Ab initio computations of atomic nuclei

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

International School of Physics "Enrico Fermi"

Course 213 - Nuclear Structure and Reactions from a Broad Perspective

Varenna, Italy, 27 June - 2 July, 2024

Work supported by the US Department of Energy

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 $$H_{\mathrm{HF}} \equiv \sum_{pq} f_p^q \hat{a}_q^\dagger \hat{a}_p$$

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

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, ... refer to occupied single-particle states (hole states), a, b, c, ... refer to unoccupied single-particle states (particle states), p, q, r, ... 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: $f_i^a = ?$

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

Mean field

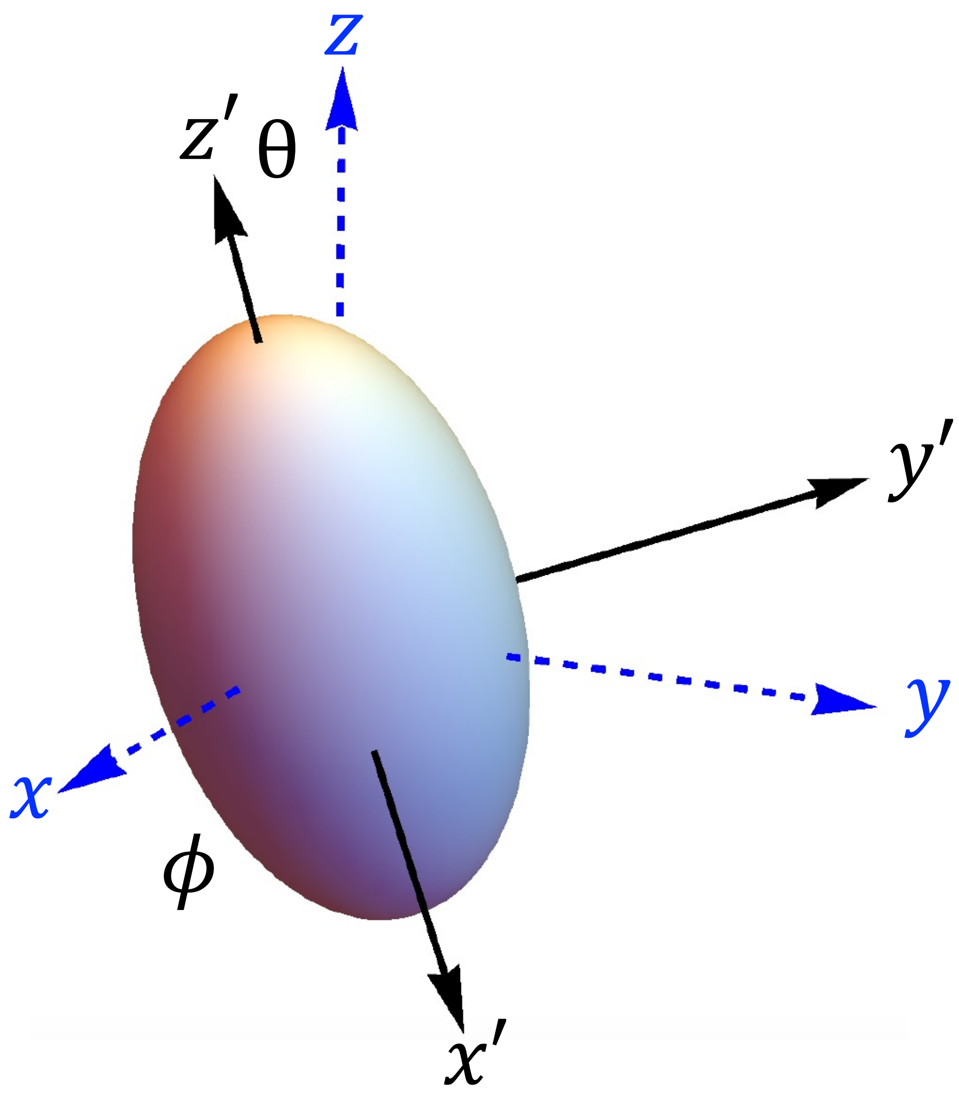
Comments:

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

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

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)

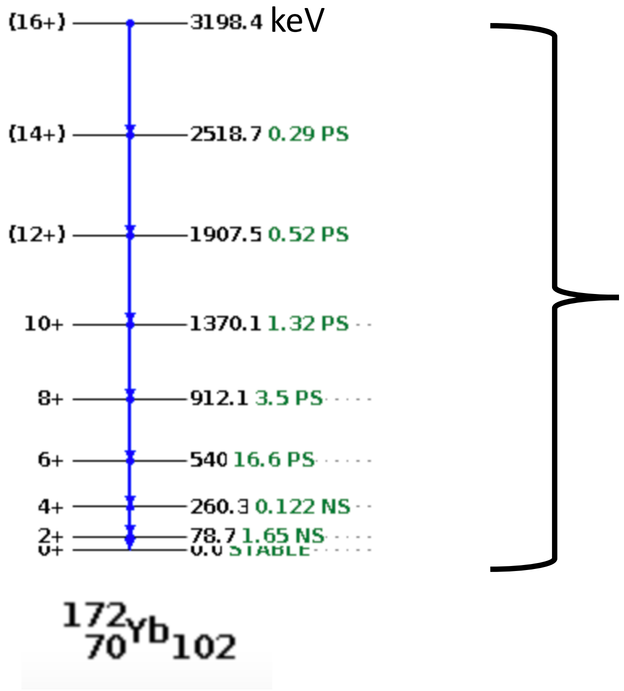
Eigenfunctions are spherical harmonics $Y_{IM}(\Omega)$

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")

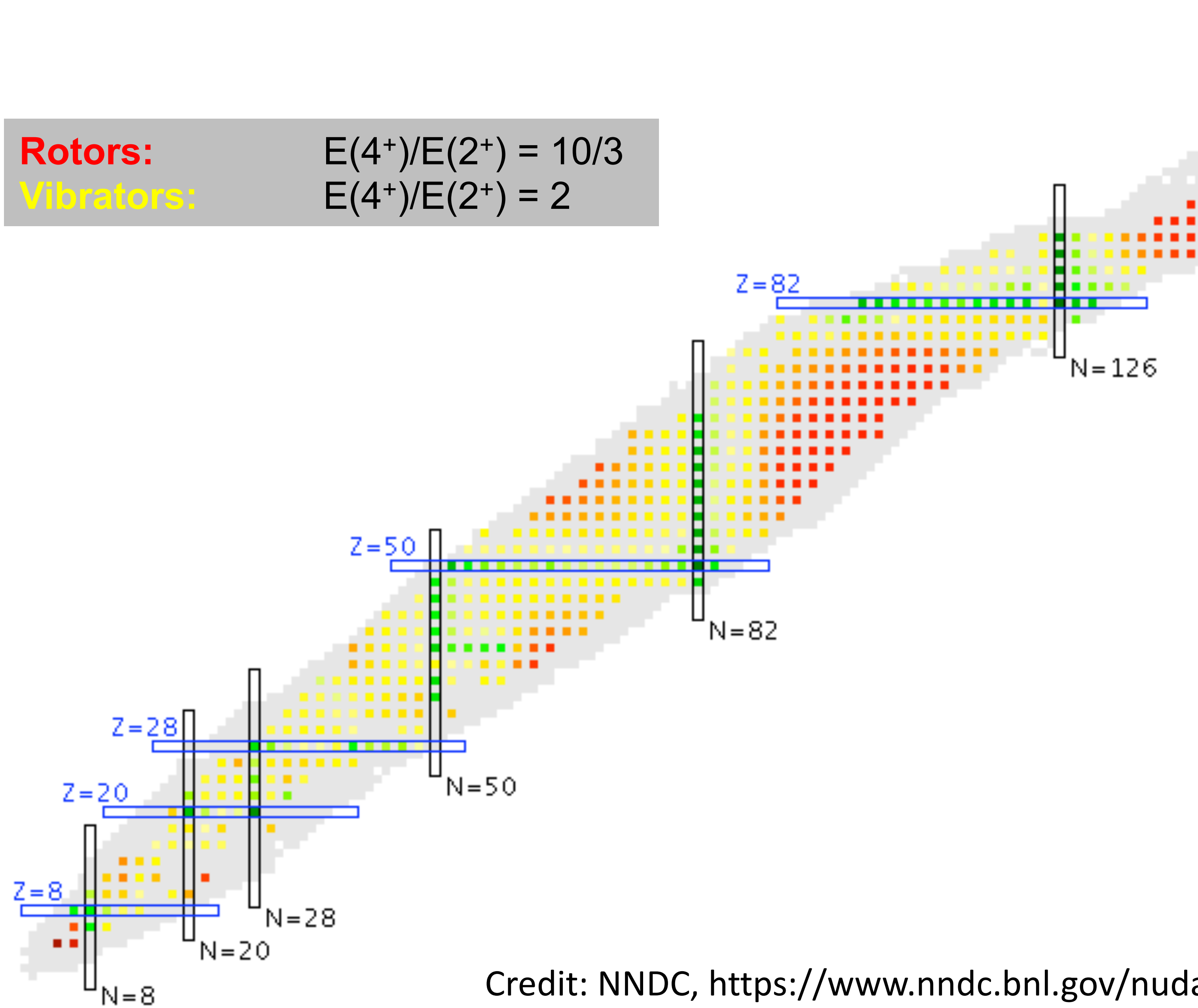
1. Deformation (HF) → rotational bands
2. Broken phases (HFB) → pairing rotational bands
3. Broken parity → bands with opposite parities close in energy

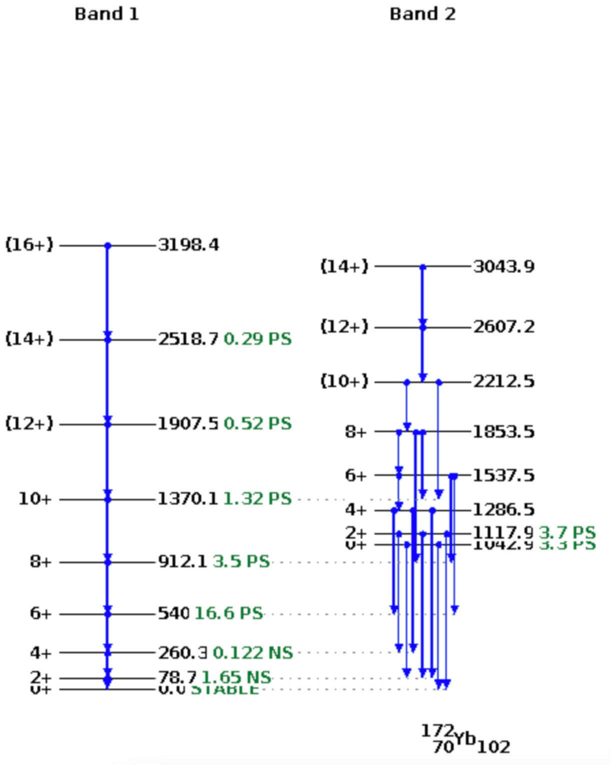
Separation of scales enable construction of effective theories

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

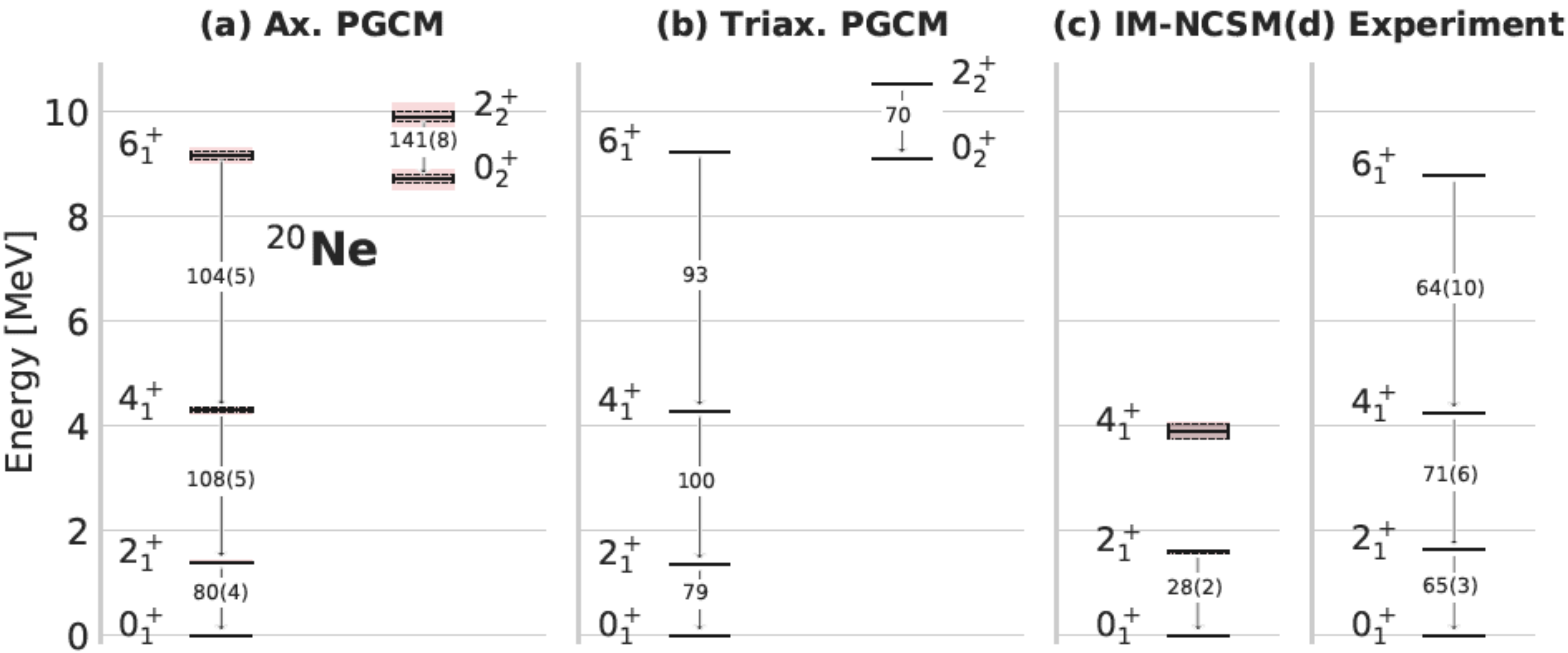
Rotors:	$E(4^+)/E(2^+) = 10/3$
Vibrators:	$E(4^+)/E(2^+) = 2$





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

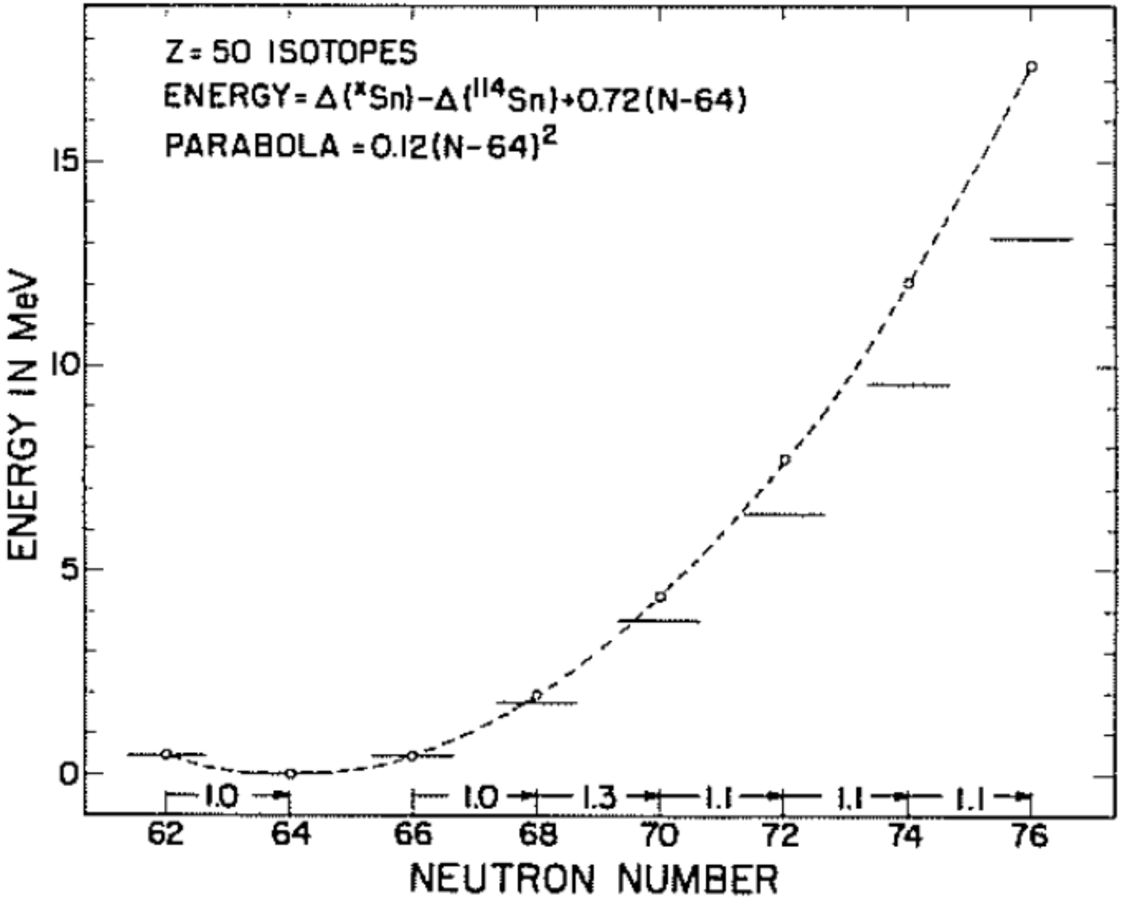
Projected Hartree-Fock-Bogoliubov calculations yield rotational bands



