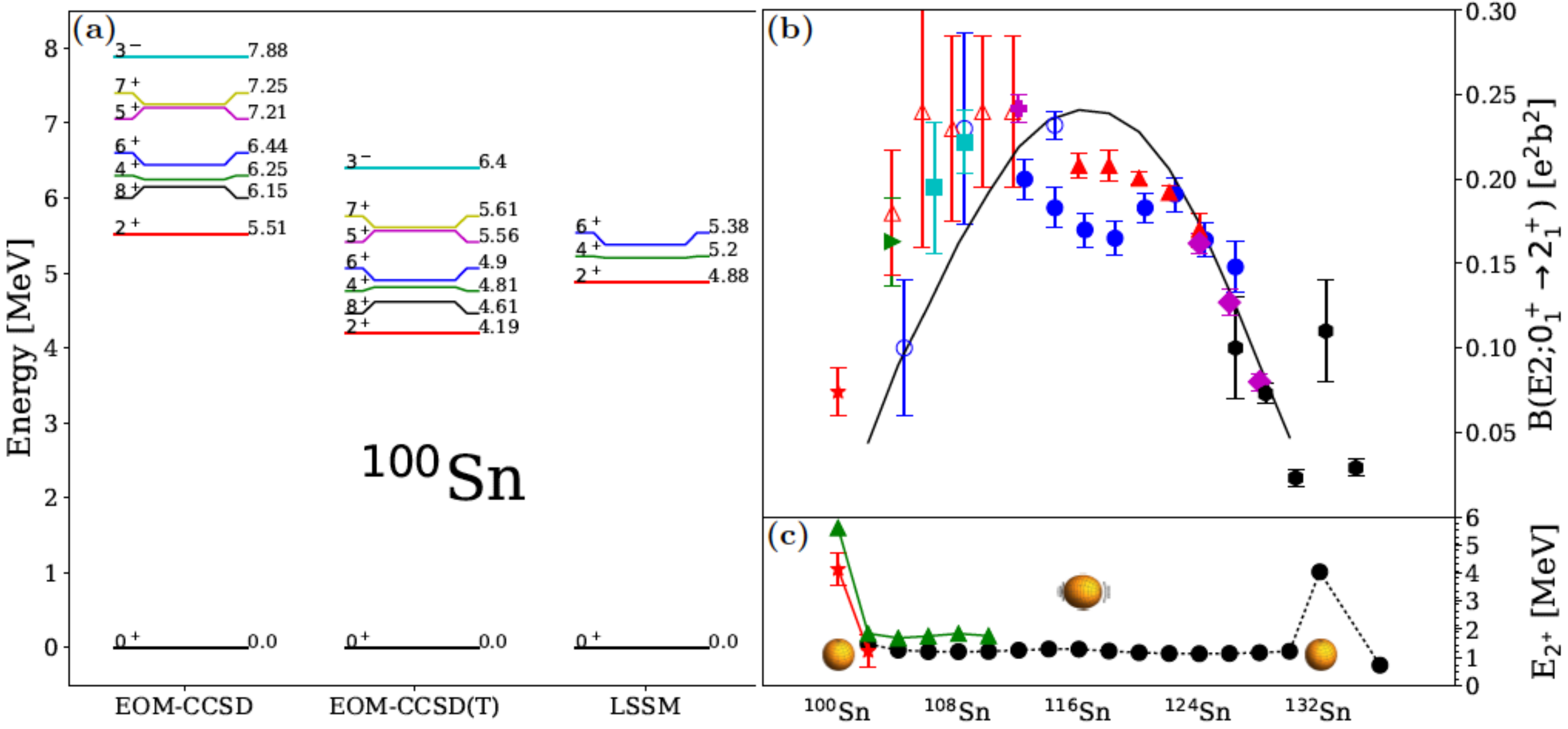
Predictions from 2016

LSSM: shell model

CC: EFT Hamiltonian, adjusted to 2,3,4 nucleons only

R. Taniuchi, C. Santamaria, P. Doornenbal, A. Obertelli, K. Yoneda et al., Nature 569, 53-58 (2019); arXiv:1912.05978

Theory predicts that ^{100}Sn (N=Z=50) is a doubly magic nucleus



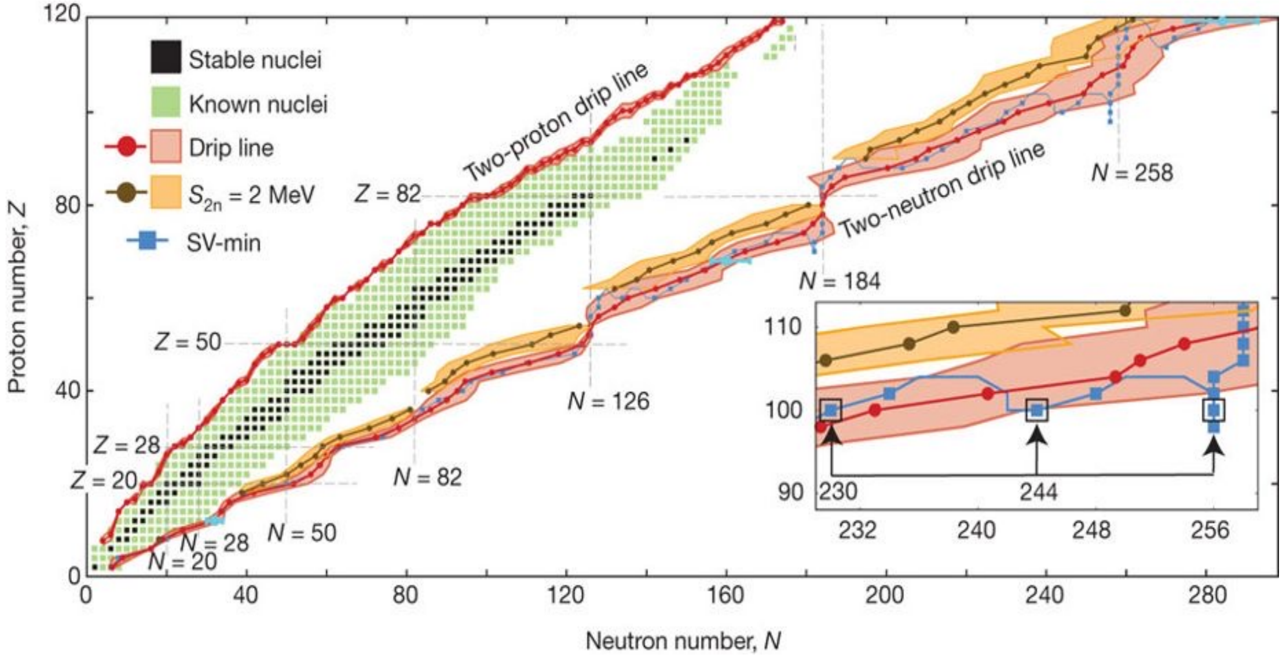
Coupled cluster based on interaction 1.8/2.0(EM); LSSM: Large Scale Shell Model [Faestermann, Gorska & Grawe (2013)]

Doubly magic nuclei are hard to excite (gap in the spectrum) and exhibit small electric quadrupole strength B(E2)

Morris, Simonis, Stroberg, Stumpf, Hagen, Holt, Jansen, TP, Roth & Schwenk, Phys. Rev. Lett. (2018)

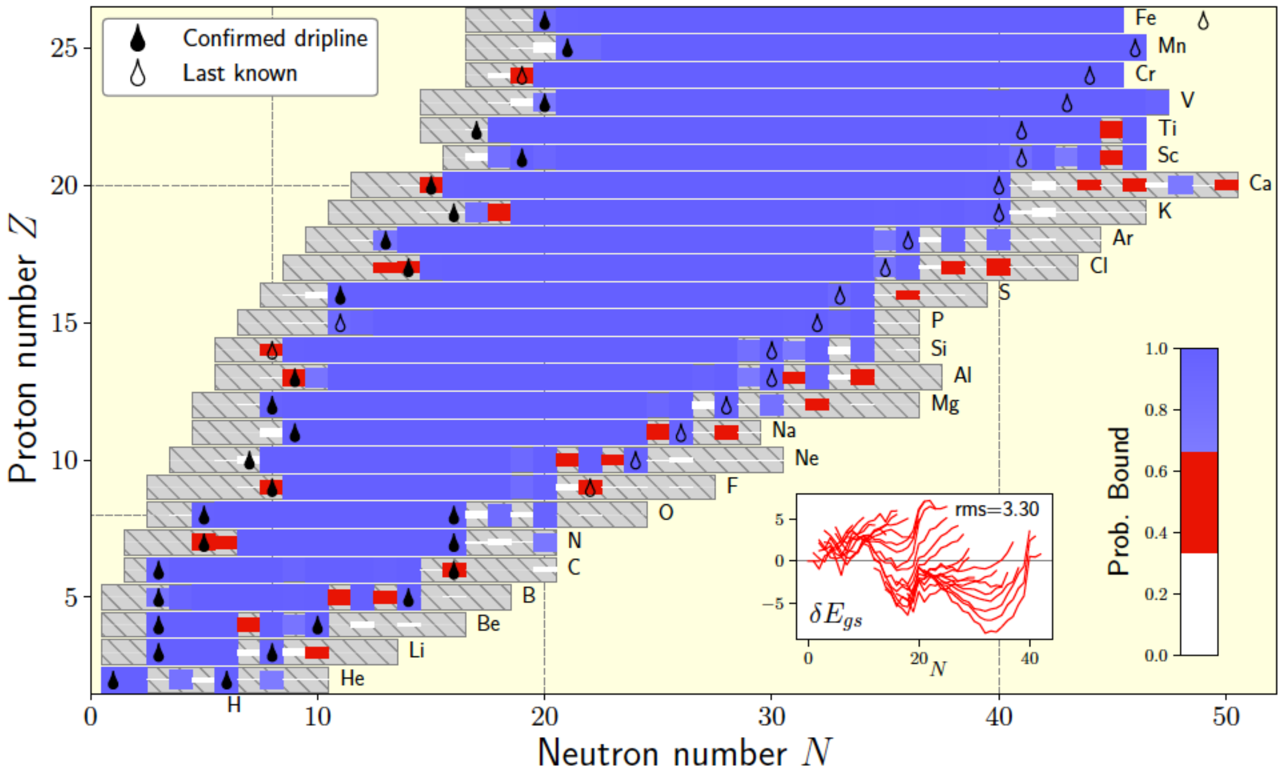
Limits of the nuclear landscape …
… coming within the limits of Hamiltonian-based methods

Nuclear DFT: Erler et al, Nature (2012)



6,900 ± 500_{syst} nuclei with $Z \leq 120$

EFT Hamiltonian: Holt, Stroberg, Schwenk & Simonis (2019)

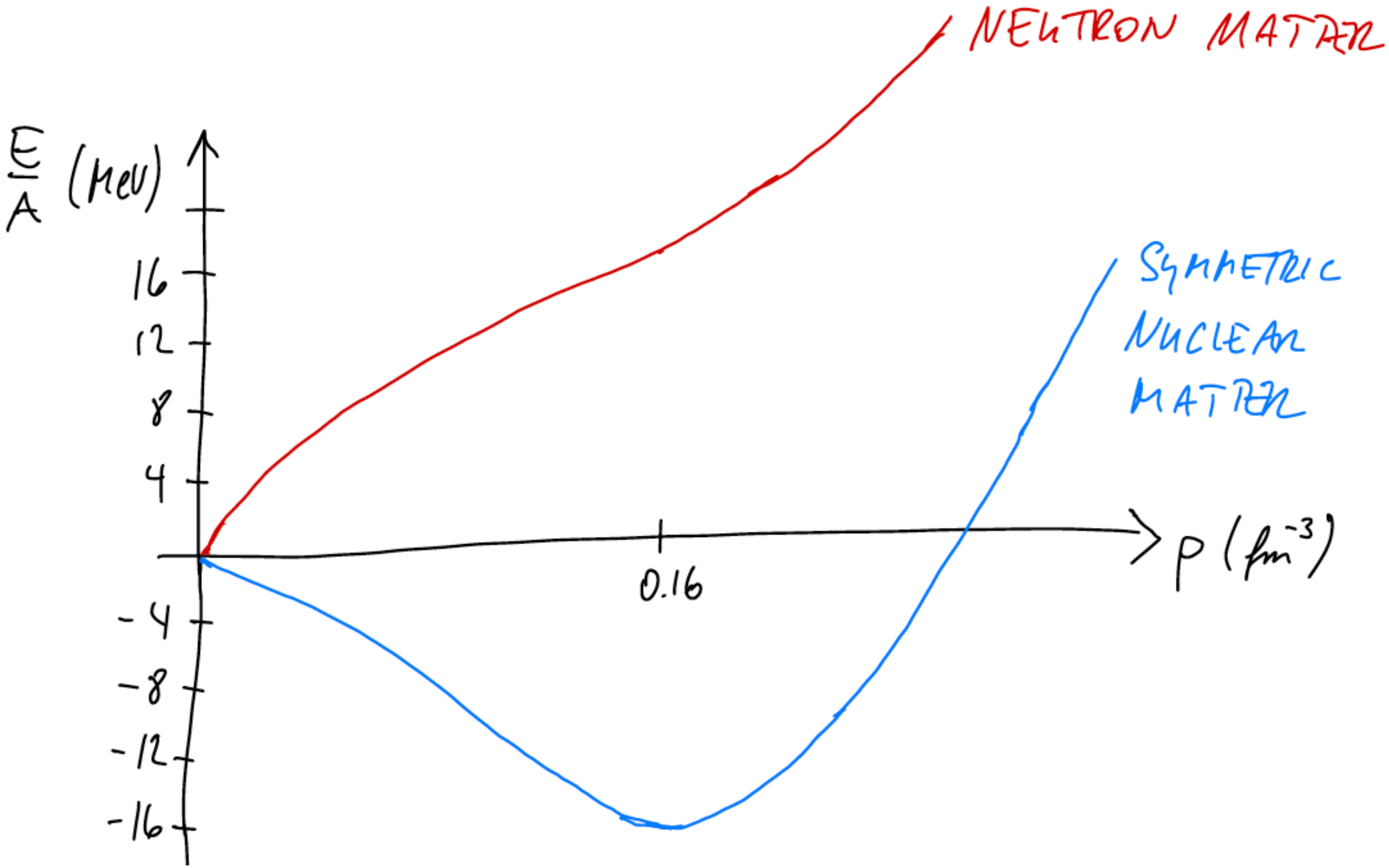


Renaissance and development of methods that scale polynomially with mass number

[Dickhoff & Barbieri; Dean & Hjorth-Jensen; Hagen, Jansen & TP; Tsukiyama, Bogner, Hergert & Schwenk; Elhatisari, Epelbaum, Lee, Lähde, Lu, Meissner; Soma & Duguet; Holt & Stroberg…]

→ Review: H. Hergert, Front. Phys. 8, 379 (2020); arXiv:2008.05061

Nuclear Equation of State
(energy per nucleon in infinite nuclear matter)

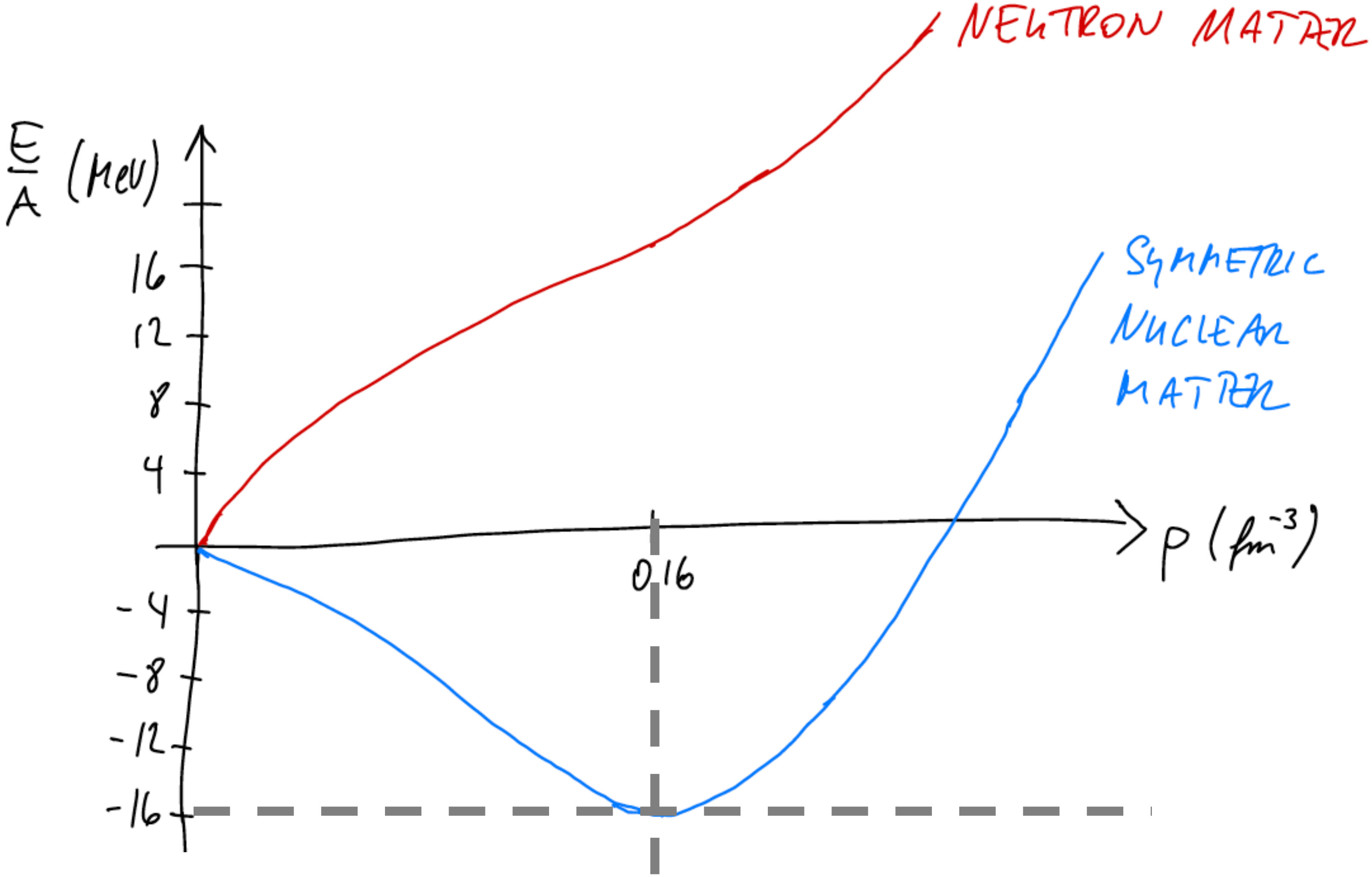


Pure neutron matter: $A = N$

Symmetric matter: $N = Z$

Note: Coulomb force neglected; electrons not included

Nuclear Equation of State



Pure neutron matter: $A = N$

Symmetric matter: $N = Z$

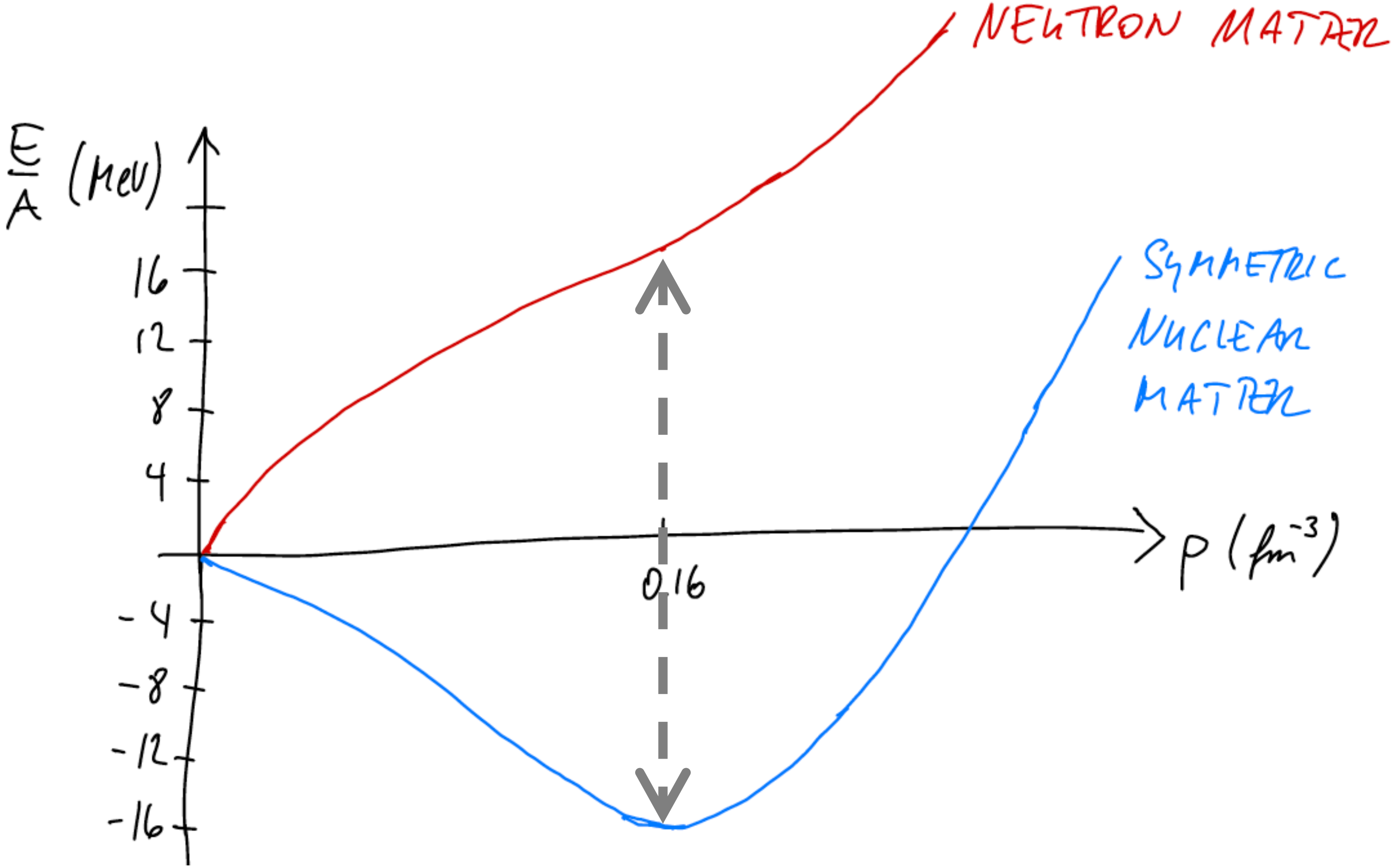
Note: Coulomb force neglected; electrons not included

Saturation point of symmetric nuclear matter

$$\frac{E_{sat}}{N} \approx -16 \text{ MeV}$$

$$\rho_{sat} \approx 0.16 \text{ fm}^{-3}$$

Nuclear Equation of State



Pure neutron matter: $A = N$

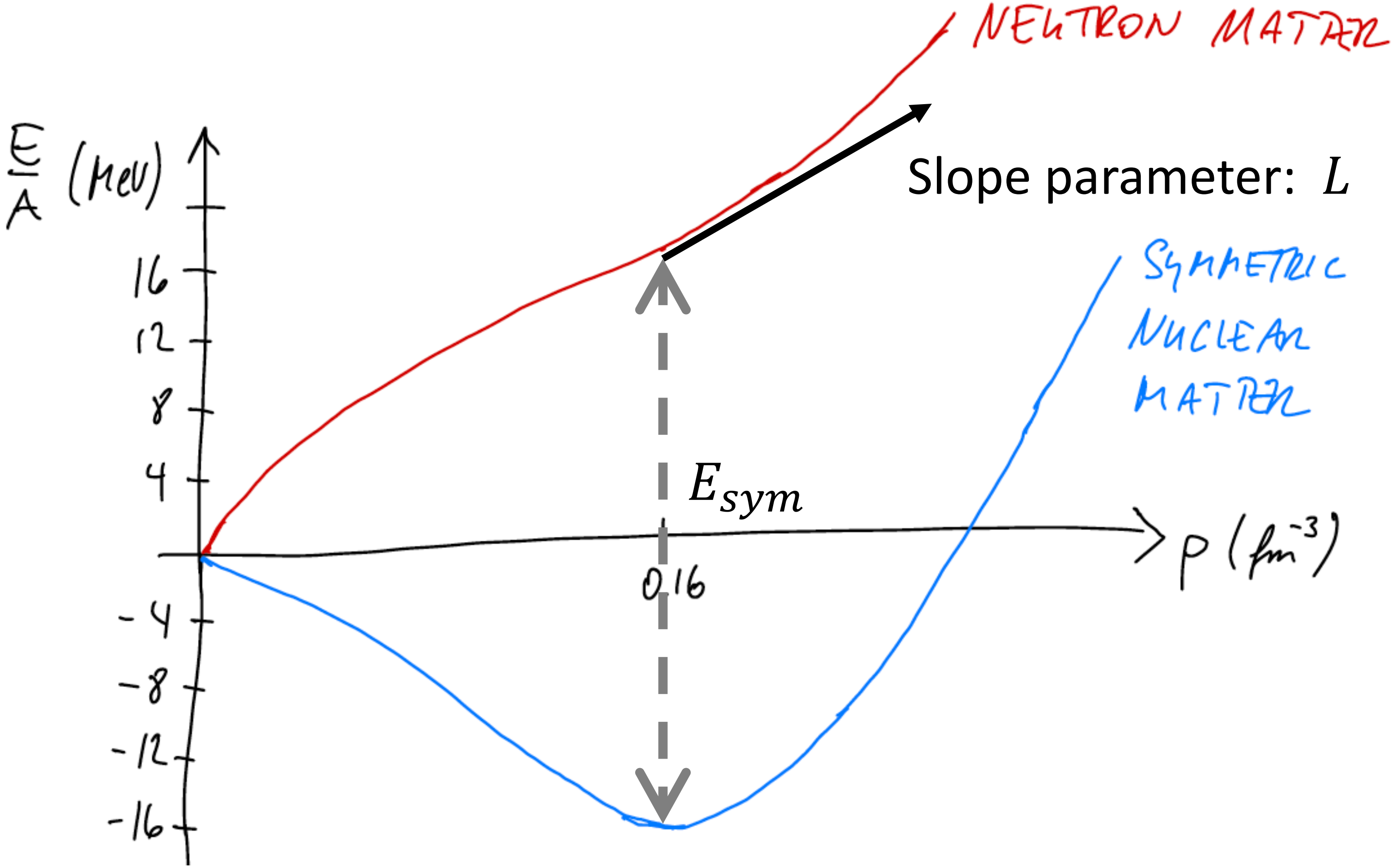
Symmetric matter: $N = Z$

Note: Coulomb force neglected; electrons not included

Symmetry energy: Difference between neutron matter and symmetric nuclear matter at saturation density