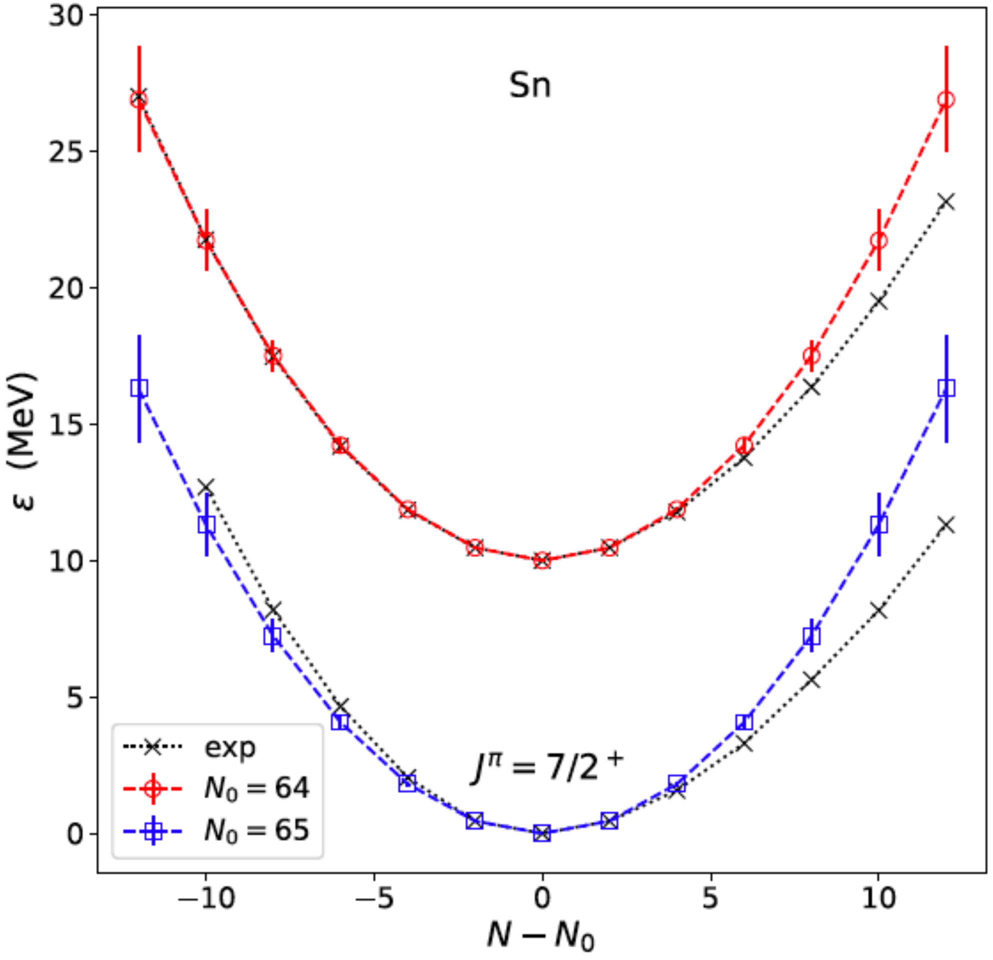
Frosini et al., Eur. Phys. J. A 58, 63 (2022); arxiv:2111.00797

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

Symmetry breaking: nuclear superfluidity



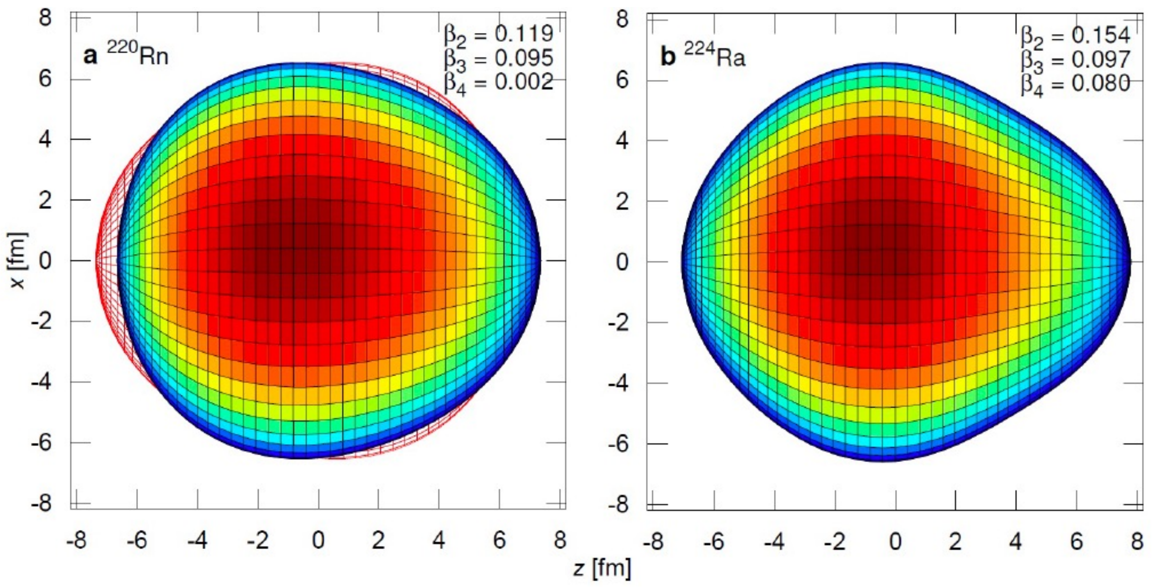
Broglia, Hansen, Riedel, Adv. Nucl. Phys. (1973)



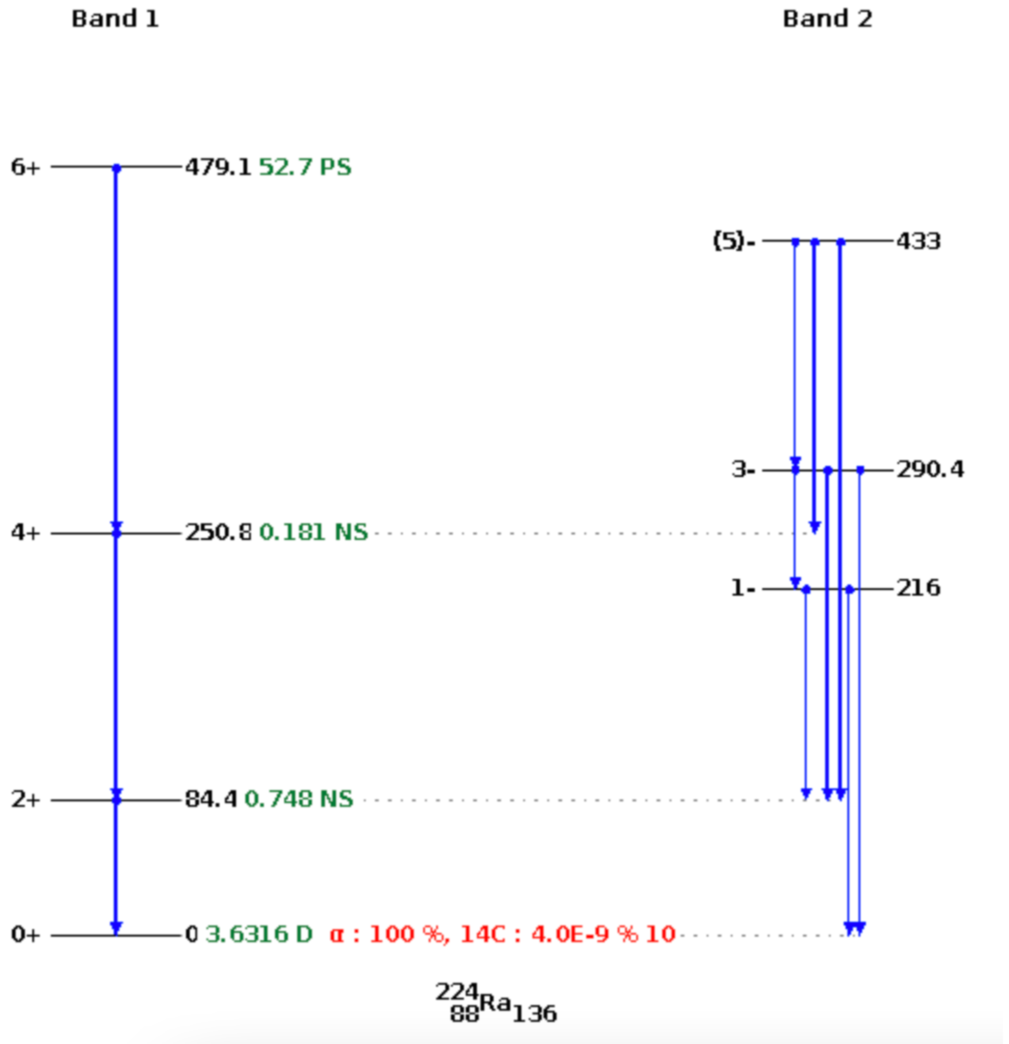
TP, Phys. Rev. C 105, 044322 (2022)

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

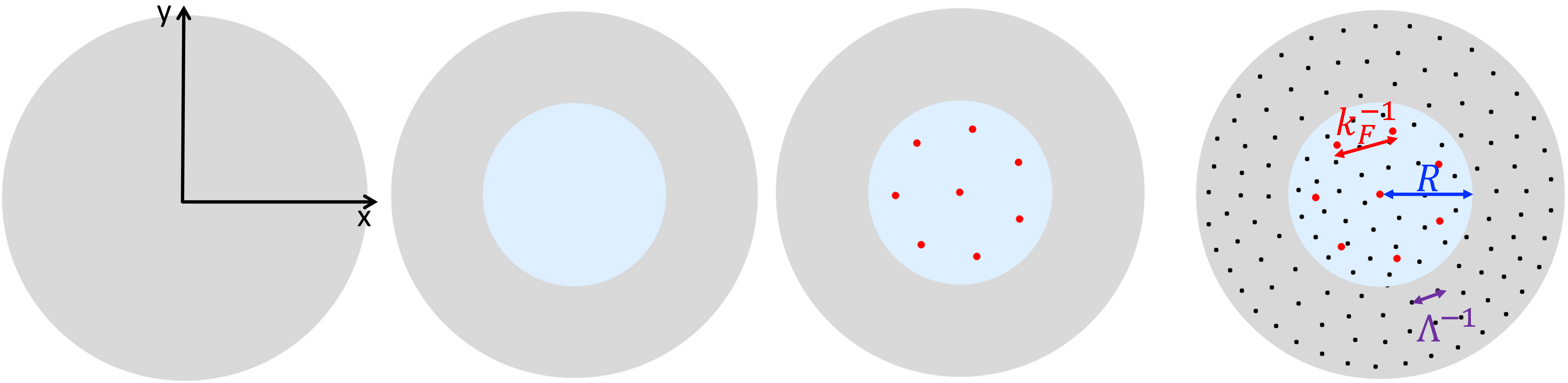


Gaffney et al. Nature 497, 199 (2013)



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

A picture of the mean-field basis in position space



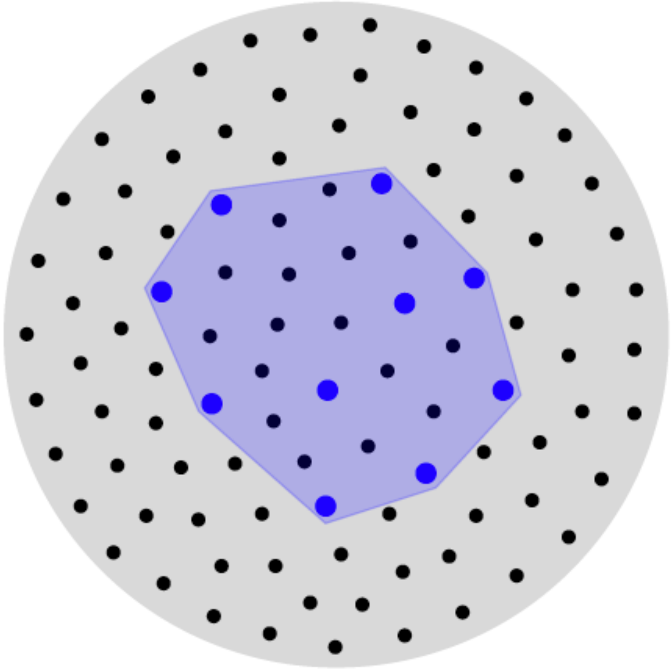
Fock space: Single-particle states fill part of position space.

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 $\sim \Lambda^{-1}$.

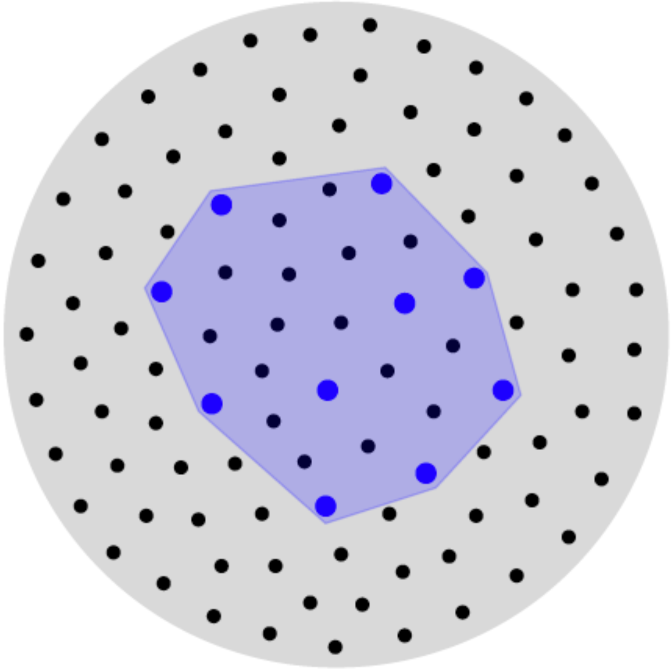
The binding energy is proportional to the mass number



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

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



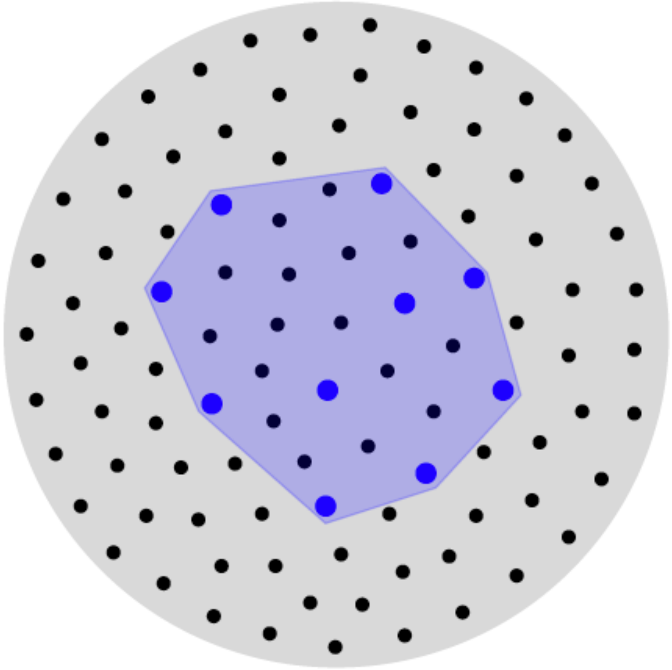
$$E_{\text{ref}} \equiv \langle\psi_0|H|\psi_0\rangle$$
$$= \sum_i \langle i|H|i\rangle + \frac{1}{2}\sum_{ij}\langle ij|H|ij\rangle + \frac{1}{6}\sum_{ijk}\langle ijk|H|ijk\rangle$$

$\propto \delta_{x_i}^{x_j}$ ← short range

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

A: The nuclear force is short ranged!

The binding energy is proportional to the mass number



$$E_{\text{ref}} \equiv \langle \psi_0 | H | \psi_0 \rangle$$

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

$\propto \delta_{x_i}^{x_j}$ ← short range

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

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

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

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

Brackets {…} indicate normal ordering

and matrix elements

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

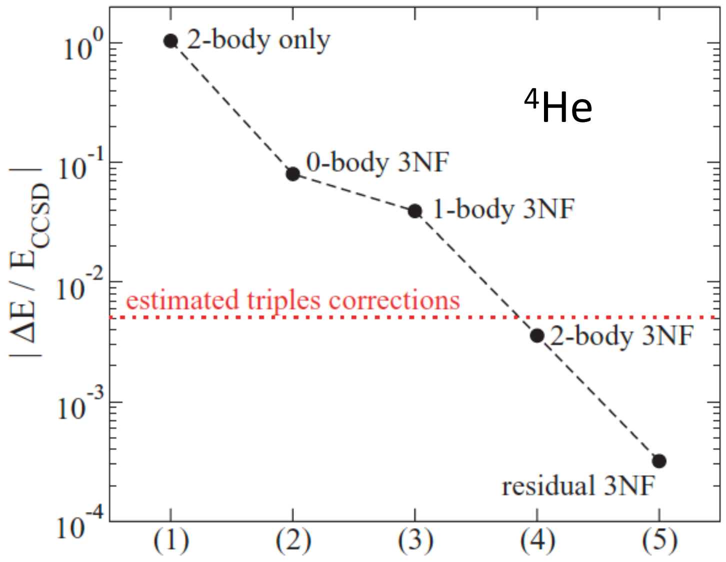
$$\langle pq|H_{\rm no}|rs\rangle = \langle pq|H|rs\rangle + \sum_i \langle pqi|H|rsi\rangle \; .$$

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

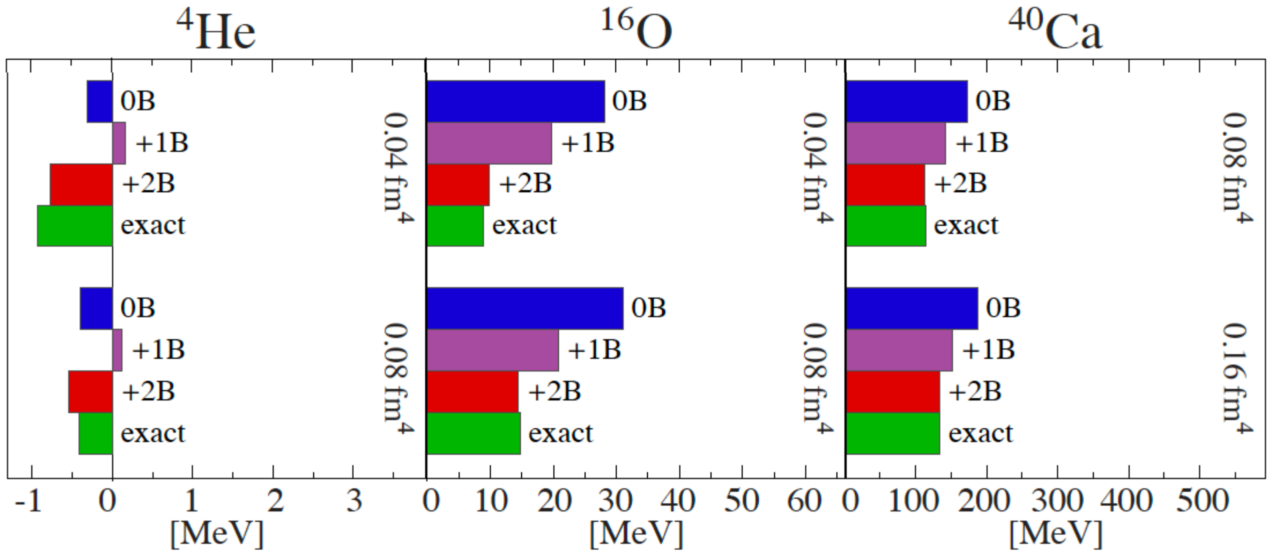
Normal-ordered two-body approximation

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)

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

Note: the cluster operator only contains excitations, but no de-excitations!

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

Computing the similarity-transformed Hamiltonian

Baker-Campbell-Hausdorff expansion

$$e^{-T}H_{\mathrm{no}}e^{T} = H_{\mathrm{no}} + [H_{\mathrm{no}}, T] + \frac{1}{2!}\left[[H_{\mathrm{no}}, T], T\right] + \frac{1}{3!}\left[\left[[H_{\mathrm{no}}, T], T\right], T\right] + \dots$$

Q: Assume that H_{no} is a two-body operator, and that $T = T_1 + T_2$.
Where does the BCH expansion end?

$$\begin{aligned} T &\equiv T_1 + T_2 \\ &= \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i + \frac{1}{4}\sum_{ijab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i \end{aligned}$$

Computing the similarity-transformed Hamiltonian

Baker-Campbell-Hausdorff expansion

$$e^{-T}H_{\mathrm{no}}e^{T} = H_{\mathrm{no}} + [H_{\mathrm{no}}, T] + \frac{1}{2!}\left[[H_{\mathrm{no}}, T], T\right] + \frac{1}{3!}\left[\left[[H_{\mathrm{no}}, T], T\right], T\right] + \ldots$$

Q: Assume that H_{no} is a two-body operator, and that $T = T_1 + T_2$.
Where does the BCH expansion end?

$$\begin{aligned} T &\equiv T_1 + T_2 \\ &= \sum_{ia} t_i^a \hat{a}_a^\dagger \hat{a}_i + \frac{1}{4}\sum_{ijab} t_{ij}^{ab} \hat{a}_a^\dagger \hat{a}_b^\dagger \hat{a}_j \hat{a}_i \end{aligned}$$

A: In this case, it ends at 4-fold nested commutators.

This is the good thing about coupled-cluster: The similarity transformation can be performed exactly.

Key properties of coupled-cluster theory

🙂 The truncation of the cluster operator 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 other similarity transformations (IMSRG)

Short-range correlations yield the bulk of the binding energy

… because the nuclear force is short ranged (Bethe 1936)

Exact expression for the correlation energy for normal-ordered two-body Hamiltonians

$$E_{\rm corr} = \sum_{ia} t_i^a \langle i|H_{\rm no}|a\rangle + \frac{1}{4}\sum_{ijab}\left(t_{ij}^{ab} + t_i^a t_j^b - t_i^b t_j^a\right)\langle ij|H_{\rm no}|ab\rangle$$

$$\underbrace{\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad}_{\propto A\,?}$$

Short-range correlations yield the bulk of the binding energy

… because the nuclear force is short ranged (Bethe 1936)

Exact expression for the correlation energy for normal-ordered two-body Hamiltonians

$$E_{\rm corr} = \sum_{ia} t_i^a \langle i|H_{\rm no}|a\rangle + \frac{1}{4}\sum_{ijab}\left(t_{ij}^{ab} + t_i^a t_j^b - t_i^b t_j^a\right)\langle ij|H_{\rm no}|ab\rangle$$

$\propto \delta_{x_i}^{x_a}$ ← locality

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

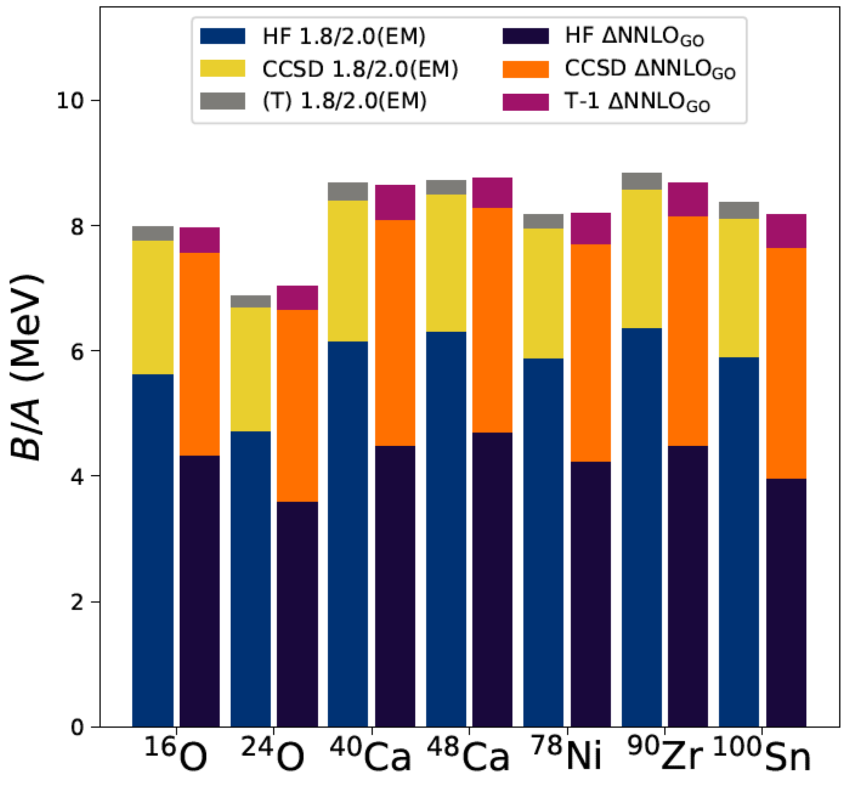
$\propto \delta_{x_i}^{x_j}\delta_{x_b}^{x_a}\,\delta_{x_i}^{x_a}$ ← short range, locality

$\propto A$

Thus, the ground-state energy is size extensive

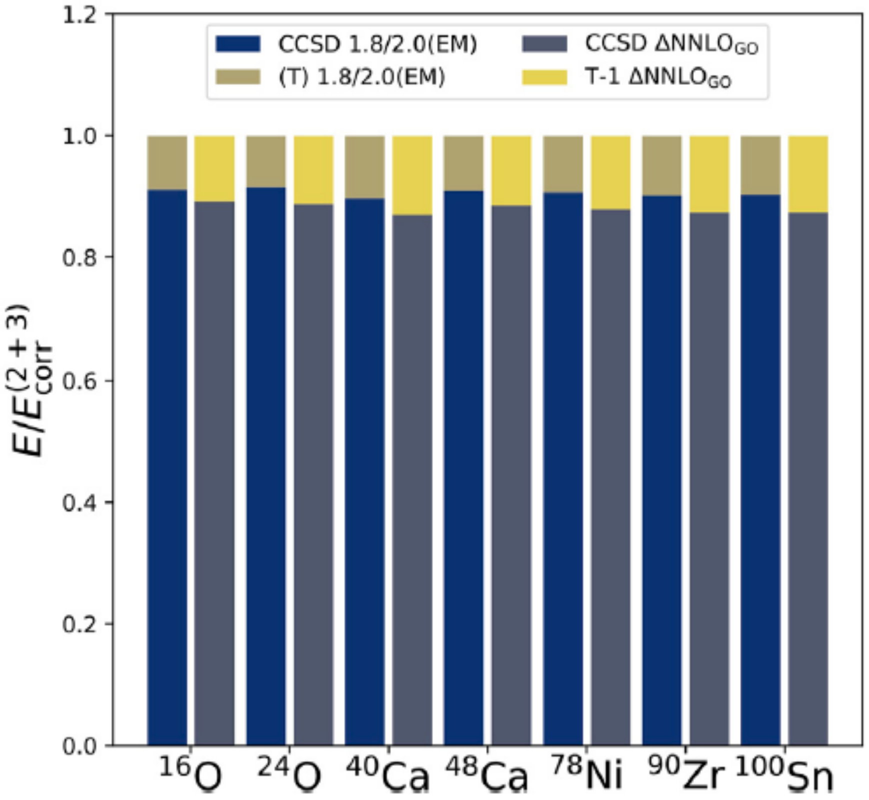
$$E_0 = E_{\rm ref} + E_{\rm corr}$$

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



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



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: Contributions to 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 contribute?

Long-range correlations and many-body correlations

$$E_{\text{corr}} = \sum_{ia} t_i^a \langle i|H_{\text{no}}|a\rangle + \frac{1}{4}\sum_{ijab}\left(t_{ij}^{ab} + t_i^a t_j^b - t_i^b t_j^a\right)\langle ij|H_{\text{no}}|ab\rangle$$

Q: How do long-range parts of T_2 or $T_3, T_4, \cdots$ contribute?
Hint: If they do not directly contribute to the energy, how can they impact the energy?

Long-range correlations and many-body correlations

$$E_{\mathrm{corr}} = \sum_{ia} t_i^a \langle i|H_{\mathrm{no}}|a\rangle + \frac{1}{4}\sum_{ijab}\left(t_{ij}^{ab} + t_i^a t_j^b - t_i^b t_j^a\right)\langle ij|H_{\mathrm{no}}|ab\rangle$$

Q: How do long-range parts of T_2 or $T_3, T_4, \cdots$ contribute?
A: They modify the short-range part of T_2

$$\bar{H}\Big|_{ij}^{ab} = (e^{-T}He^{T})\Big|_{ij}^{ab} = H_{ij}^{ab} + [H,T\,]\Big|_{ij}^{ab} + \cdots = 0$$

Higher-rank clusters contribute as follows: $[H, T_3 + T_4]|_{ij}^{ab} \neq 0$ but $[H, T_5]|_{ij}^{ab} = 0$.

Long-range clusters contribute to short-range physics: $\left[H, T_{long}\right]|_{ij}^{ab} \rightarrow \bar{H}_{short}|_{ij}^{ab} + \bar{H}_{long}\Big|_{ij}^{ab}$

Short-range clusters only contribute to short-range physics: $[H, T_{short}]|_{ij}^{ab} \rightarrow \bar{H}_{short}|_{ij}^{ab}$

Renormalization of particle-hole correlations

We want to better understand dynamical correlations!