$$E_{sym} \approx 32 \text{ MeV}$$

Nuclear Equation of State



Pure neutron matter: $A = N$

Symmetric matter: $N = Z$

Note: Coulomb force neglected; electrons not included

Symmetry energy: Difference between neutron matter and symmetric nuclear matter at saturation density

$E_{sym} \approx 32$ MeV

L less well known

Neutron Radii in Nuclei and the Neutron Equation of State

Alex Brown

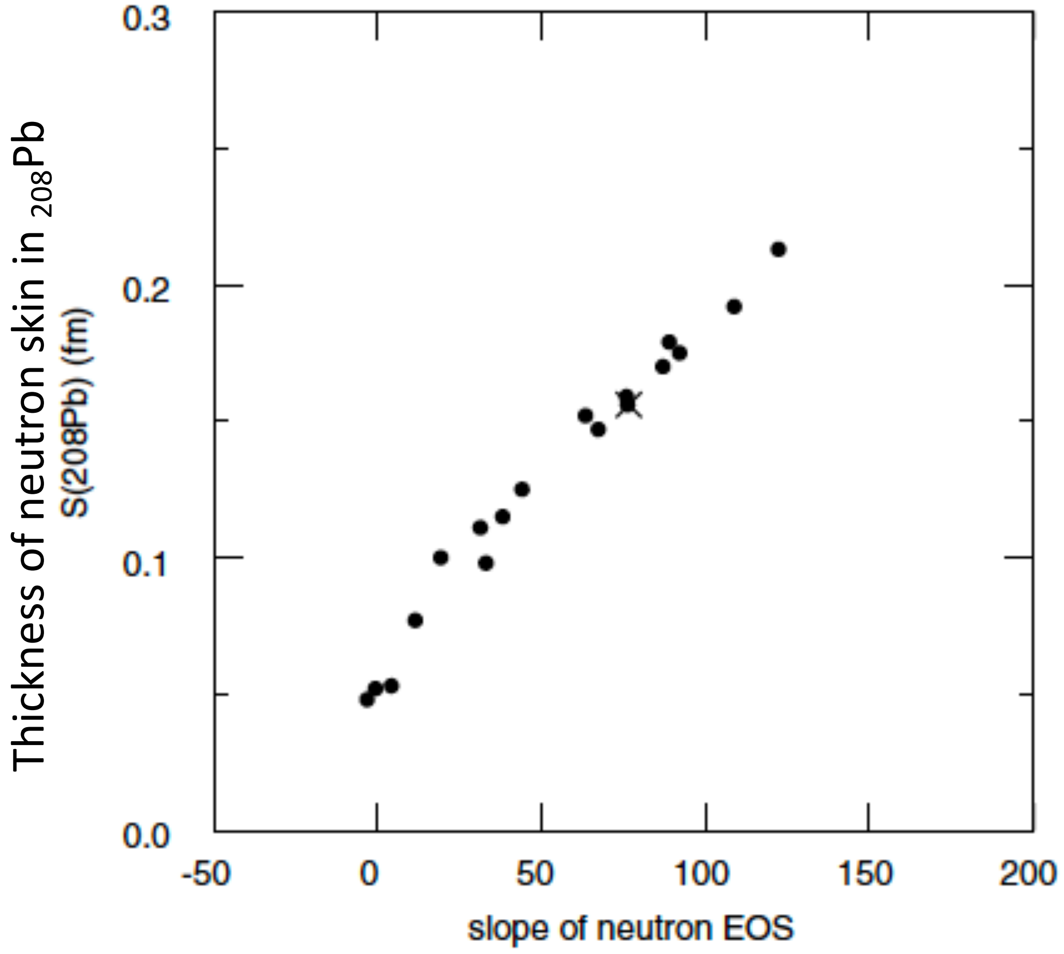
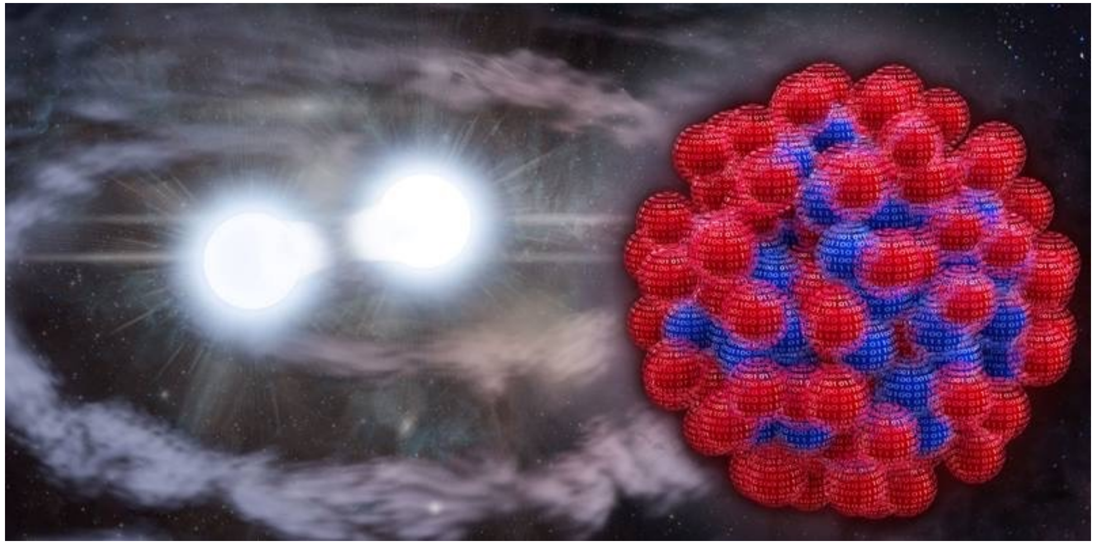
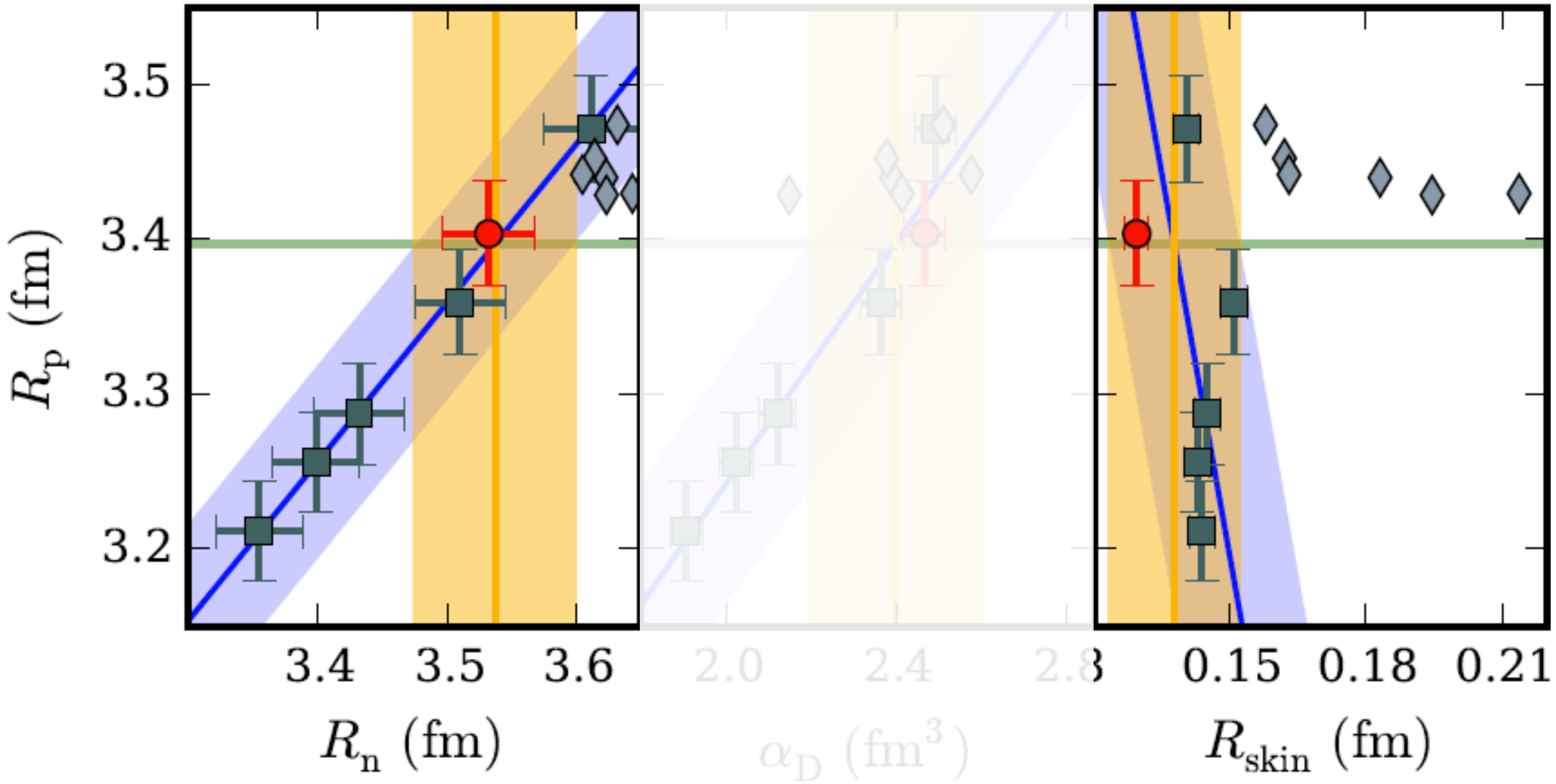


FIG. 3. The derivative of the neutron EOS at $\rho_n = 0.10$ neutron/fm^3 (in units of MeV fm^3/neutron) vs the S value in ^{208}Pb for 18 Skyrme parameter sets. The cross is SkX.



Credit: Andy Sproles, ORNL

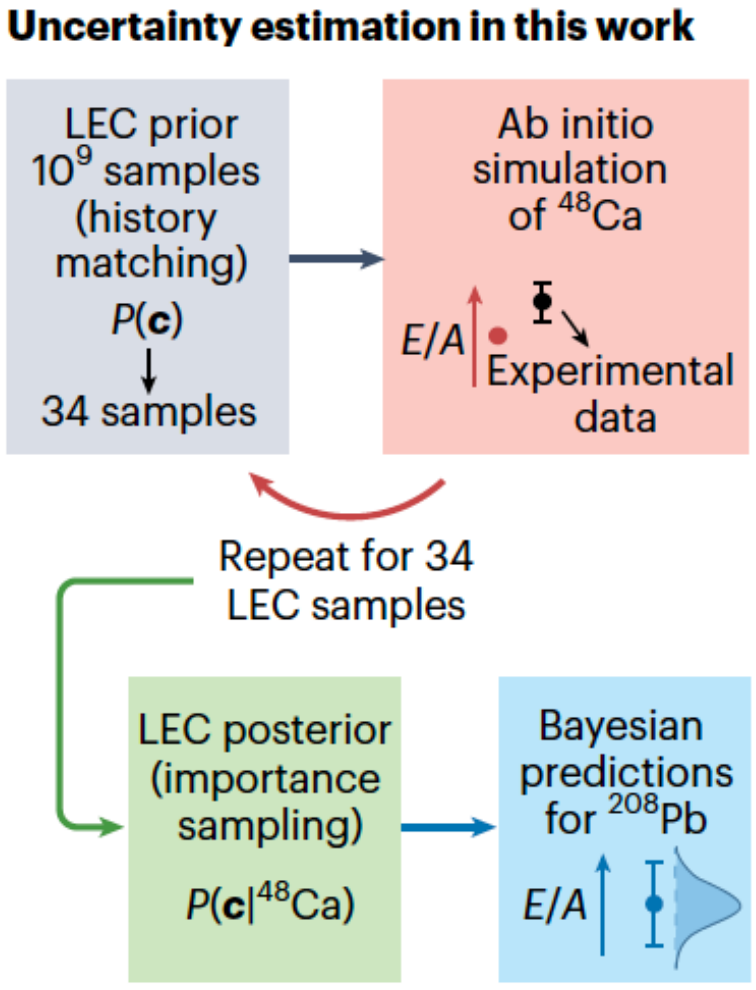
Neutron skin in ^{48}Ca



Uncertainty estimates from family of chiral interactions
[NNLO$_{sat}$, potentials by Hebeler *et al*. (2011), and DFT].

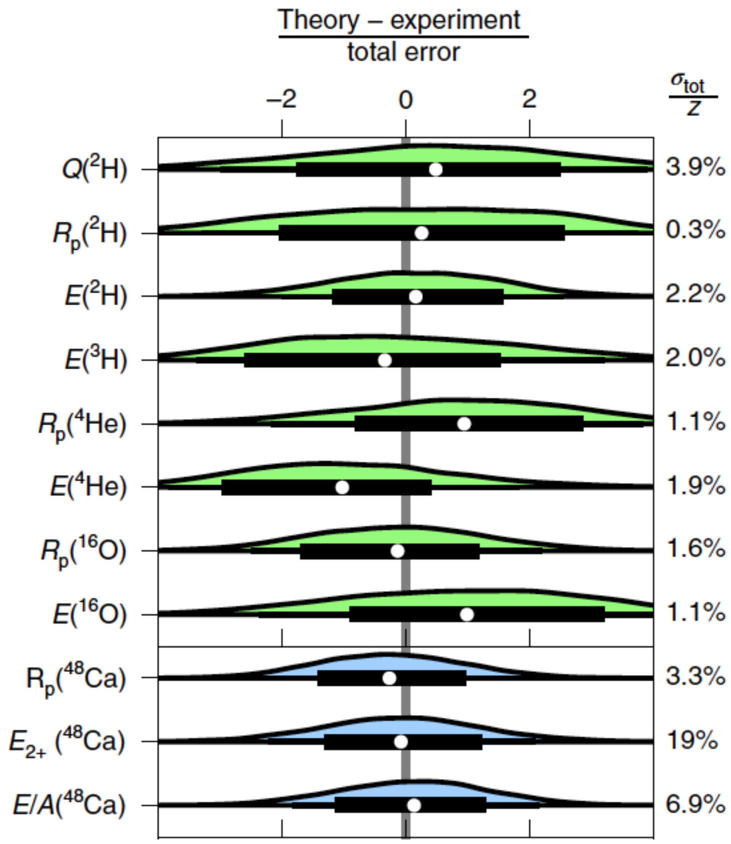
G. Hagen *et al*., Nature Physics 12, 186 (2016)

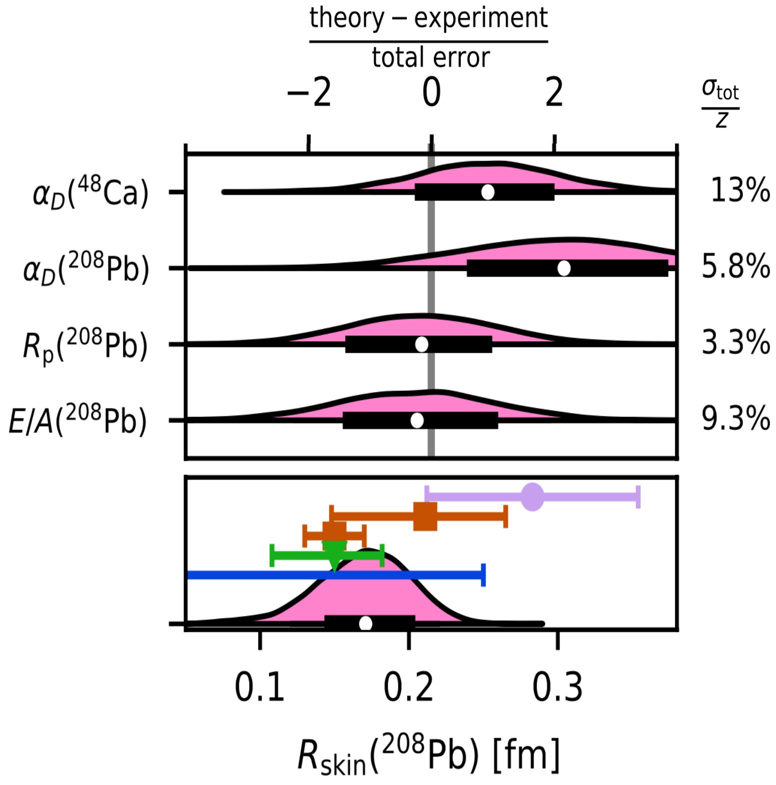
CREX, PREX, nuclear structure, and neutron stars



Arnau Rios, Nature News & Views 2022

Emulators sieved through 10^8 EFT interactions; 34 non-implausible forces yield $R_{skin}(^{208}Pb)$ = 0.14 – 0.20 fm

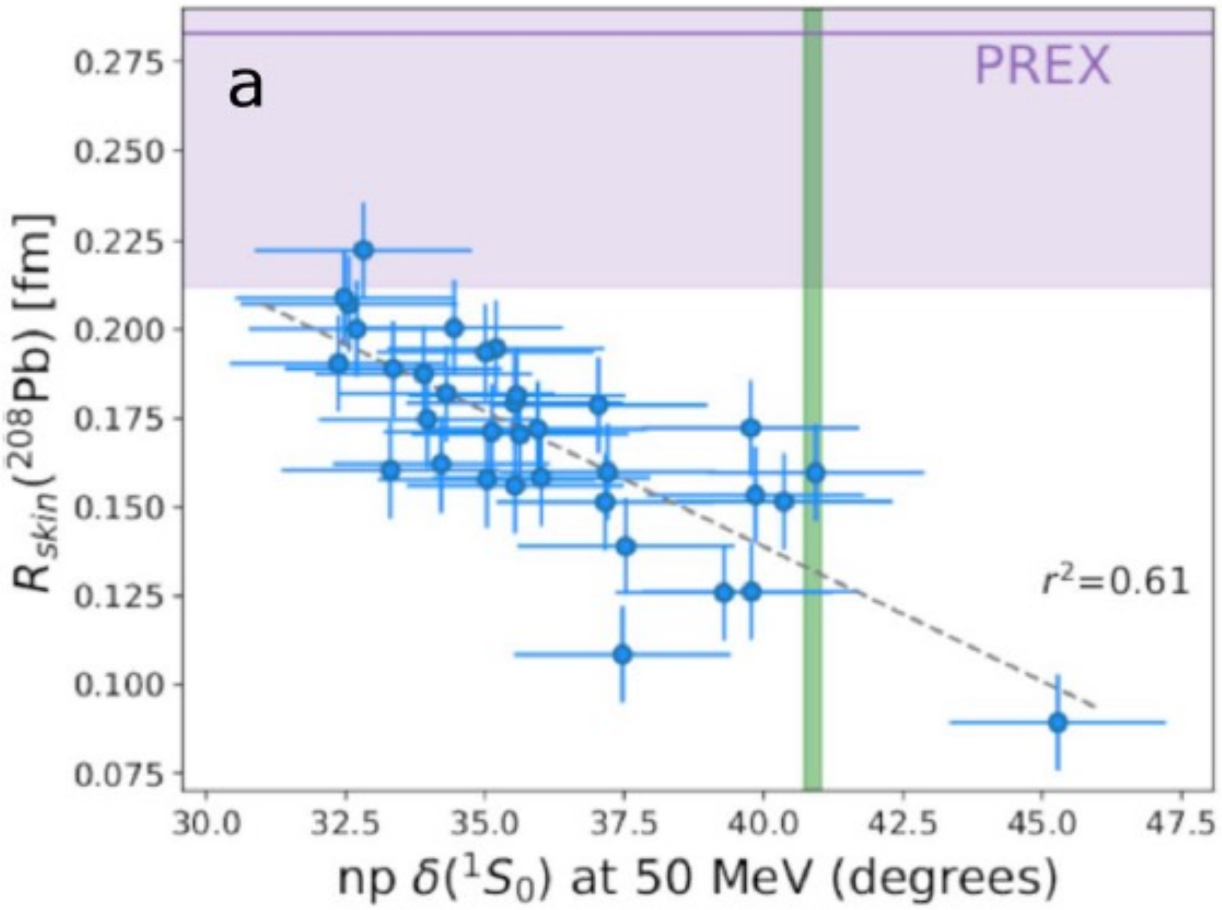




Baishan Hu, Weiguang Jiang, Takayuki Myagi, Zhonghao Sun, et al, Nature Physics 18, 1196 (2022)

Tremendous progress in quantifying uncertainties; PREX not precise enough to strongly constrain theory…

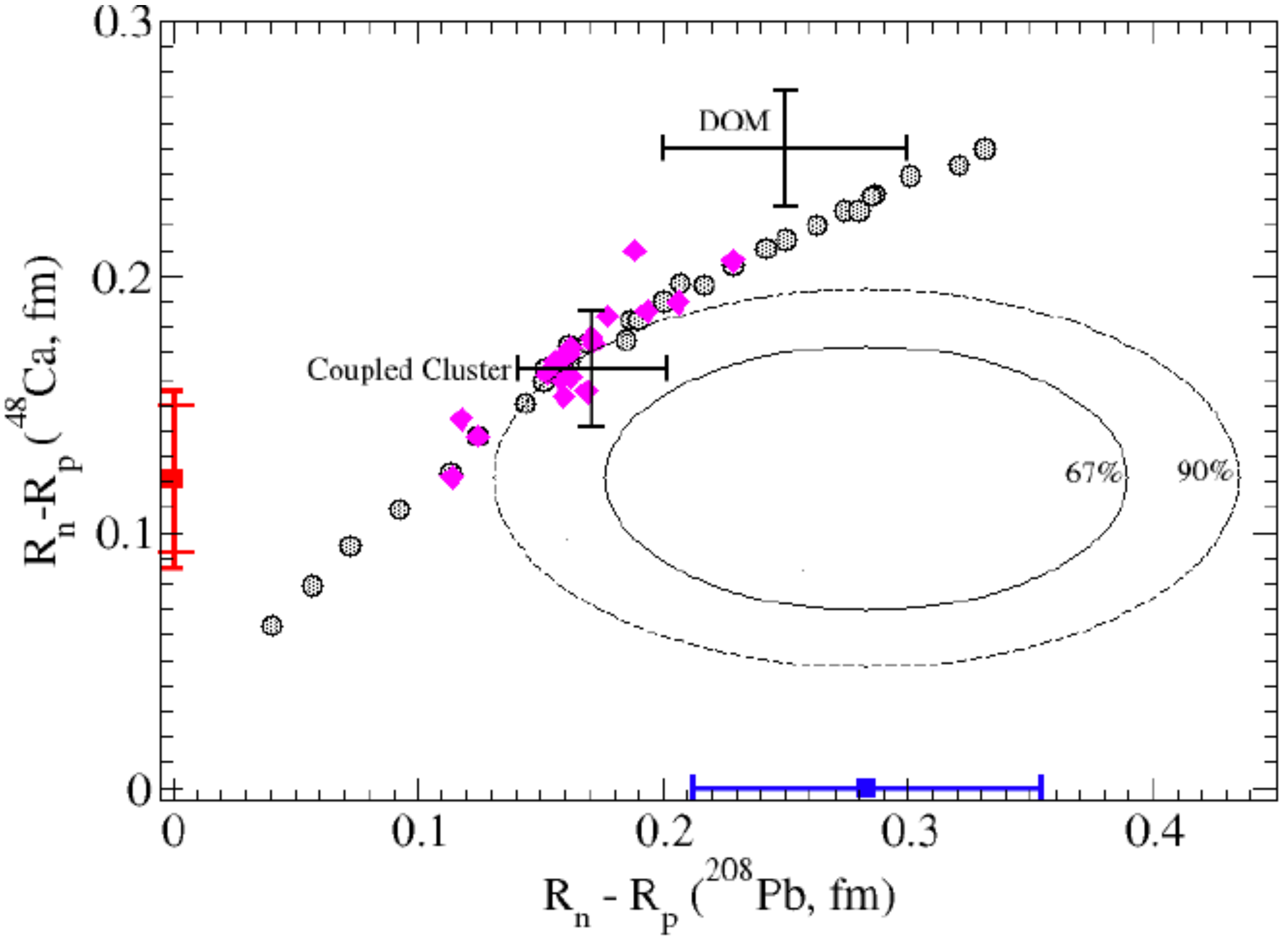
NN scattering precludes large neutron skins