Proposal: Apply Lepage's insights to many-body computations

- CCSD computations ($T = T_1 + T_2$) lack triples (T_3), i.e. three-body correlations
- Assume: Triples mainly induce short-range correlations

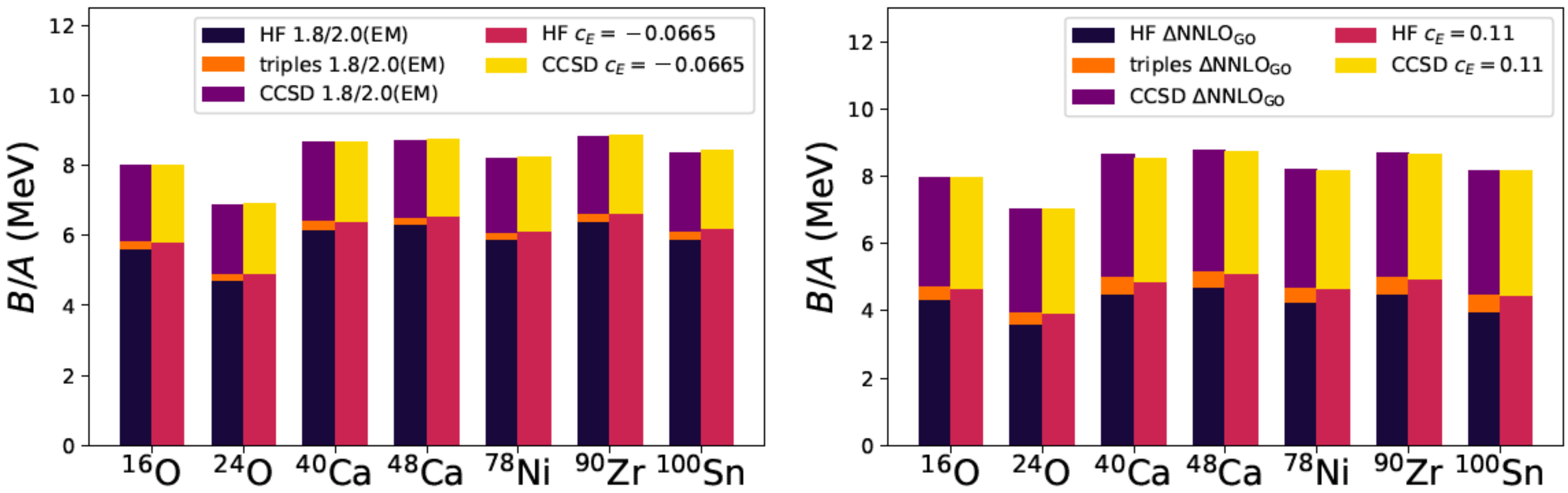
  "integrating out" of triples then requires renormalization of three-body contact

Interaction	Name	c_E
A	1.8/2.0(EM)	−0.12 [52]
A renorm.		−0.0665
B	ΔNNLO$_{\rm GO}$(394)	−0.002 [67]
B renorm.		0.11

	Interaction and method				Exp.
	A renorm. CCSD	A Λ-CCSD(T)	B renorm. CCSD	B CCSDT-1	
^{16}O	127.8	127.8	127.5	127.5	127.62
^{24}O	166	165	169	169	168.96
^{40}Ca	346	347	341	346	342.05
^{48}Ca	420	419	419	420	416.00
^{78}Ni	642	638	636	639	641.55
^{90}Zr	798	795	777	782	783.90
^{100}Sn	842	836	816	818	825.30

Zhonghao Sun, Charles Bell, G. Hagen, TP, Phys. Rev. C 106, L061302 (2022)

Renormalization of particle-hole correlations



Left figure: results for 1.8/2.0(EM) interaction; right for ΔNNLO$_{GO}$; from Sun et al, PRC 106, L061302 (2022)
Compare the $T = T_1 + T_2 + T_3$ result to those from an interaction with renormalized three-nucleon forces

Q: What would one (presumably) need to do if one wanted to limit computations to Hartree Fock $T = T_1$?

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}	$E_{CCSD(T)}$	$E_{Proj.}$	$\langle J_{HF}\rangle$	$\langle J_{CCSD(T)}\rangle$
^{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

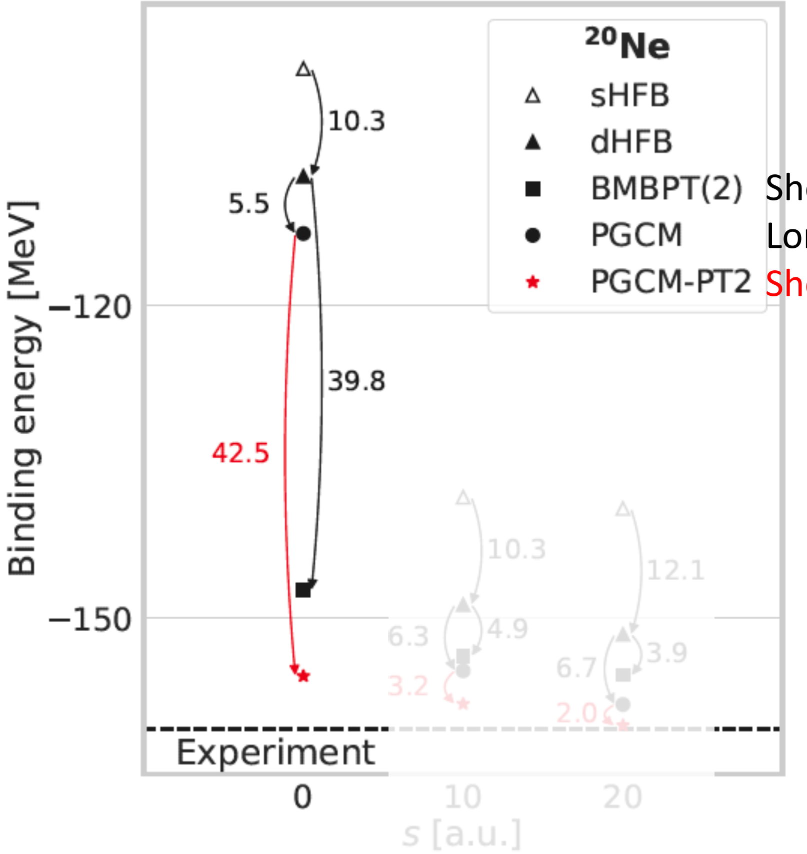
Coester and Kümmel (1960), “Short-range correlations in nuclear wave functions”
Lipkin (1960): “Collective motion in many-particle systems: Part 1. the violation of conservation laws”

	E_{HF}	$E_{CCSD(T)}$	$E_{Proj.}$	$\langle J_{HF} \rangle$	$\langle J_{CCSD(T)} \rangle$
^{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?
Q: Why does the energy contribution from symmetry projection decrease with increasing mass number?

This partitioning of the energy into large contributions from dynamical and small static correlations is universal



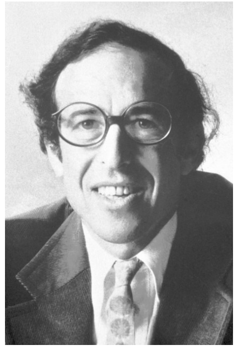
Short-range correlations
Long-range correlations
Short-range correlations

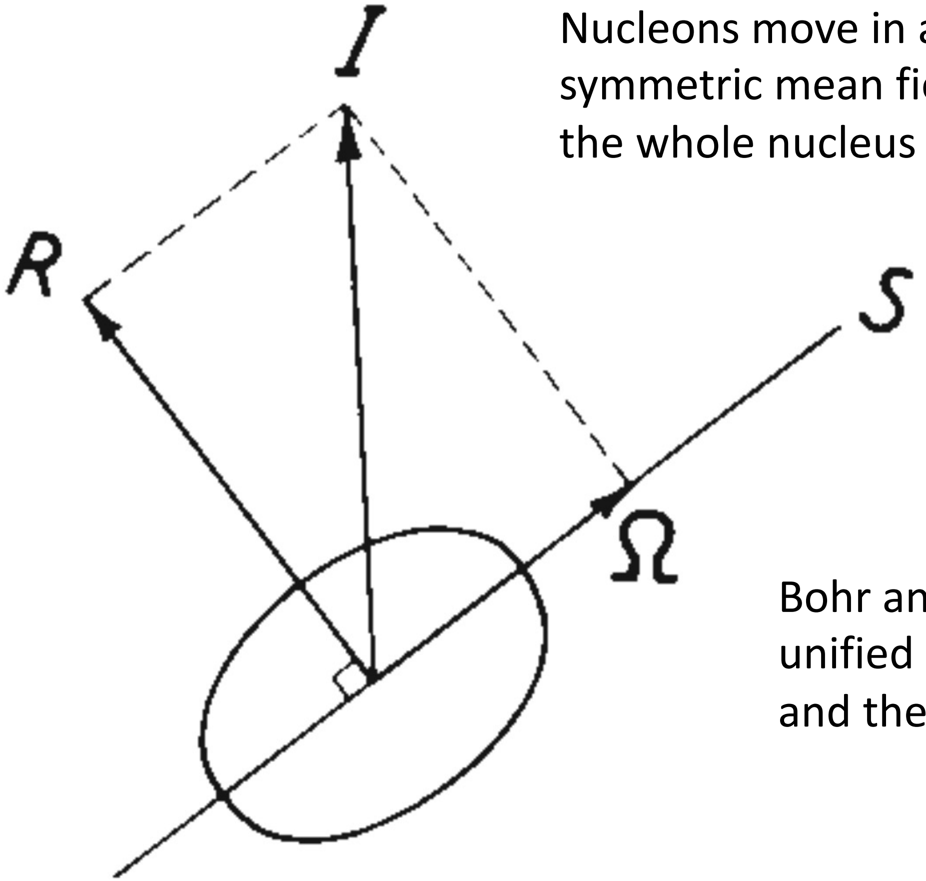
Frosini et al., Eur. Phys. J. A 58, 63 (2022); arXiv:2111.00797

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

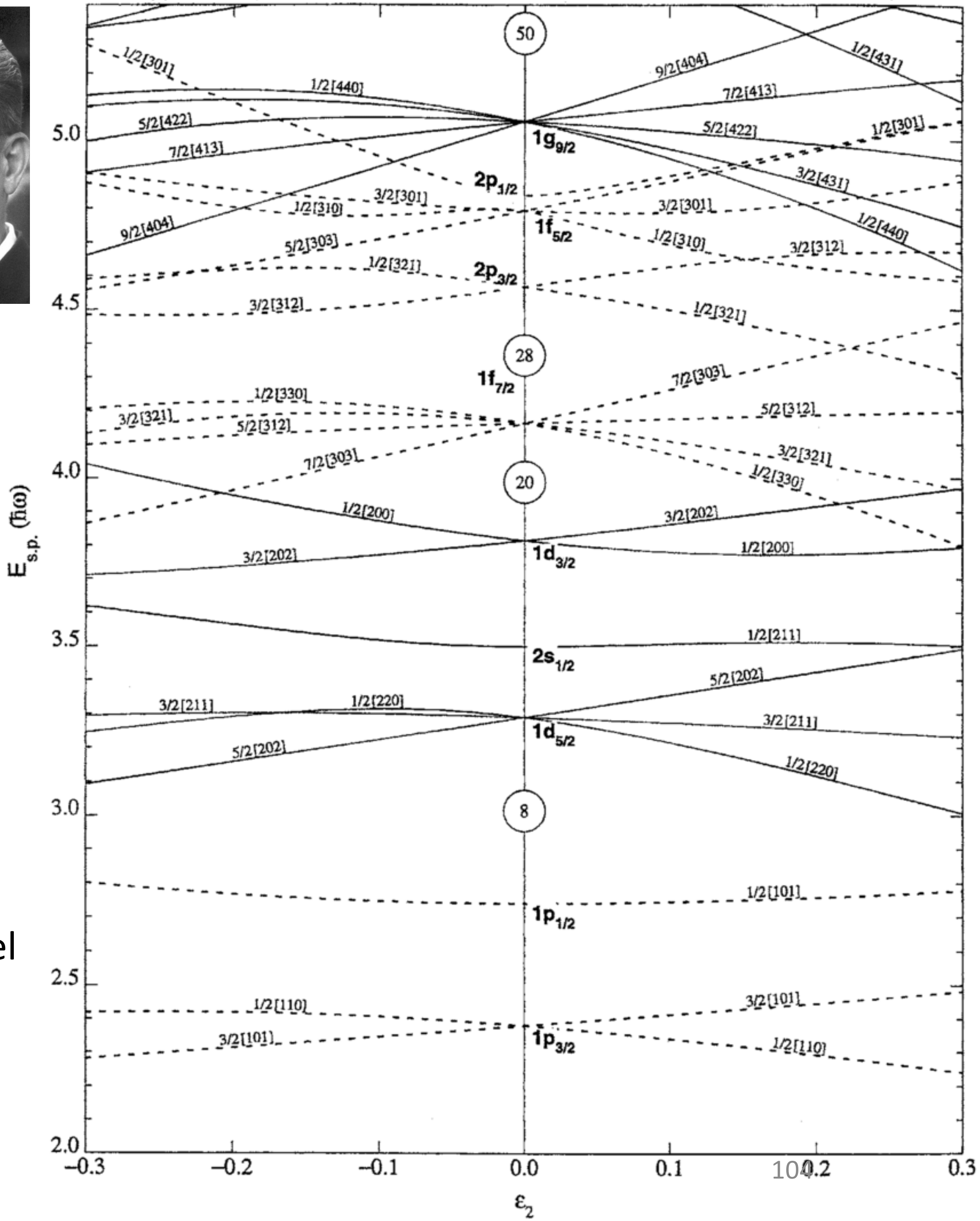



A. Bohr (1950s)

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

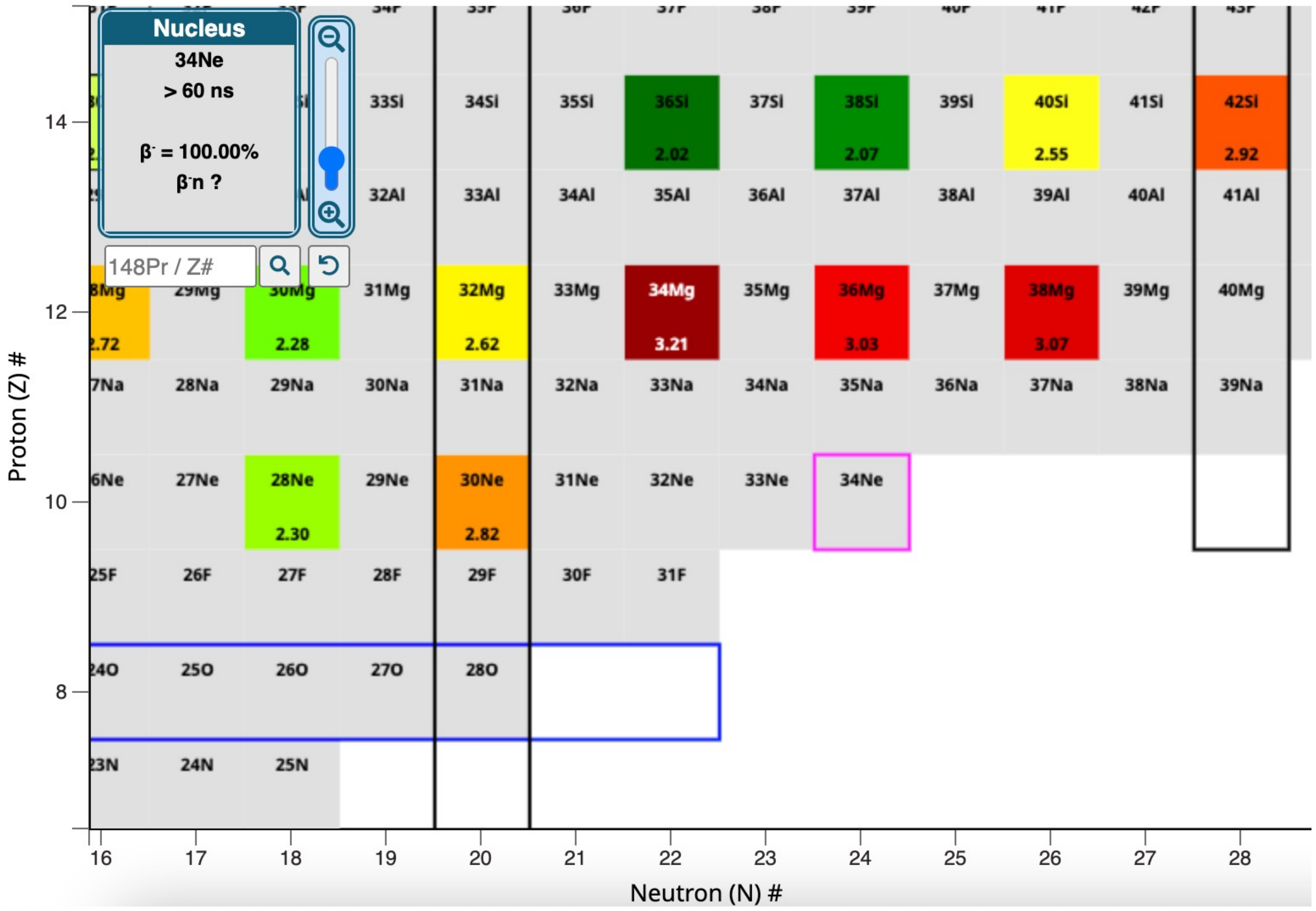
1. Take Hamiltonians from chiral effective field theory: $H = T + V_{NN} + V_{NNN}$
2. Perform Hartree-Fock or Hartree-Fock-Bogoliubov computation
    a. Yields non-trivial vacuum state $|\psi_0\rangle$
    b. Informs us about nuclear deformation and superfluidity
    c. Introduces Fermi momentum $k_F \approx 1.35$ 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