Nuclear matter properties			
Observable	median	68% CR	90% CR
E_0/A	-16.9	$[-17.9, -15.4]$	$[-19.1, -14.9]$
ρ_0	0.167	$[0.150, 0.181]$	$[0.142, 0.194]$
S	31.1	$[29.1, 33.2]$	$[27.6, 34.6]$
L	52.7	$[38.3, 68.5]$	$[23.9, 76.2]$
K	287	$[242, 331]$	$[216, 362]$
Neutron skins			
Observable	median	68% CR	90% CR
$R_{\text{skin}}(^{48}\text{Ca})$	0.164	$[0.141, 0.187]$	$[0.123, 0.199]$
$R_{\text{skin}}(^{208}\text{Pb})$	0.171	$[0.139, 0.200]$	$[0.120, 0.221]$

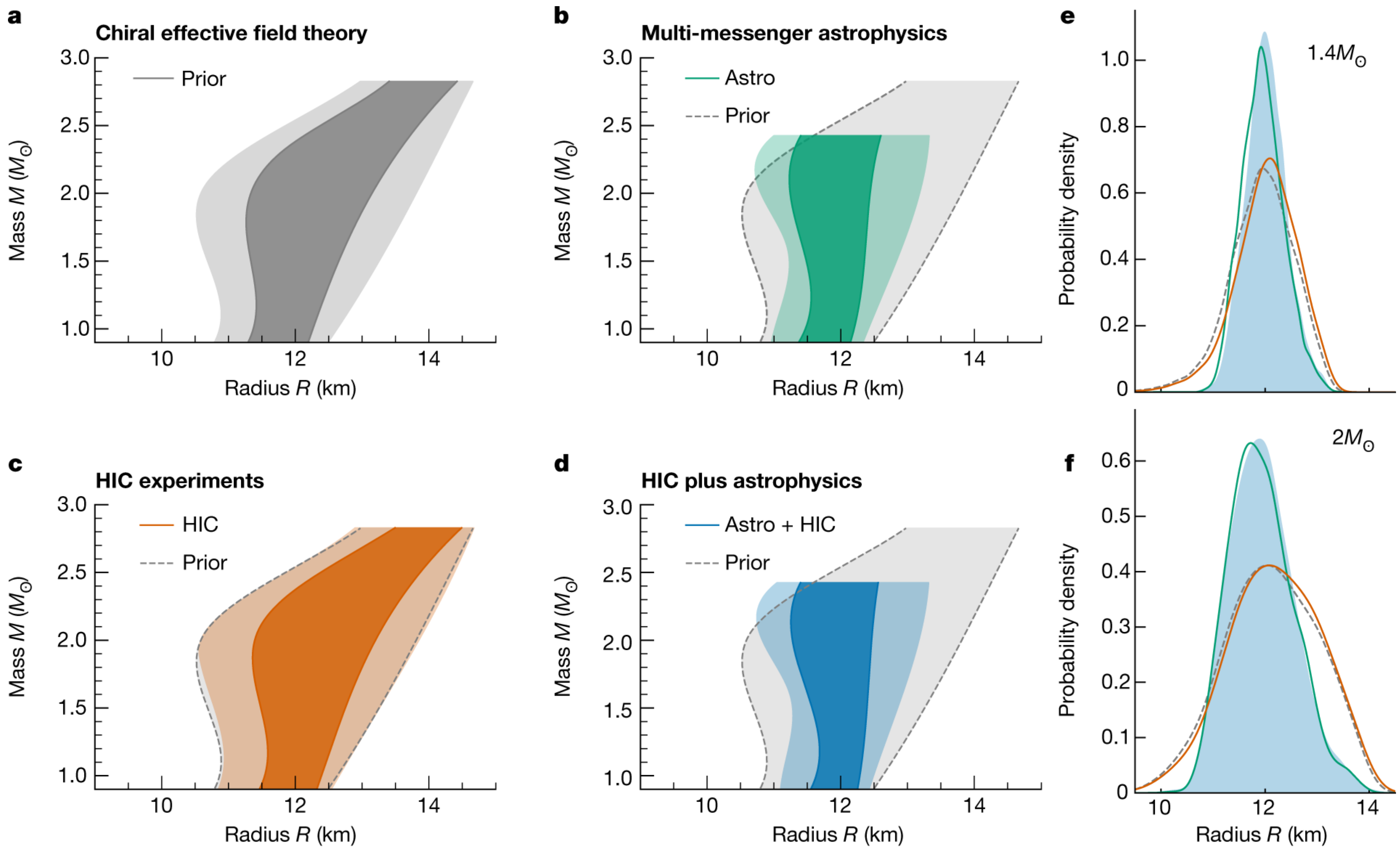
Baishan Hu, Weiguang Jiang, Takayuki Myagi, Zhonghao Sun, et al, Nature Physics 18, 1196 (2022)

CREX, PREX vs theory



Adhikari et al., Phys. Rev. Lett. 129, 042501 (2022)

Multi-messenger constraints on neutron stars

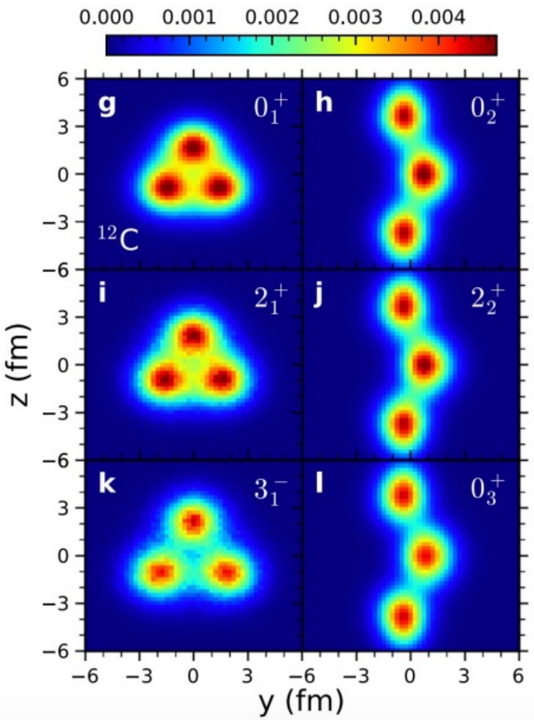


Huth et al, Nature 606, 276 (2022)

Emergent geometry and duality in the carbon nucleus

Objectives

- We perform *ab initio* lattice calculations of the spectrum, form factors, transitions, and intrinsic shapes of the low-lying states of carbon-12.
- We compute full *A*-body density correlations and provide a model-independent picture of the intrinsic geometry of each nuclear state.



Intrinsic shapes of the low-lying states of carbon-12. Panels **g**, **i**, **k** show members of the ground state rotational band. These states have an equilateral triangle geometry. Panels **h** and **j** show members of the Hoyle state rotational band, and Panel **l** shows the third 0^+ state. These states have an obtuse triangle geometry

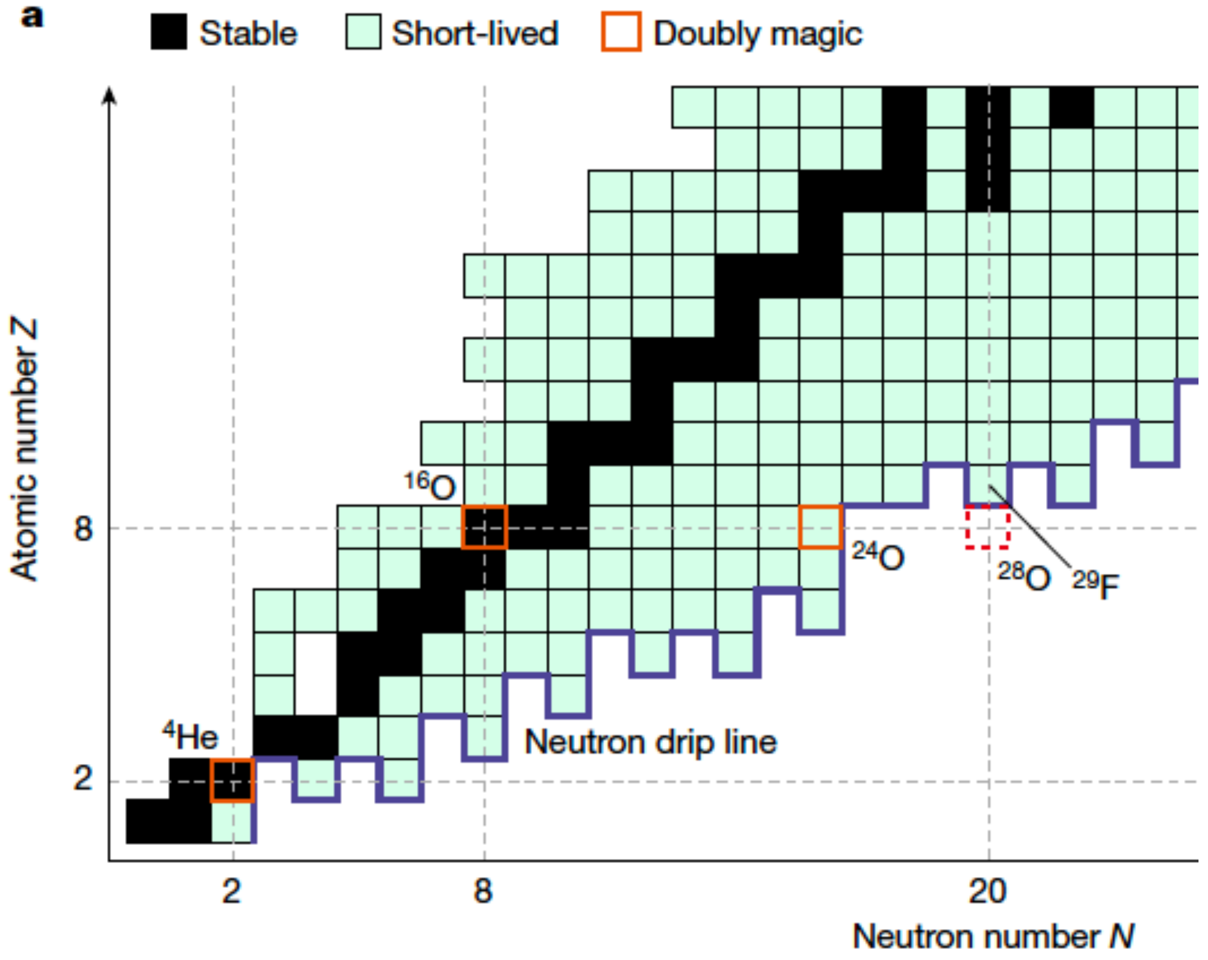
Impact (as of now)

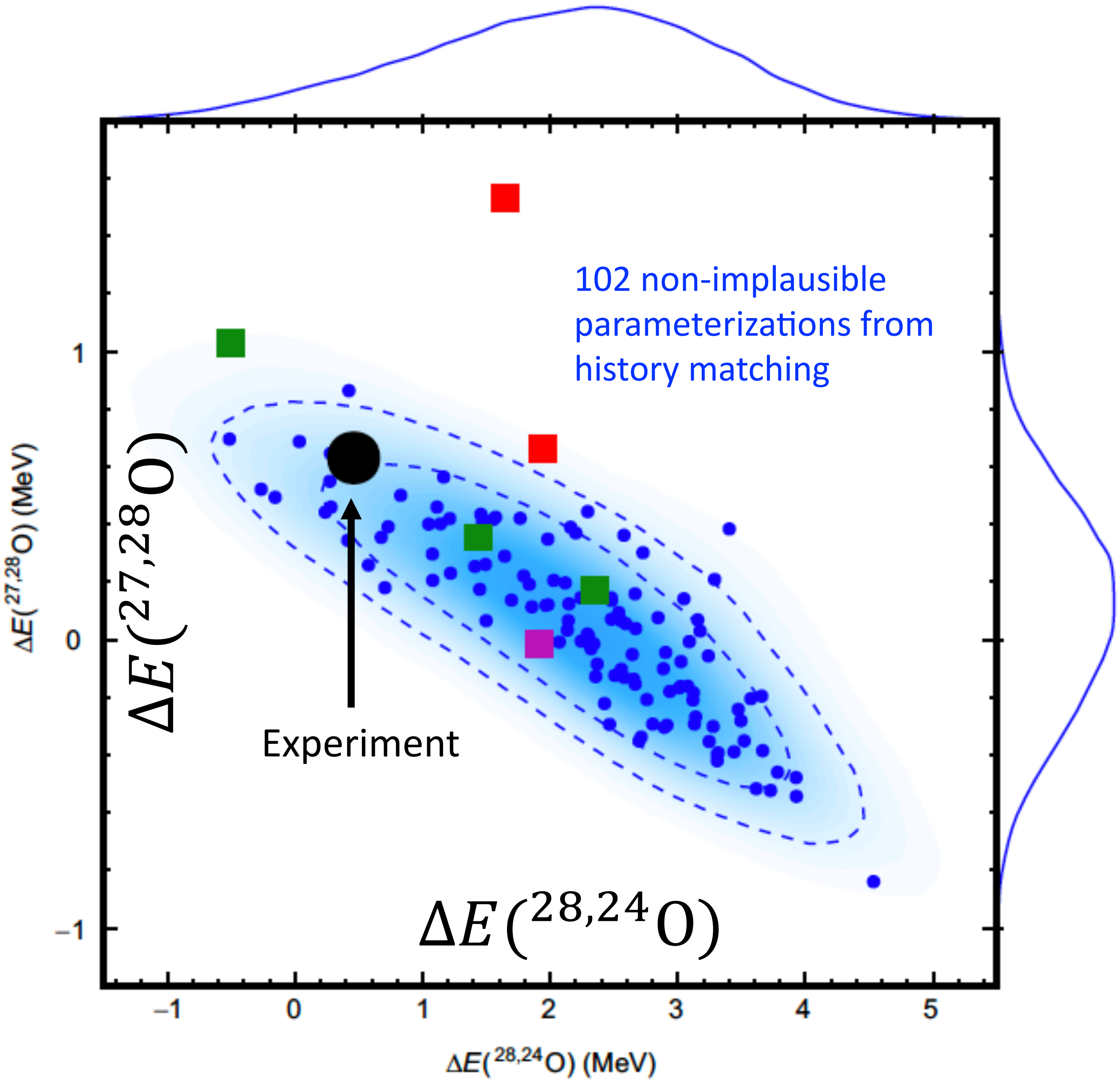
- We find that the low-lying states of carbon-12 have one of two geometries: either an equilateral triangle or an obtuse triangle composed of alpha clusters.
- The states with an equilateral triangle geometry also have a simple dual description in terms of the nuclear shell model.
- The states with an obtuse triangle geometry have no simple description in terms of the nuclear shell model.

Accomplishments (as of now)

- Shihang Shen, Serdar Elhatisari, Timo A. Lähde, Dean Lee, Bing-Nan Lu, Ulf-G. Meißner, Emergent geometry and duality in the carbon nucleus, Nat. Commun. 14, 2777 (2023).
- https://www.eurekalert.org/news-releases/989300
- https://www.youtube.com/watch?reload=9&v=s2wUQ0tFE1o

First observation of ^{28}O





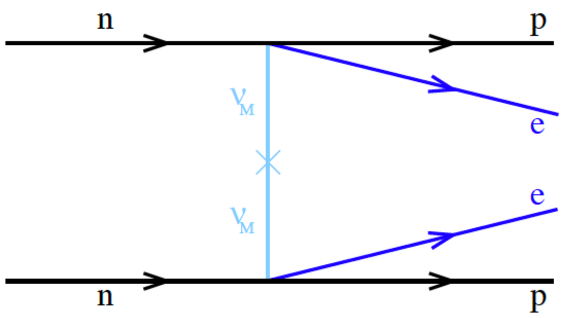
Q: Is ^{28}O = 8 protons + 20 neutrons a bound nucleus?

A: It is not! Kondo *et al.*, Nature **620**, 965 (2023)

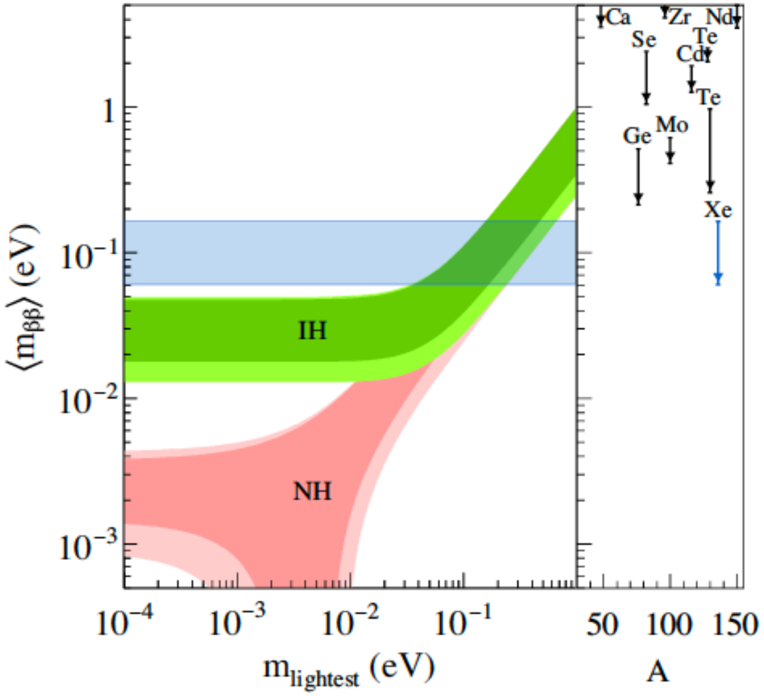
Challenges: Nuclear matrix element for neutrinoless $\beta\beta$ decay

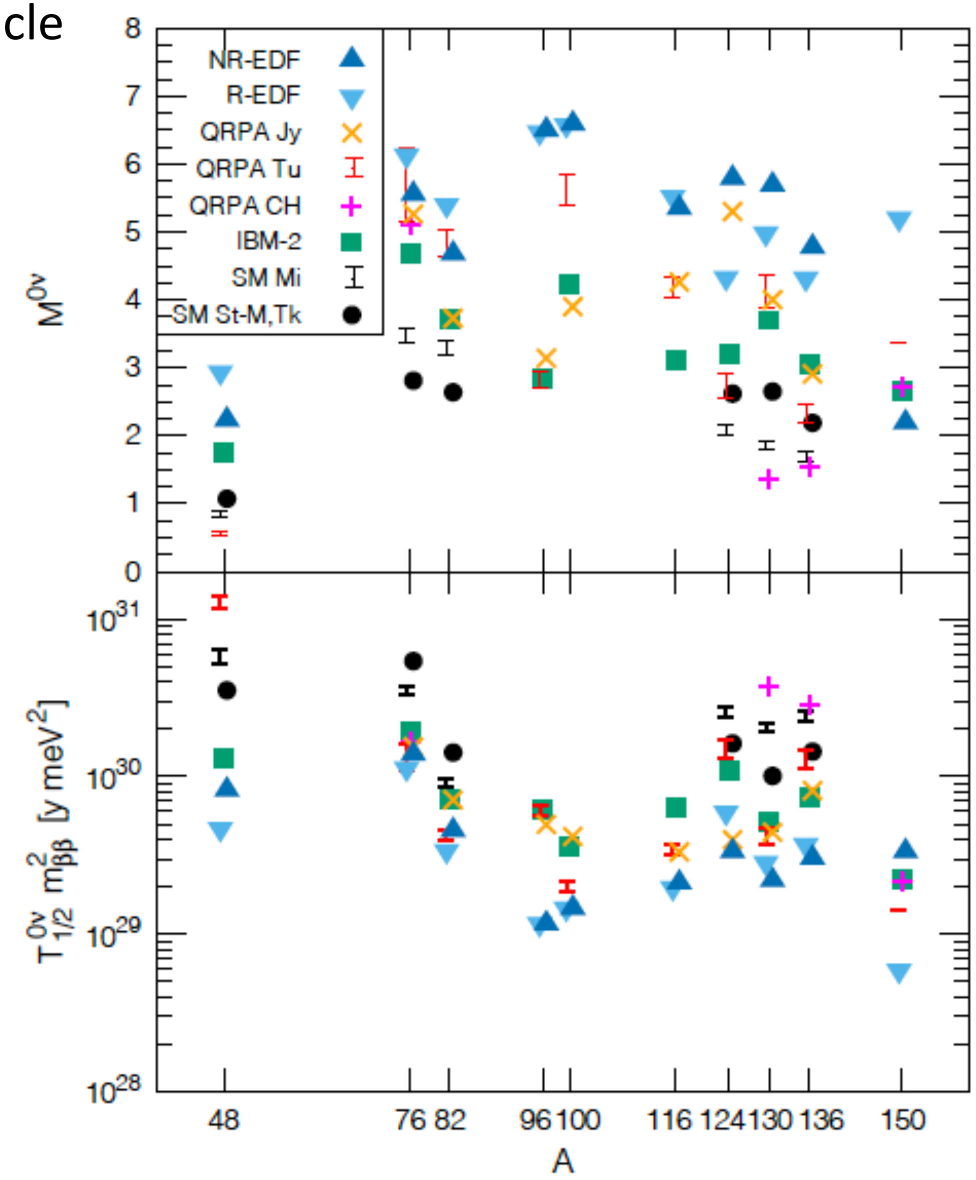
Hypothesis: The neutrino is a Majorana fermion, i.e. its own antiparticle
→ Search for neutrinoless $\beta\beta$ decay
Interest: Next-generation experiments will probe inverted hierarchy
Need: Nuclear matrix element to relate lifetime (if observed) to neutrino mass scale

Light Majorana-neutrino exchange in $\beta\beta$ decay



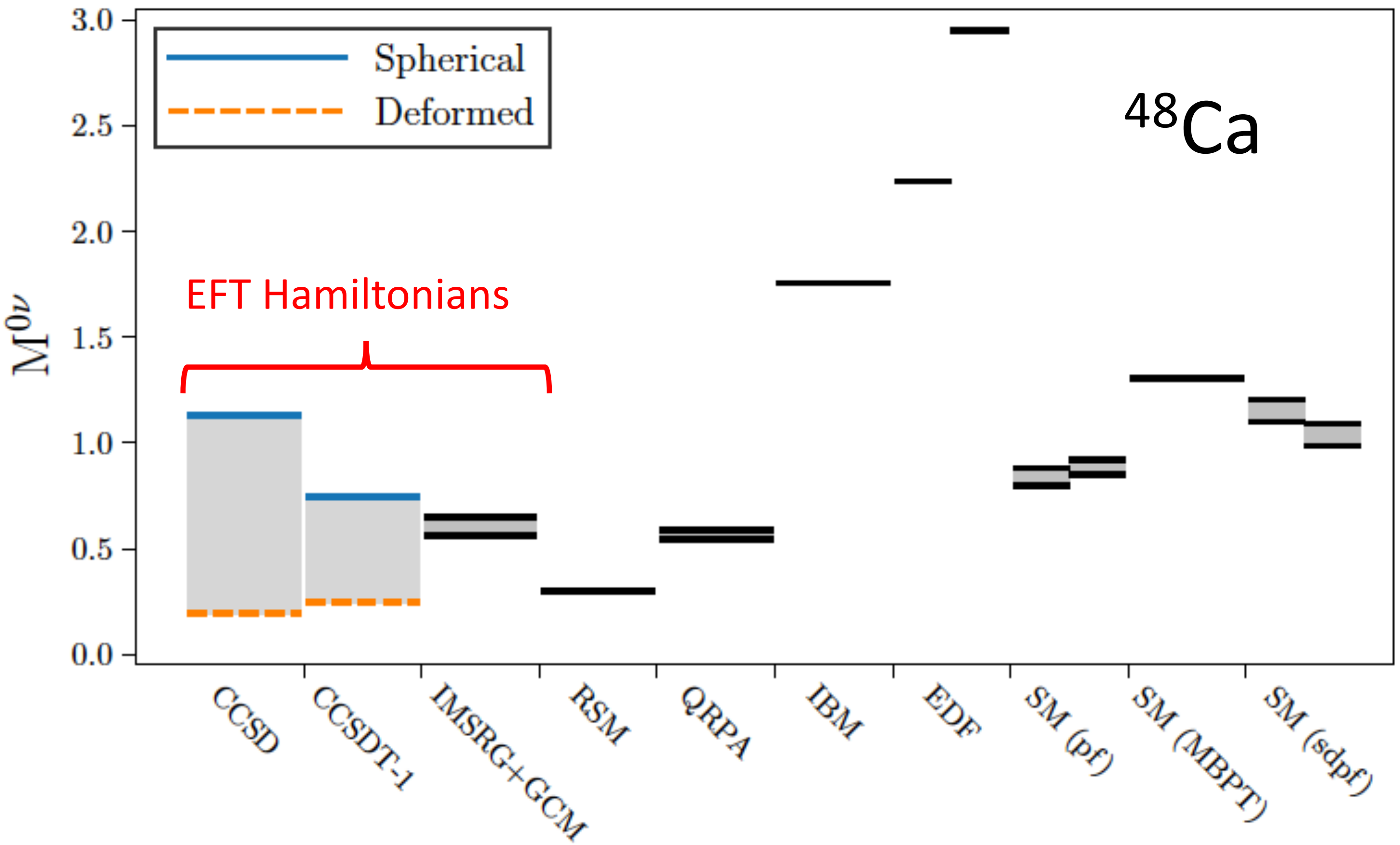
IH inverted hierarchy
NH normal hierarchy