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

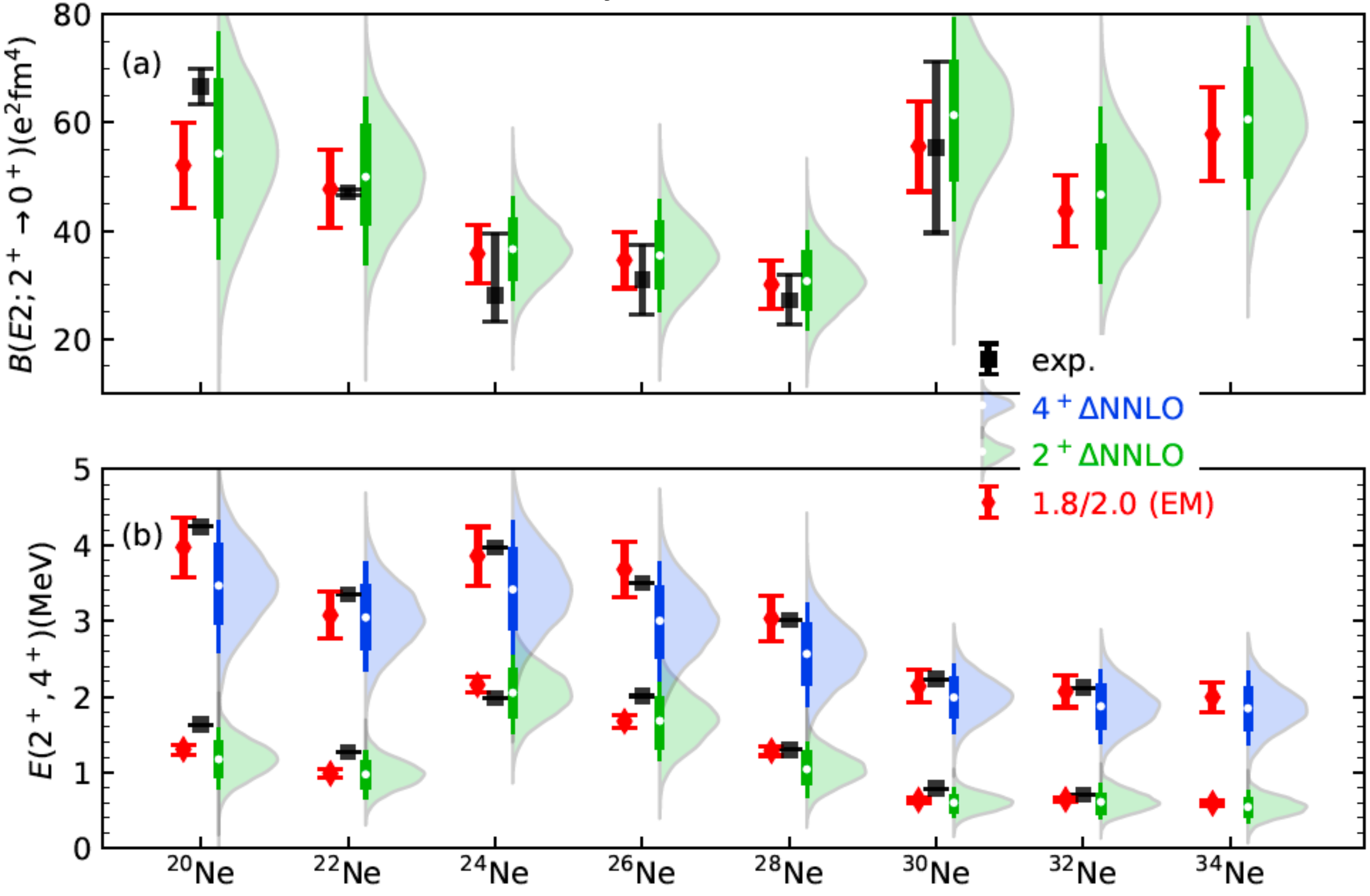
$R_{4/2} = 10/3$ for a rigid rotor

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

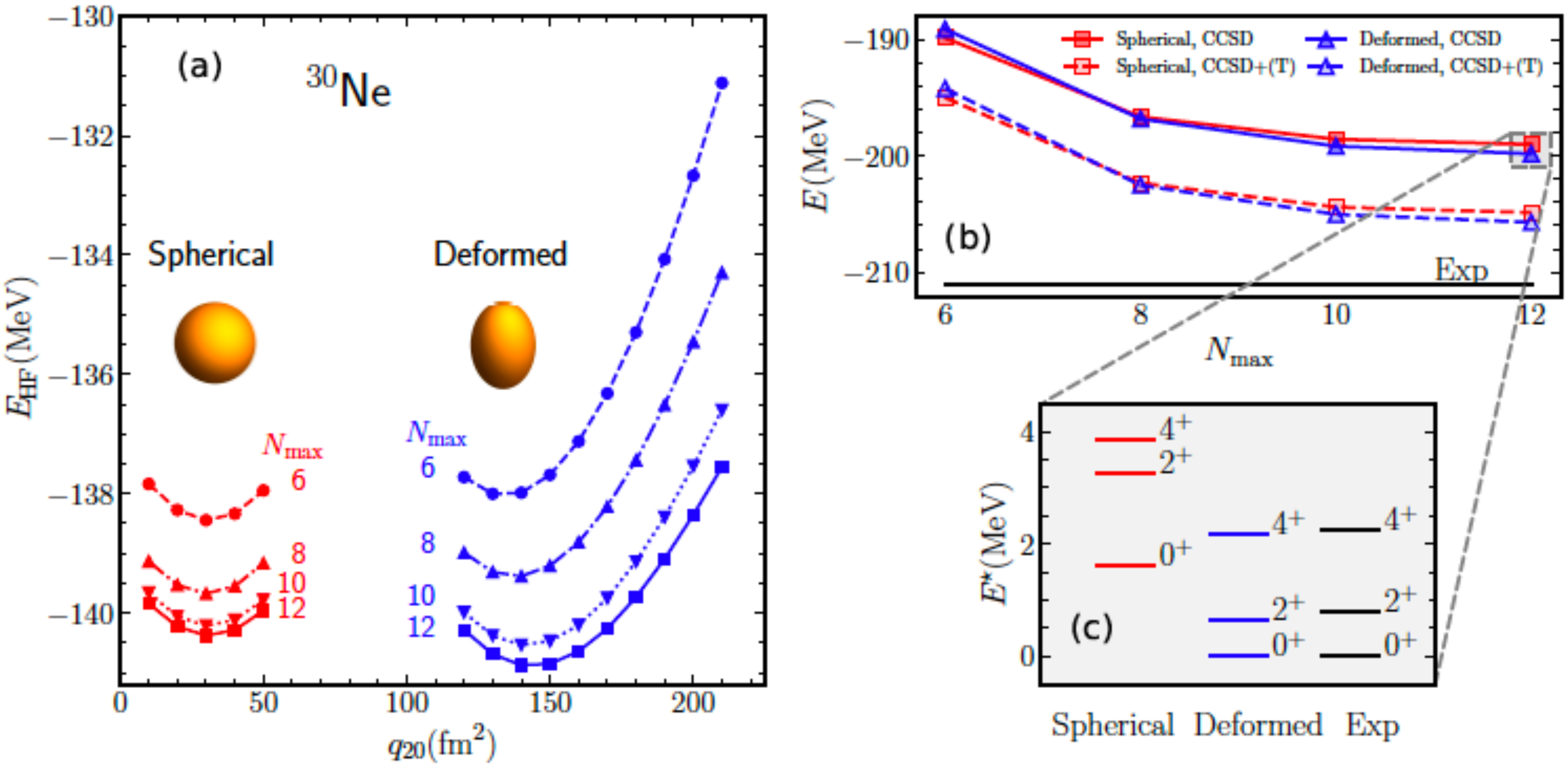
States with different shapes that are close in energy

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).

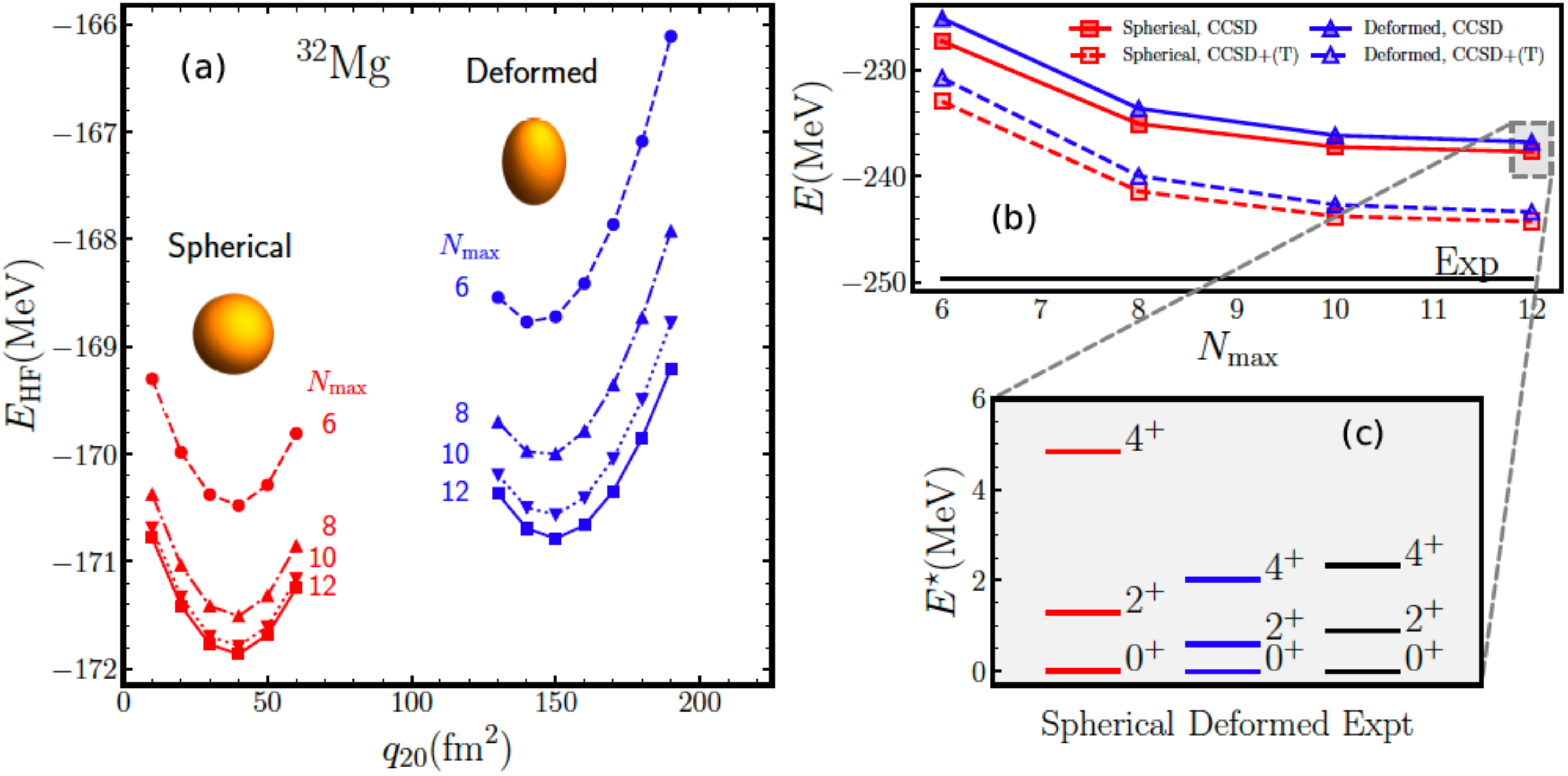
Theoretical descriptions: Reinhard et al., Phys. Rev. C 60, 014316 (1999); Rodríguez-Guzmán, Egido, and Robledo, Nucl. Phys. A 709, 201 (2002); Péru and Martini, Eur. Phys. J. A 50, 88 (2014); Caurier, Nowacki, and Poves, Phys. Rev. C 90, 014302 (2014); see also Tsunoda et al., Nature 587, 66 (2020).

Prediction: Shape coexistence in ^{30}Ne



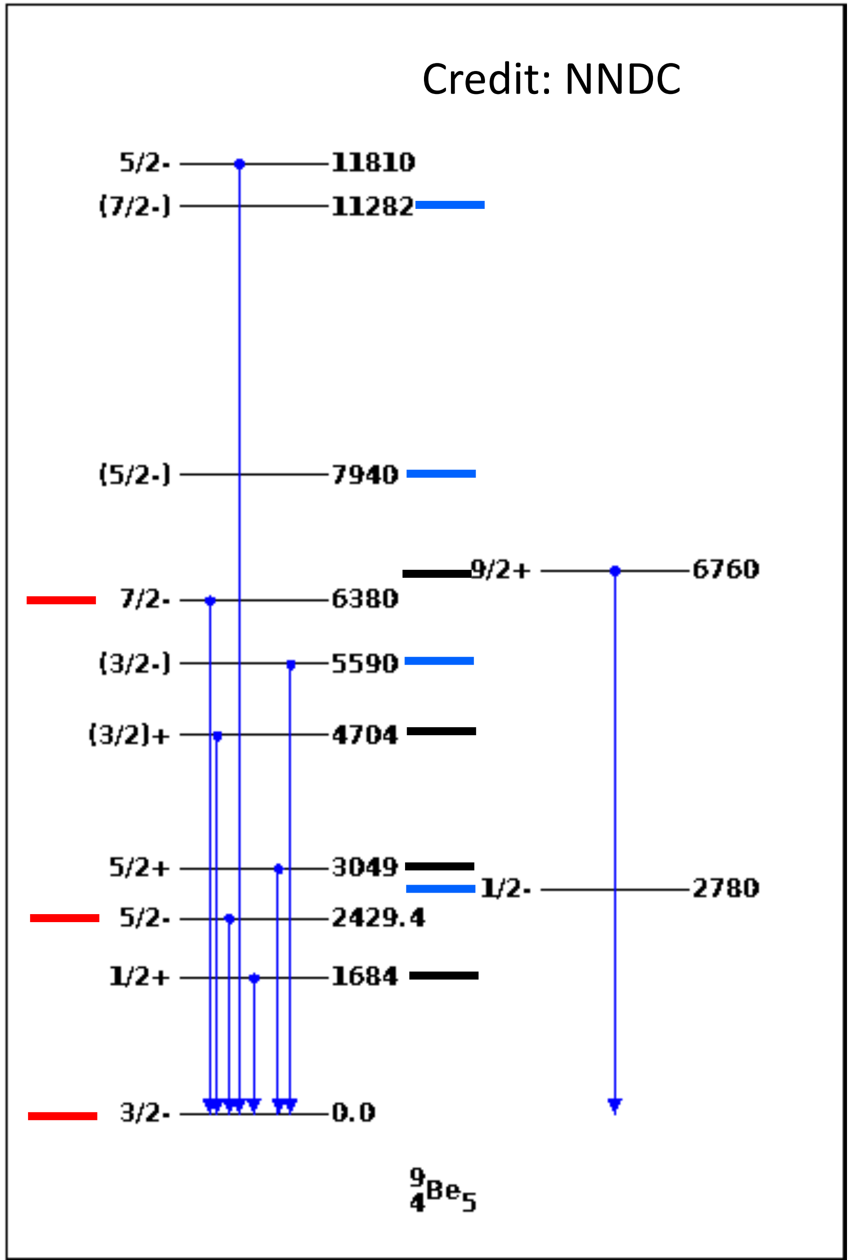
Zhonghao Sun et al., arXiv:2404.00058

Confirmation: Shape coexistence in ^{32}Mg



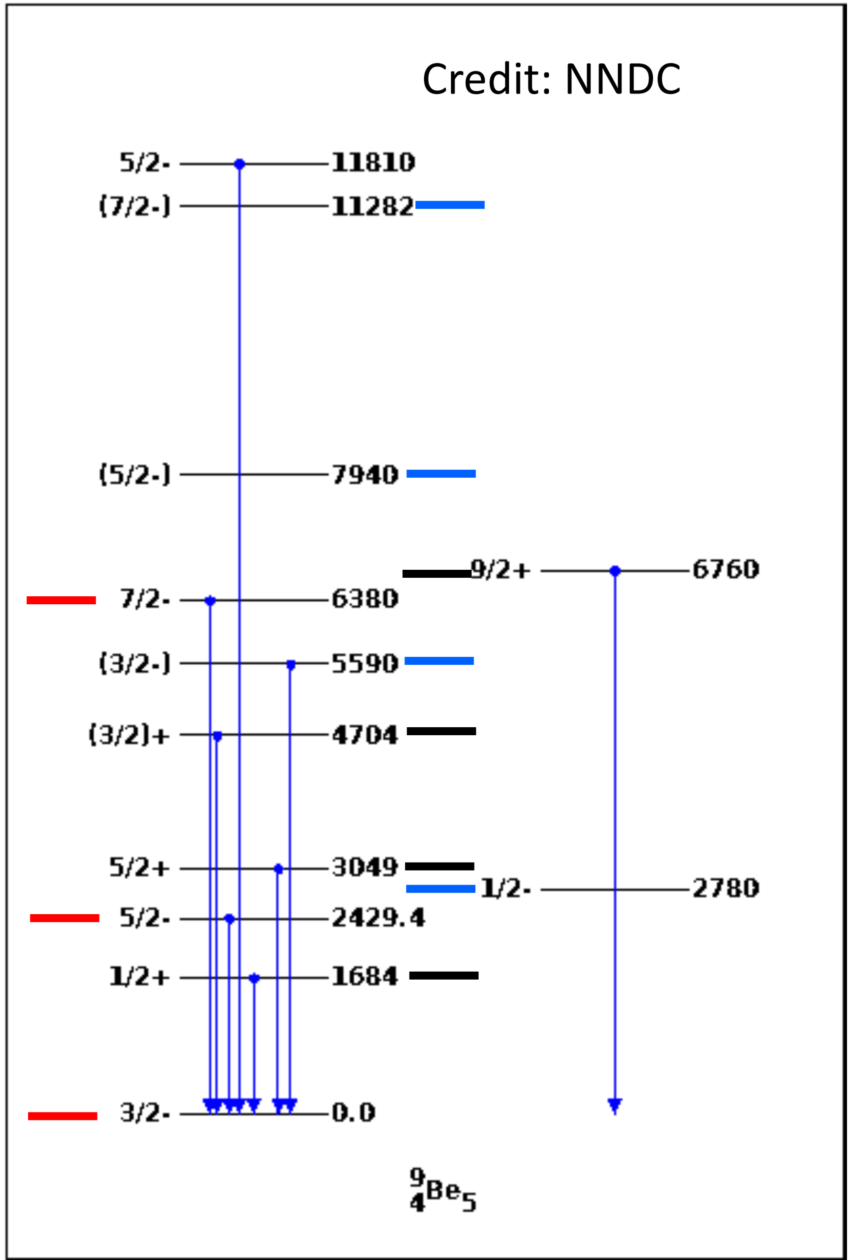
Zhonghao Sun et al., arXiv:2404.00058

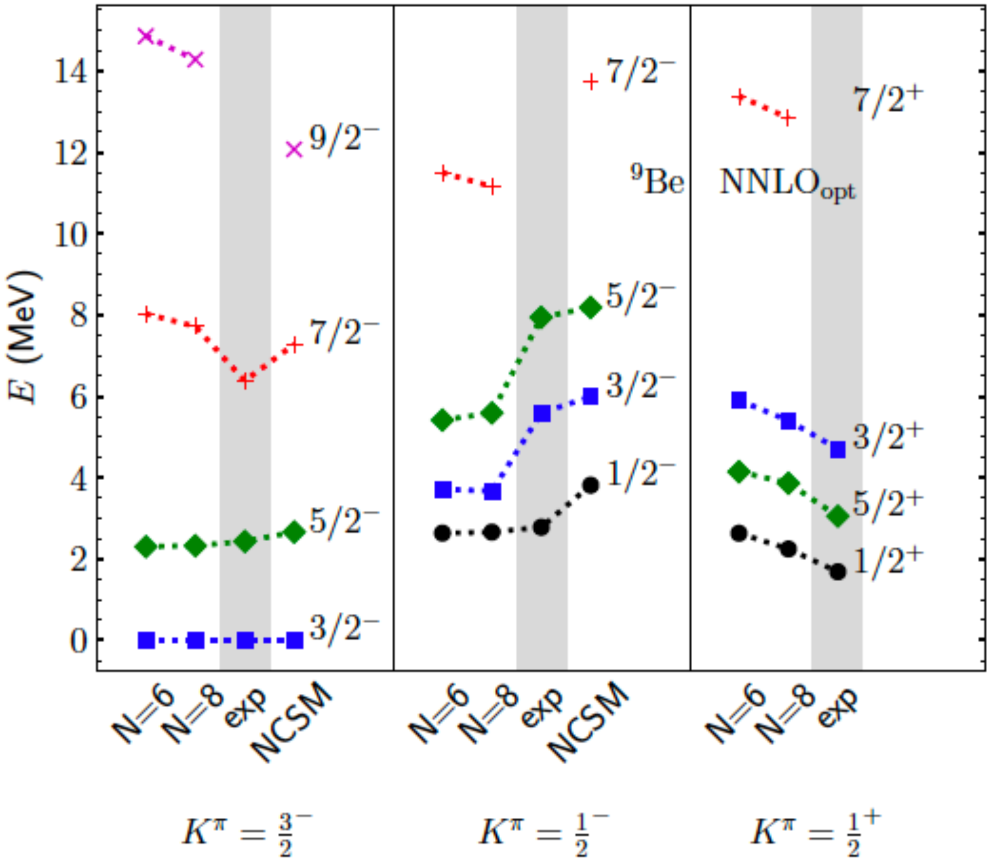
Odd-mass deformed nuclei



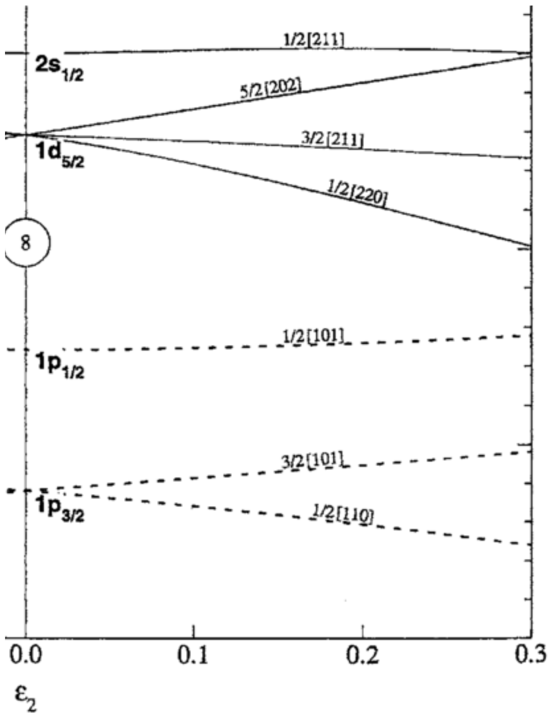
Rhetorical Q: Who sees patterns here?
Who sees a stamp collection?

Odd-mass deformed nuclei



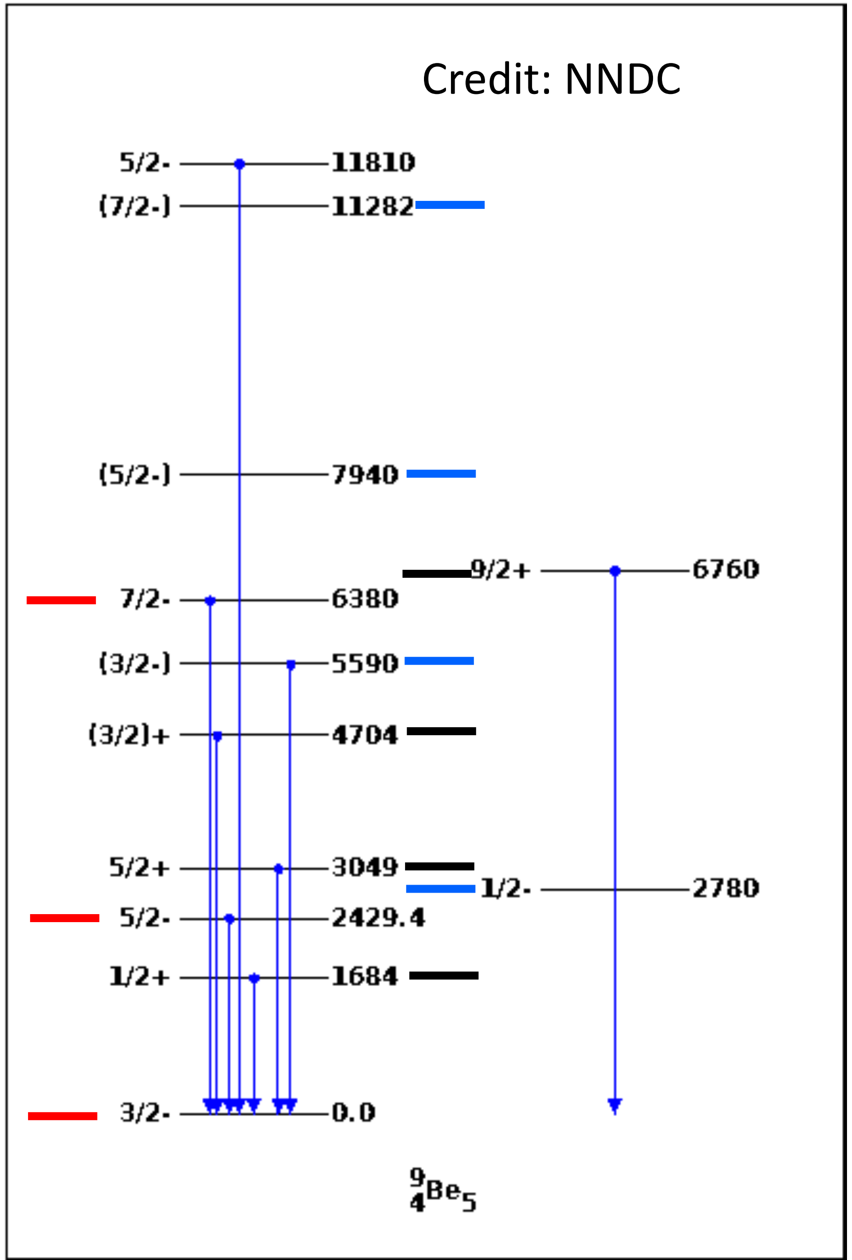


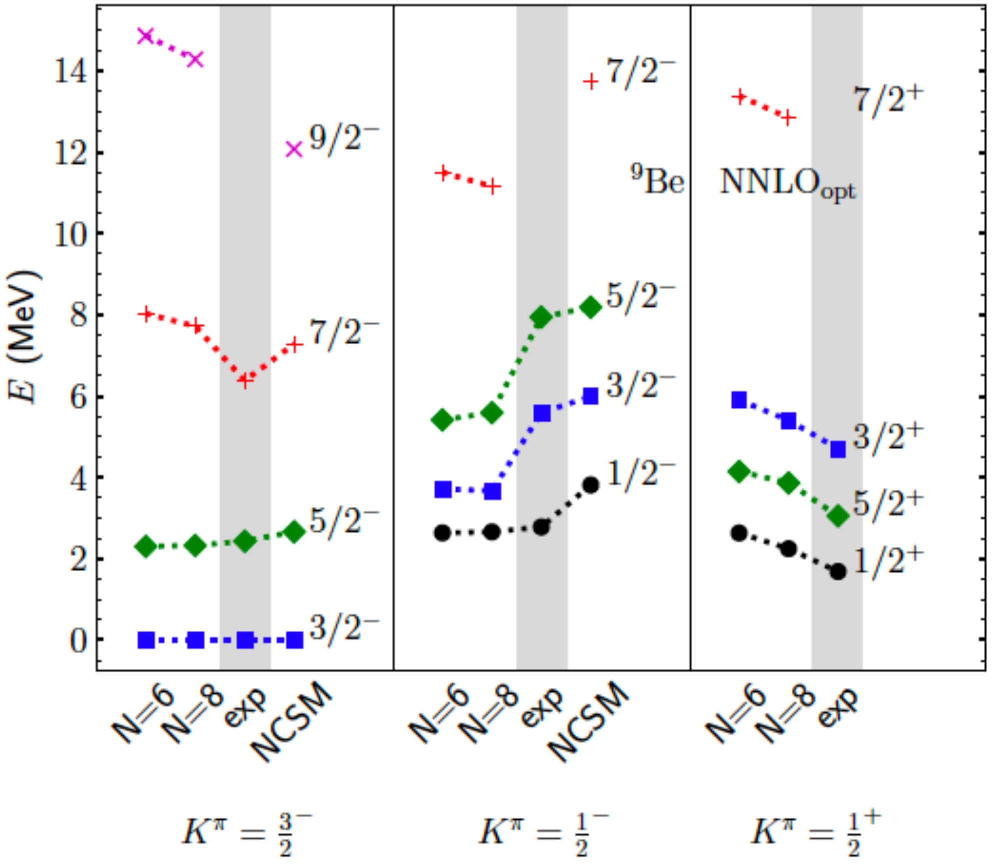
Zhonghao Sun et al., in preparation
NCSM: Caprio et al., Int. J. Mod. Phys. E 24, 1541002 (2015).



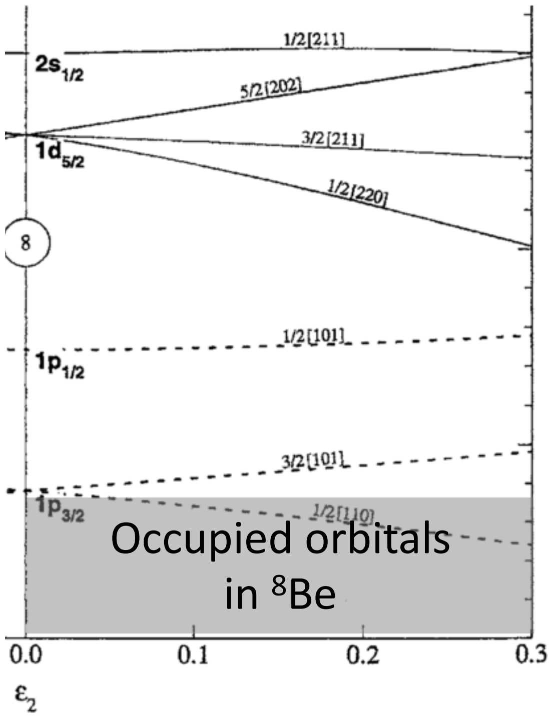
Q: For ^{9}Be (Z=4, N=5), can you place the odd neutron in the Nilsson diagram for each of the bands shown in the middle?