Engel & Menéndez, Rep. Prog. Phys. 80, 046301 (2017); arXiv:1610.06548

Challenges: Nuclear matrix element for neutrinoless $\beta\beta$ decay



J. M. Yao et al., Phys. Rev. Lett. 124, 232501 (2020); arXiv:1908.05424.
S. J. Novario et al., Phys. Rev. Lett. 126, 182502 (2021); arXiv:2008.09696

Challenges:

- Higher precision
- ^{76}Ge, mass 130 nuclei are used in detectors (and not ^{48}Ca)
- Contact of unknown strength also enters (to keep RG invariance), [Cirigliano, Dekens, de Vries, Graesser, Mereghetti, Pastore, van Kolck, Phys. Rev. Lett. 120, 202001 (2018); arXiv:1802.10097]

Ab Initio Uncertainty Quantification of Neutrinoless Double-Beta Decay in ^{76}Ge

U.S. DEPARTMENT OF ENERGY | Office of Science

NUCLEI Nuclear Computational Low-Energy Initiative

Objective

The observation of neutrinoless double beta decay (NLDBD) would yield profound insights into the nature of neutrinos, their mass, and it might help explain the dominance of matter over antimatter in our universe.

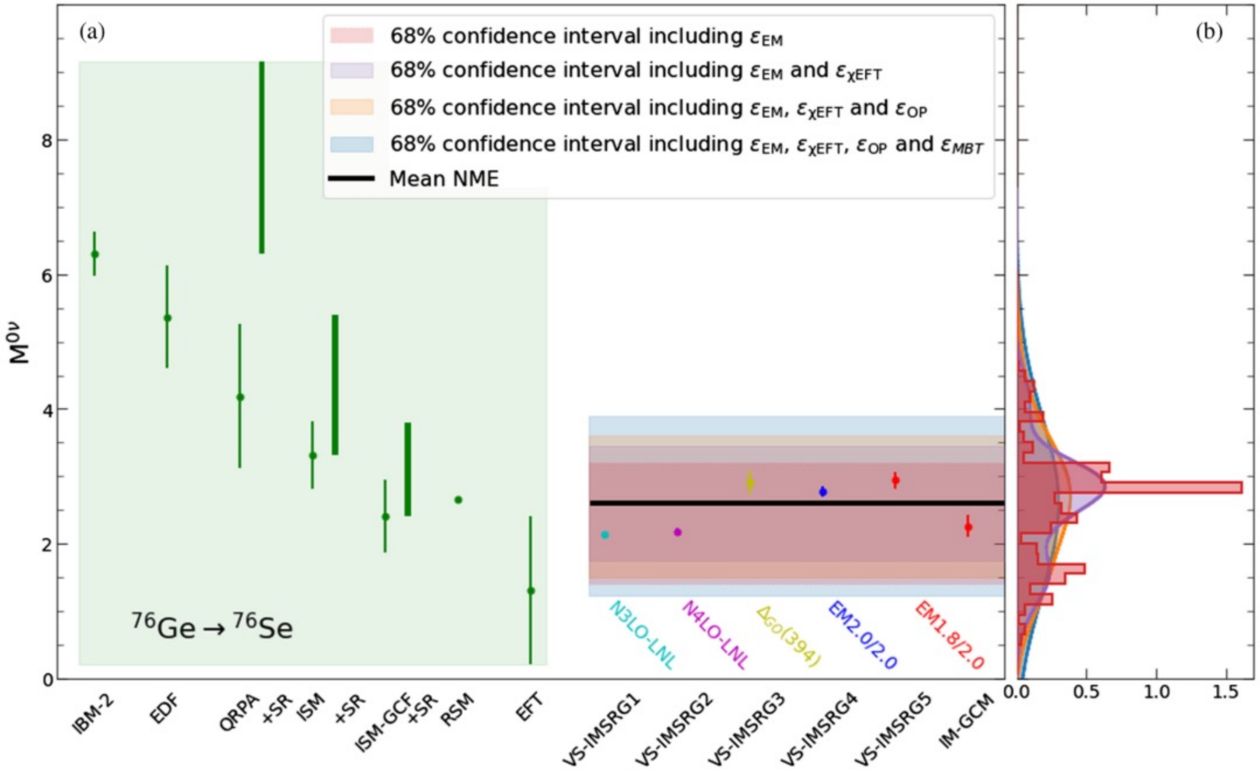
Impact

We perform *ab initio* calculations (called VS-IMSRG and IM-GCM) of the nuclear (decay) matrix elements (NMEs) in ^{76}Ge, which are necessary to reliably extract the neutrino mass scale from experimental data, and to identify the primary drivers of theoretical uncertainties in current state-of-the-art approaches.

Accomplishments

- Published in [PRL 132, 182502 (2024)](https://doi.org/10.1103/PhysRevLett.132.182502)

Comparison of NLDBD NMEs in ^{76}Ge from nuclear models and *ab initio* calculations.



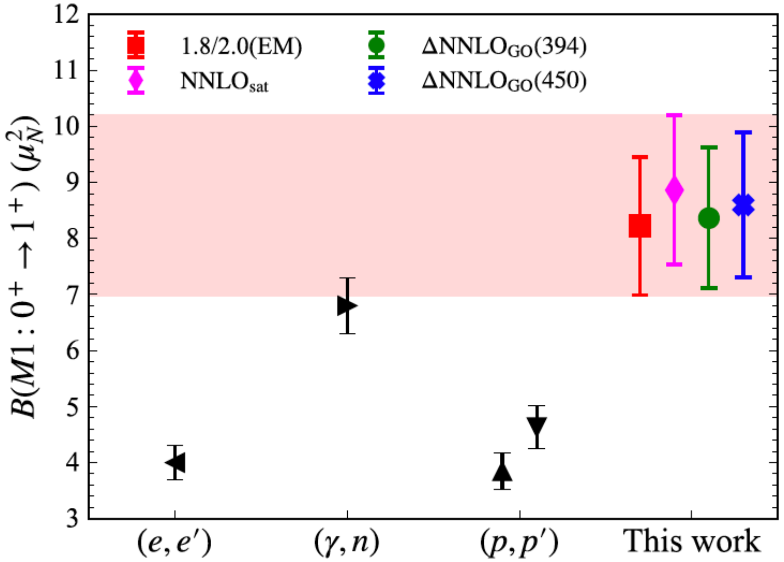
(a) NMEs from phenomenological models and results from VS-IMSRG and IM-GCM using different chiral interactions. Error bars of phenomenological NMEs reflect the discrepancy between calculations from different groups.

(b) Posterior distribution function of the NME using a novel VS-IMSRG emulator with 8188 non-implausible chiral interactions from which confidence intervals are extracted.

Magnetic excitations of the nucleus ^{48}Ca: theory input to an experimental controversy

Objectives

- There is an experimental controversy regarding the magnetic dipole transition in the nucleus ^{48}Ca. This makes it interesting to see what first principles computations would reveal.
- Resolving the controversy is important because our understanding of magnetic dipole transitions also impacts how physicists model hard-to-pin-down neutrino-nucleus interactions that happen in exploding stars.



The magnetic dipole strength carried by the 1^+ state at 10.23 MeV in ^{48}Ca. Data from electron scattering (e,e'), photon scattering (γ, n) and proton scattering (p,p') experiments are compared to the calculations of this work.