Odd-mass deformed nuclei



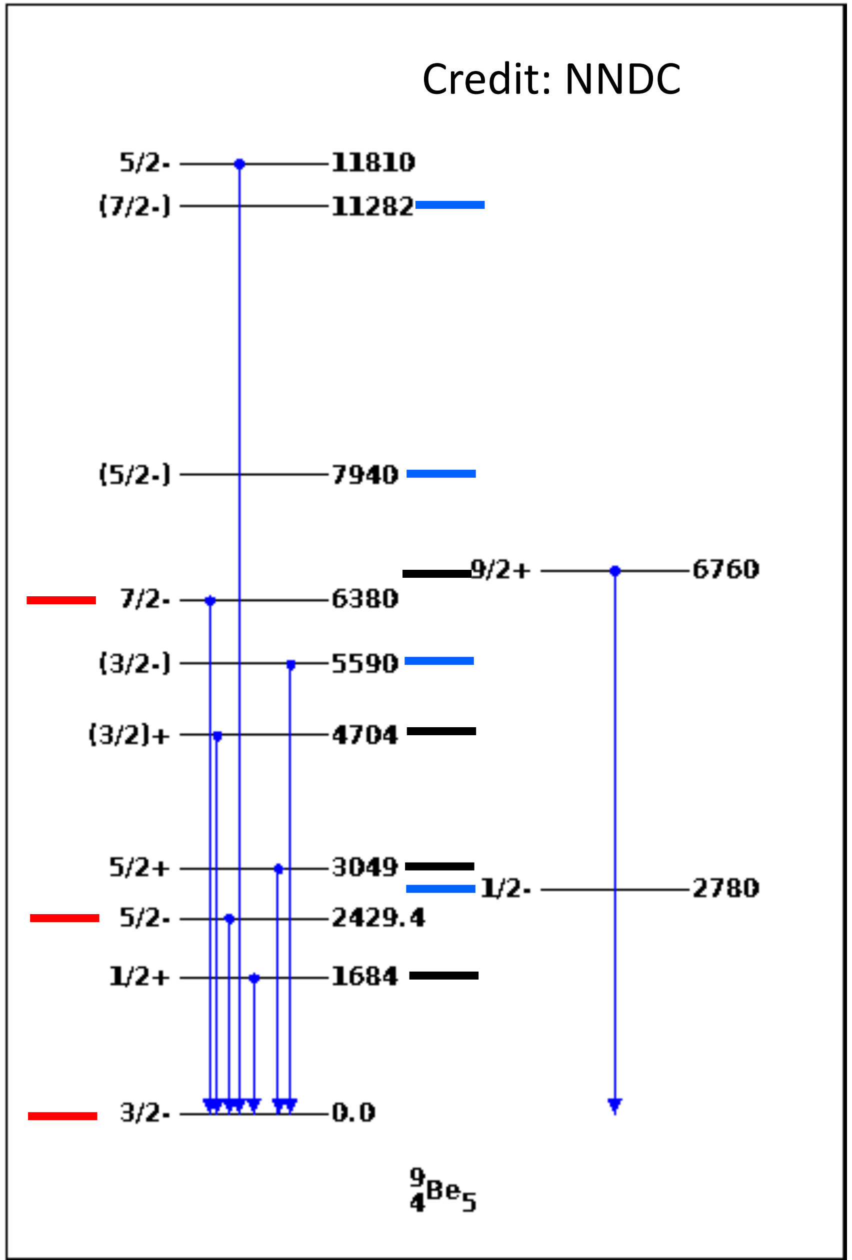


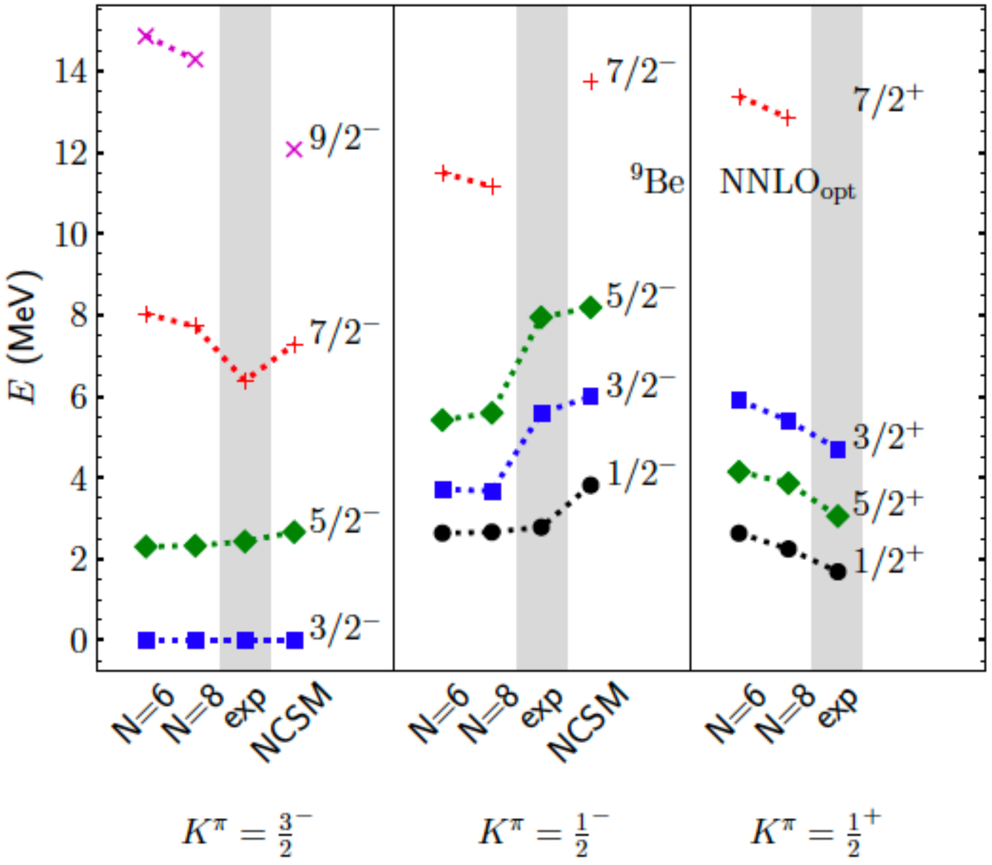
Zhonghao Sun et al., in preparation
NCSM: Caprio et al., Int. J. Mod. Phys. E 24, 1541002 (2015).



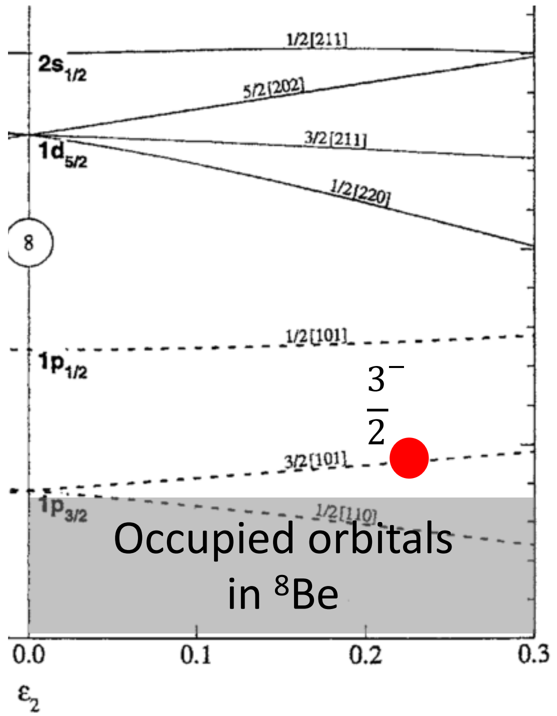
Q: For ^{9}Be (Z=4, N=5), can you place the odd neutron in the Nilsson diagram for each of the bands shown in the middle?

Odd-mass deformed nuclei



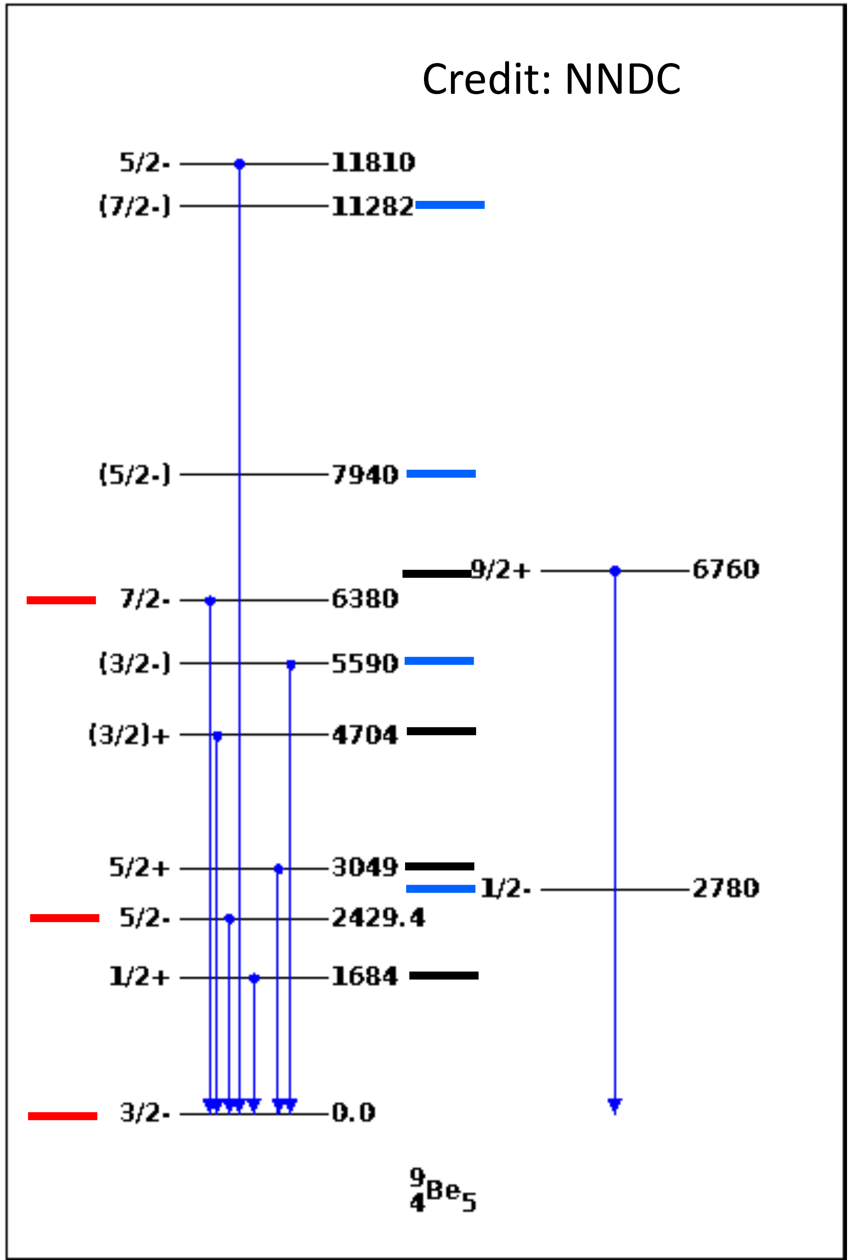


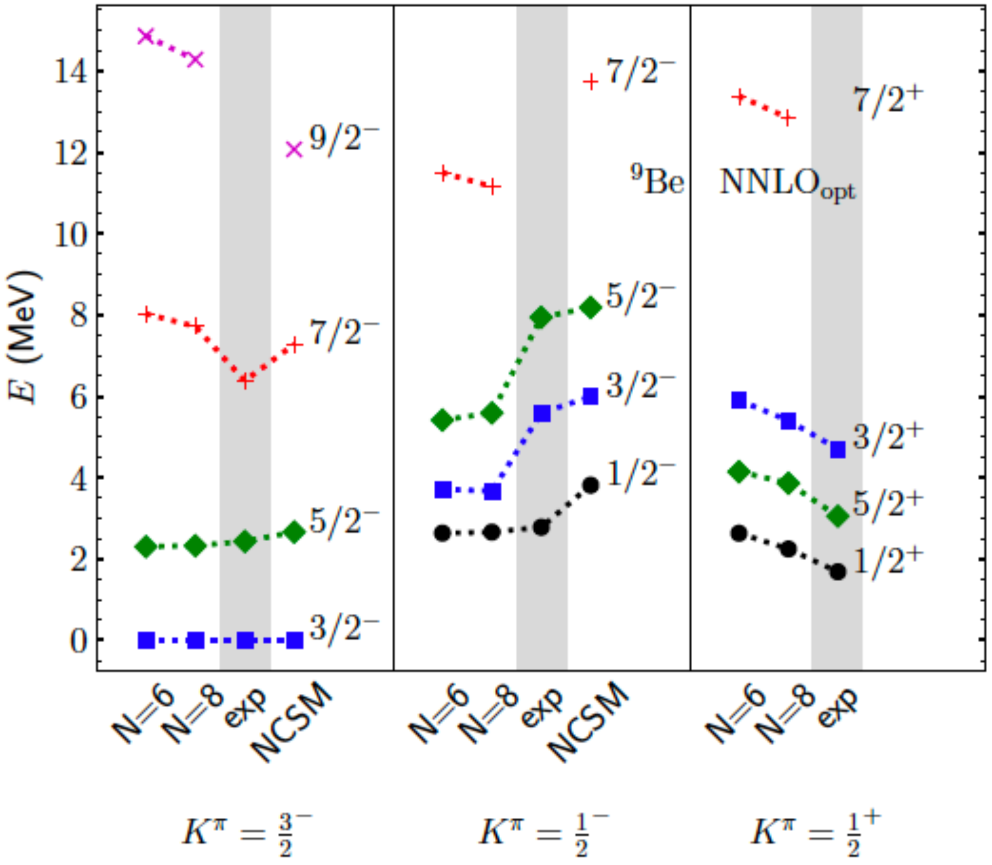
Zhonghao Sun et al., in preparation
NCSM: Caprio et al., Int. J. Mod. Phys. E 24, 1541002 (2015).



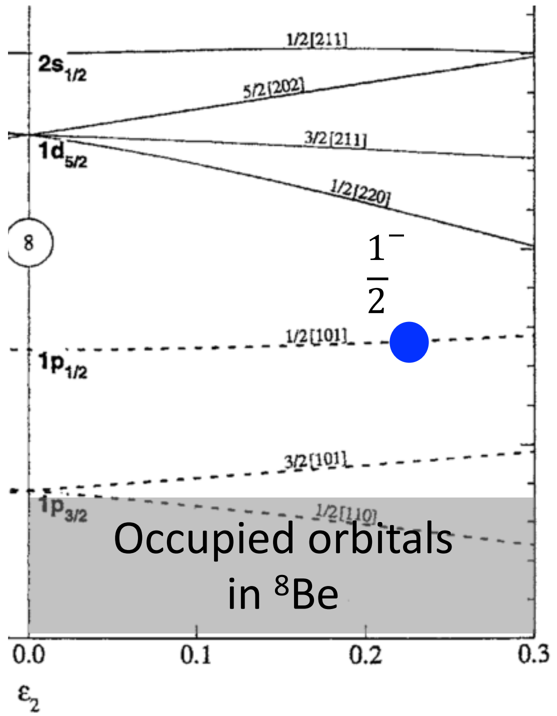
Q: For ^{9}Be (Z=4, N=5), can you place the odd neutron in the Nilsson diagram for each of the bands shown in the middle?