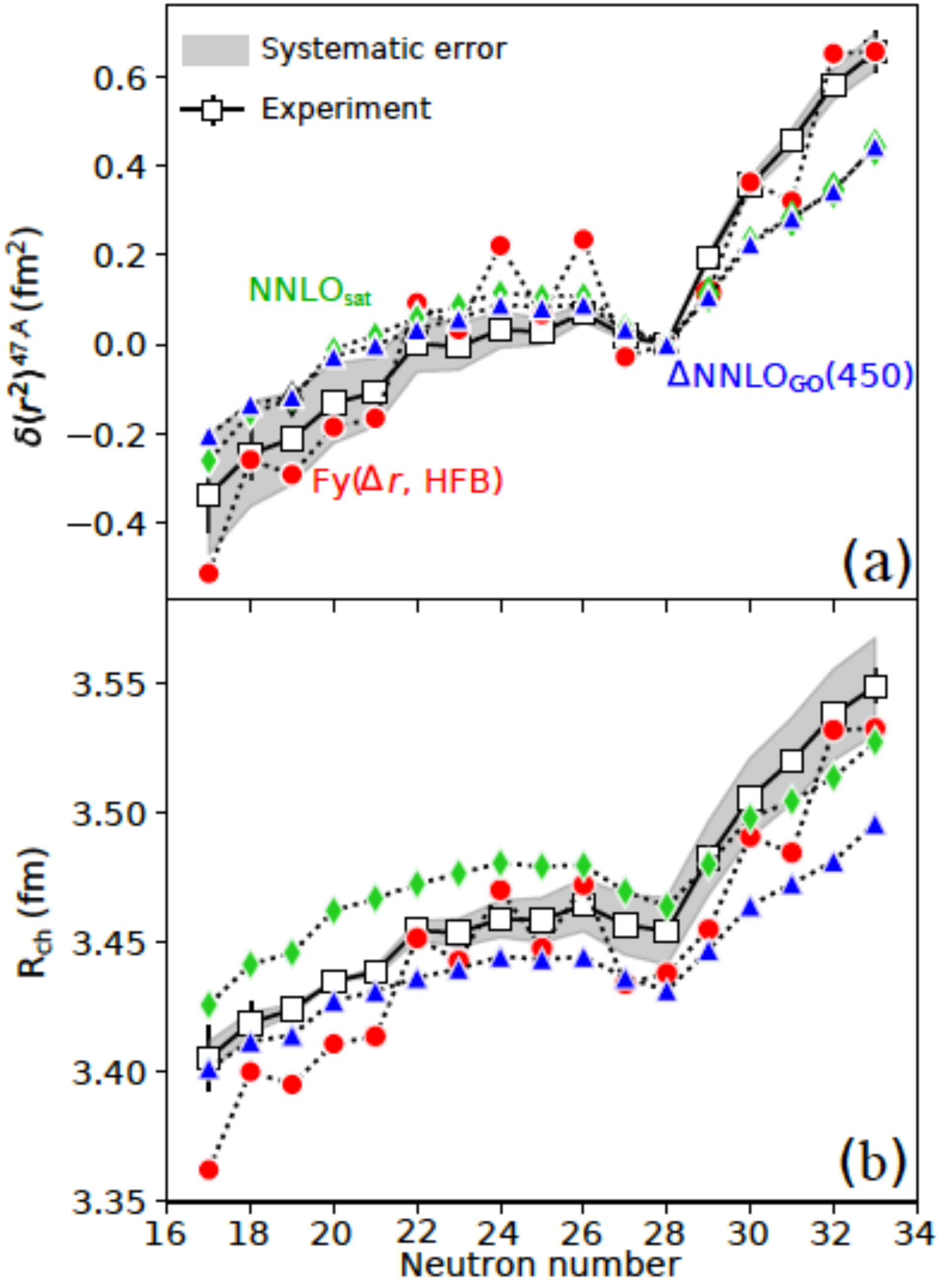
Impact

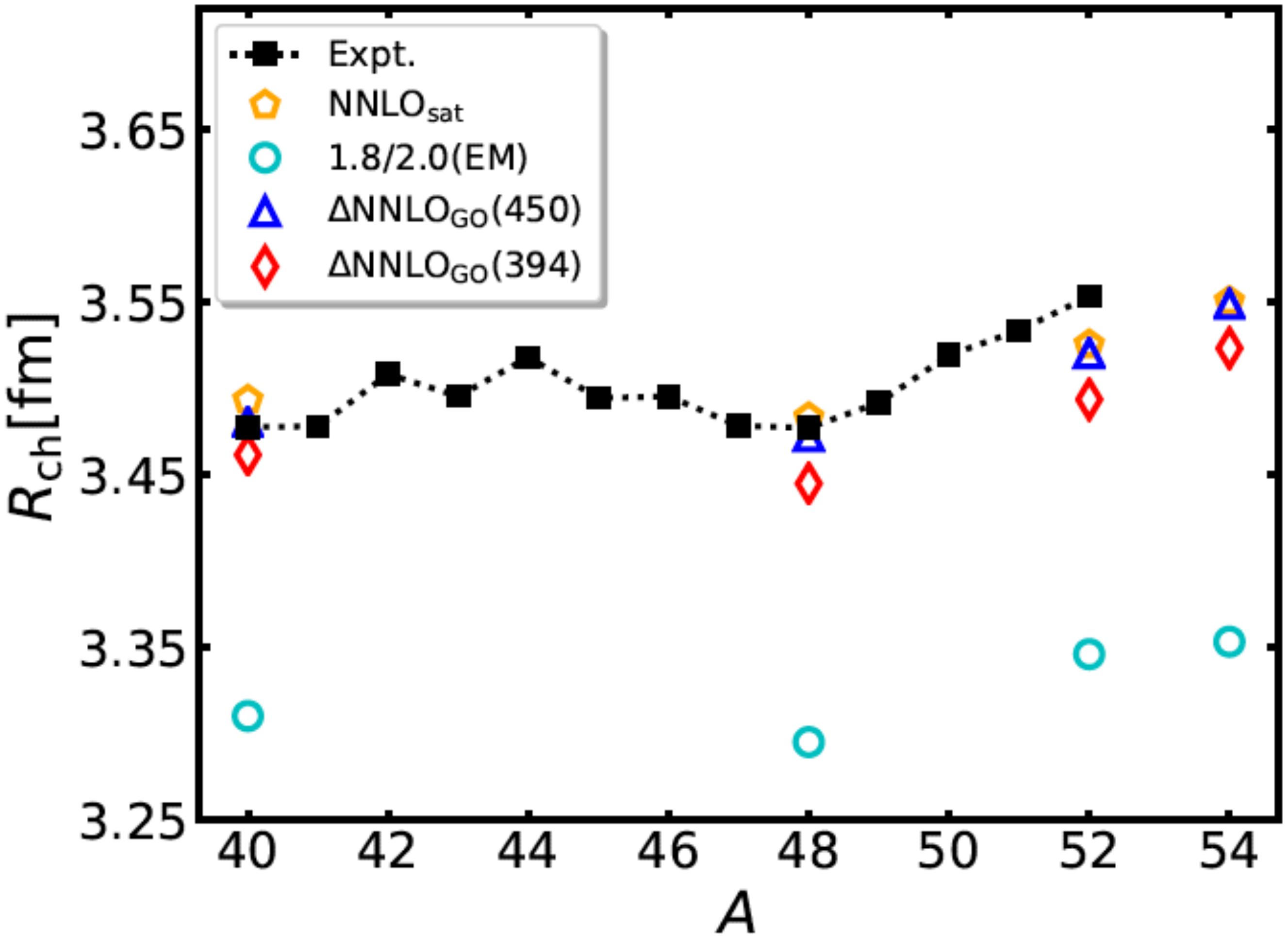
- Within uncertainties, computations are consistent with the photon scattering (γ, n) experiment.
- Two-body currents, i.e. magnetic transitions that happen while two nucleons interact, do not yield a reduction in the magnetic strength. This is a somewhat unexpected result because similar two-body currents reduce the rates of beta decays.
- The results from the calculations cast some doubts on earlier approaches to neutrino-nucleus scattering that built on the (e,e') scattering data (which saw much smaller magnetic transition strengths).
- The computations put the ball back into the experimenters' court. It is important that the experimental disagreement gets clarified.

Accomplishments

- B. Acharya, B.S. Hu, S. Bacca, G. Hagen, P. Navrátil, T. Papenbrock, Phys. Rev. Lett. 132, 232504 (2024)

Challenges: Charge radii



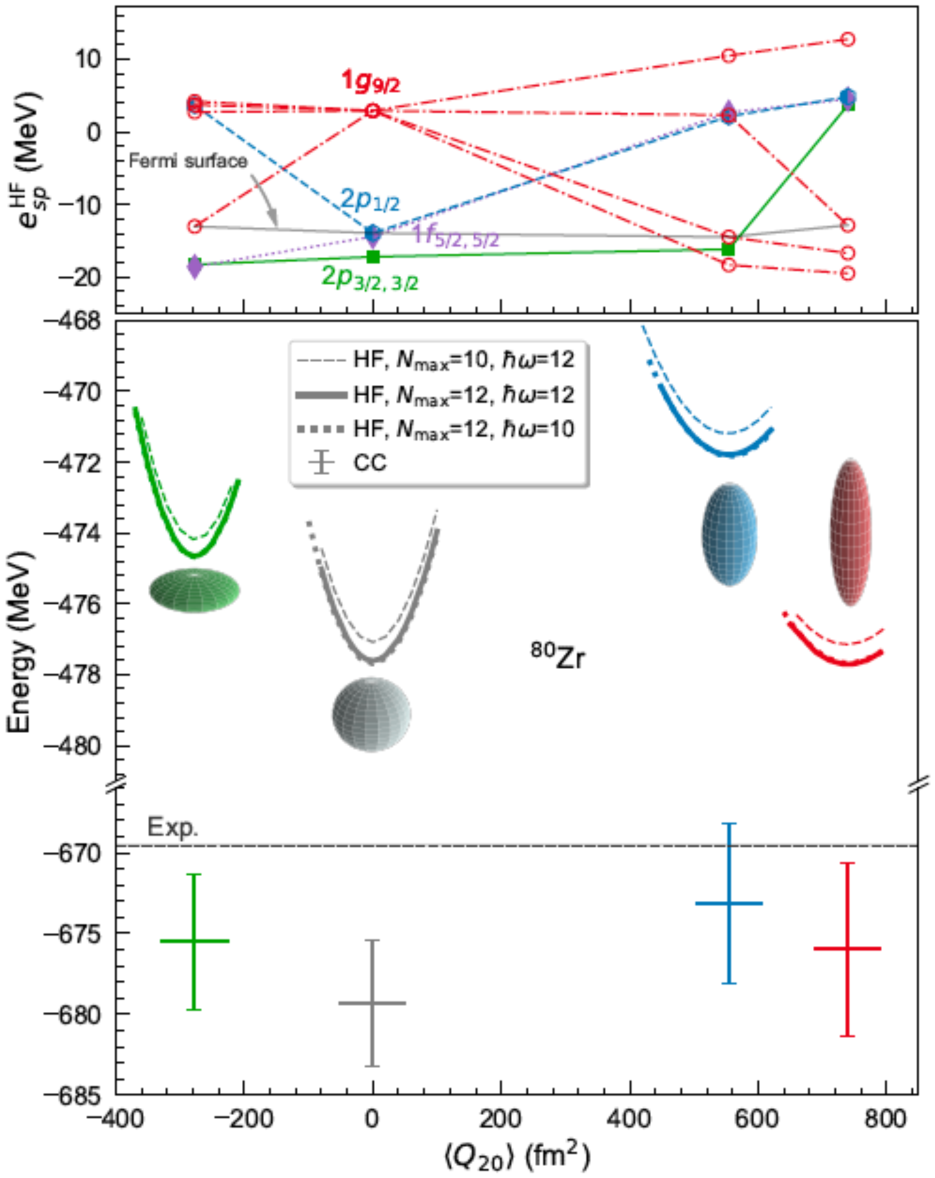


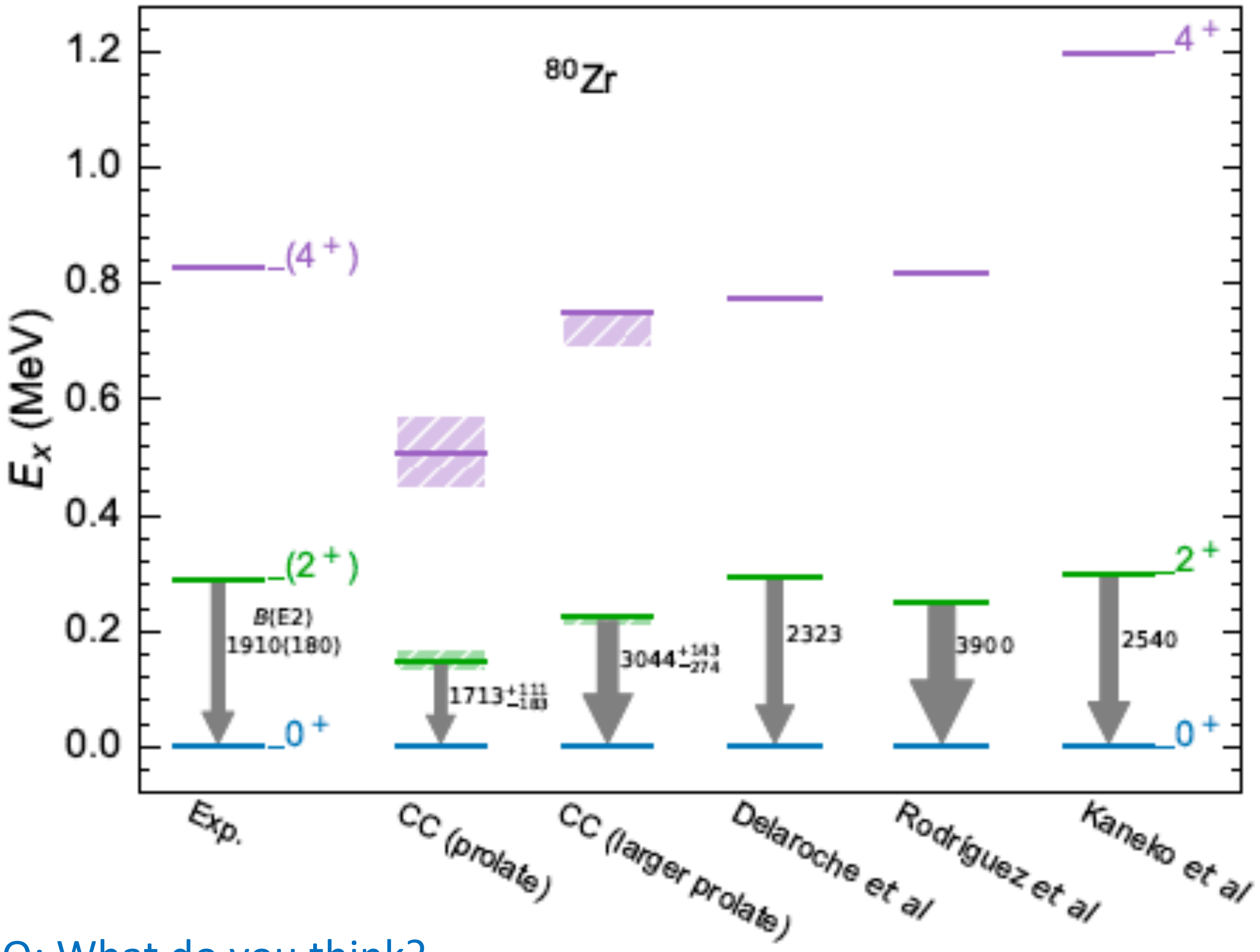
W.G. Jiang et al, arXiv:2006.16774

Sharp increase beyond N=28 not reproduced by EFT Hamiltonians

A. Koszorus, X. F. Yang et al, Nature Physics 17, 439 (2021); arXiv:2012.01864

Challenges: What is the shape of the ground state?





Q: What do you think?
Hint: Compare ground-state energies, rotational bands, and electromagnetic transition strengths $B(E2)$!

Baishan Hu, Zhonghao Sun, G. Hagen, TP, arXiv:2405.05052

Summary successes and challenges

- 🙂 Computations based EFT Hamiltonians now reach mass numbers $A \sim 100$
- 🙂 Link nuclear structure to forces between 2 and 3 nucleons

- 🤔 What causes the dramatic increase of charge radii beyond neutron number $N = 28$?
- 🤔 What is the nuclear matrix element for neutrinoless $\beta\beta$ decay?
- 🤔 How does nuclear binding depend on the pion mass?
- 🤔 What is the nuclear equation of state at multiples of the saturation energy?
- 🤔 Identifying shape coexistence is not hard; getting the correct shape of the ground state is hard
- 🤔
- 🤔

Thank you for your attention, participation, and questions!