Odd-mass deformed nuclei



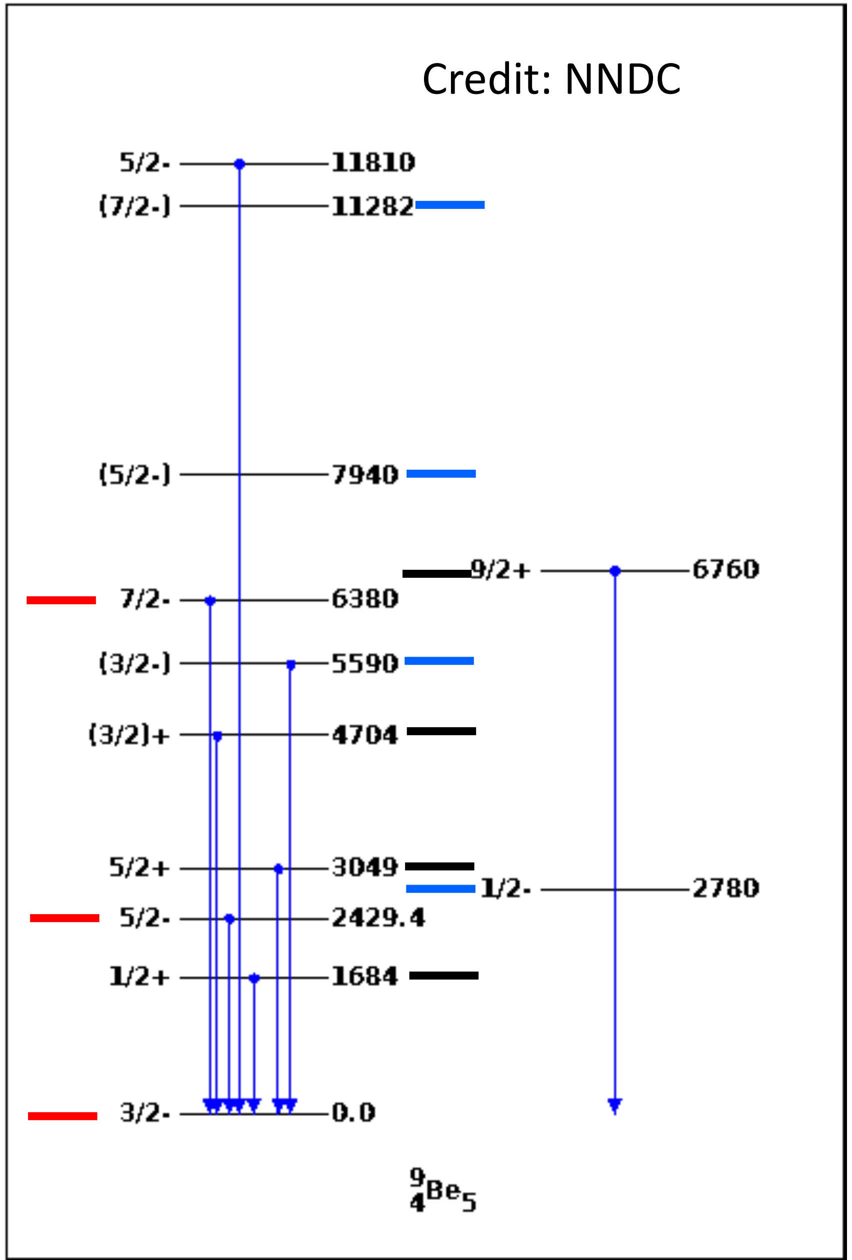


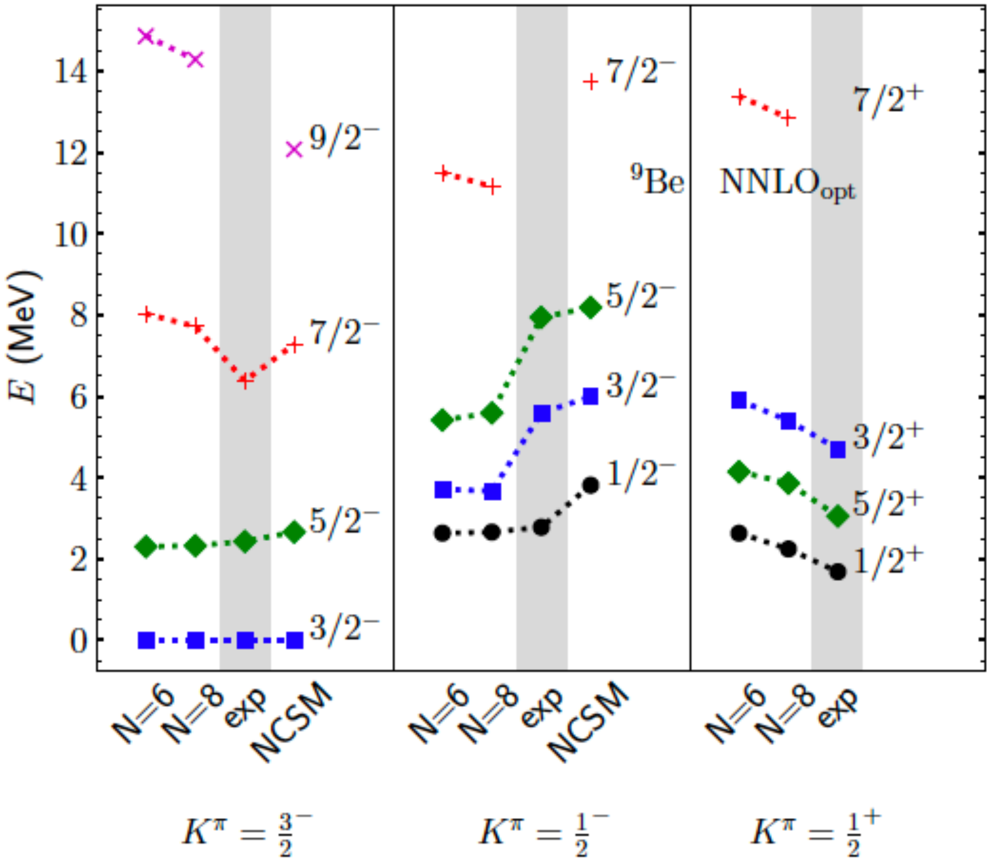
Zhonghao Sun et al., in preparation
NCSM: Caprio et al., Int. J. Mod. Phys. E 24, 1541002 (2015).



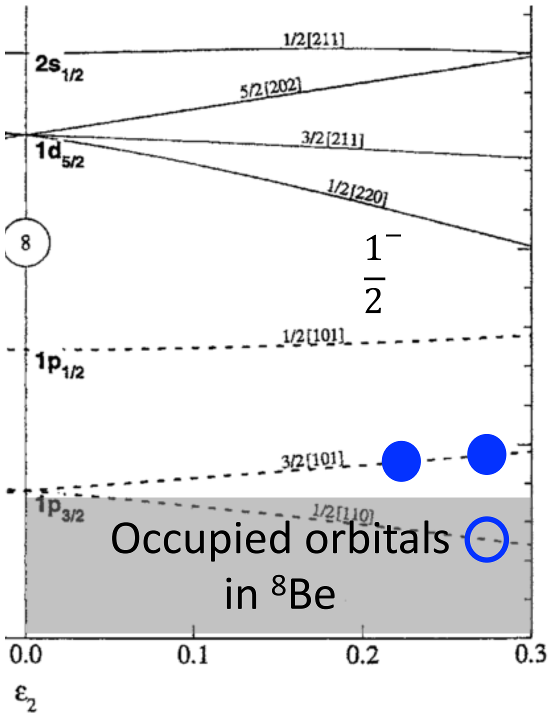
Q: For ^{9}Be (Z=4, N=5), can you place the odd neutron in the Nilsson diagram for each of the bands shown in the middle?

Odd-mass deformed nuclei



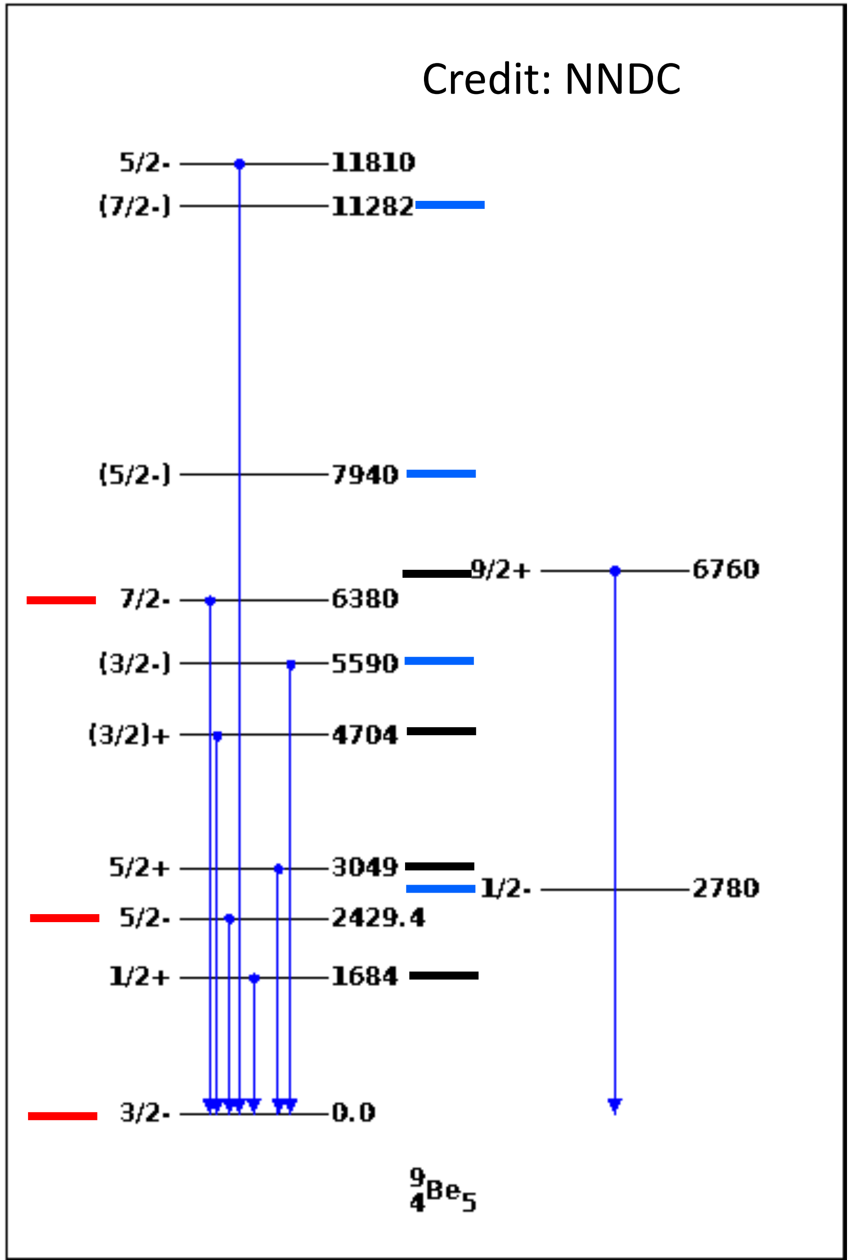


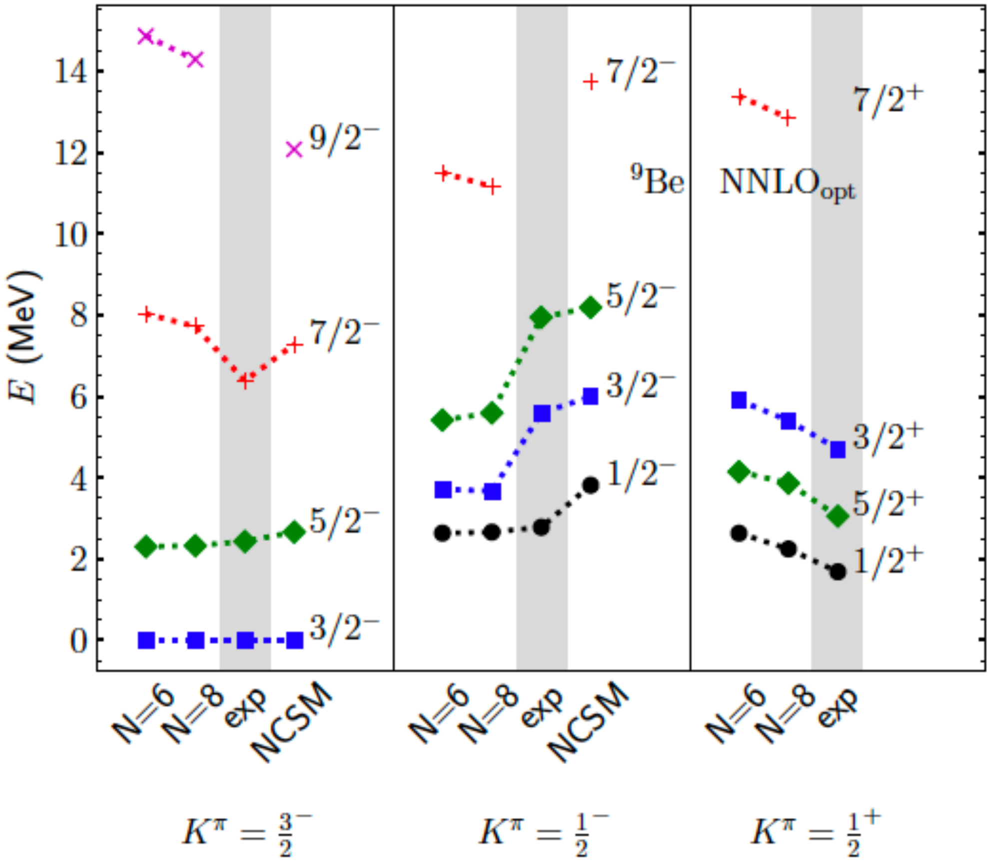
Zhonghao Sun et al., in preparation
NCSM: Caprio et al., Int. J. Mod. Phys. E 24, 1541002 (2015).



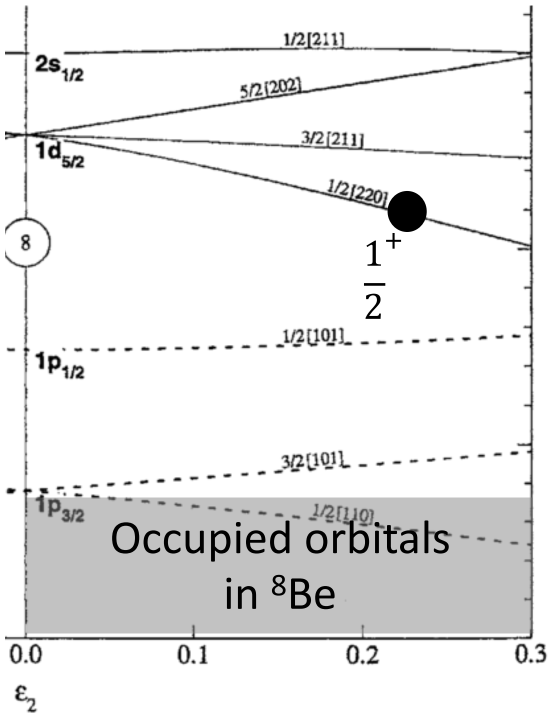
Q: For ^{9}Be (Z=4, N=5), can you place the odd neutron in the Nilsson diagram for each of the bands shown in the middle?

Odd-mass deformed nuclei





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?

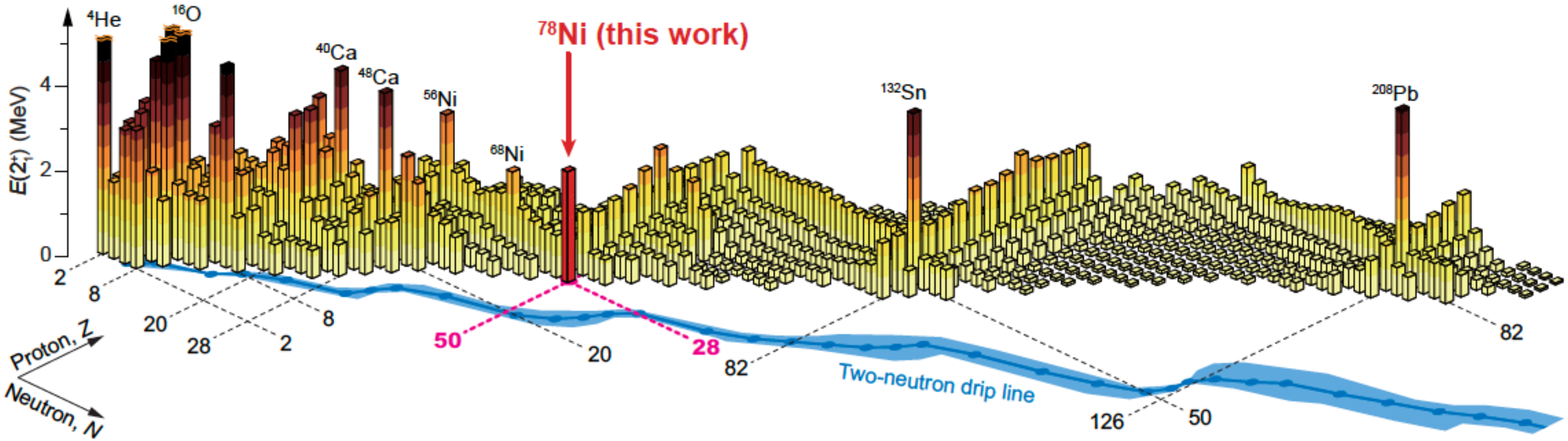
Summary: Ab initio computations

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

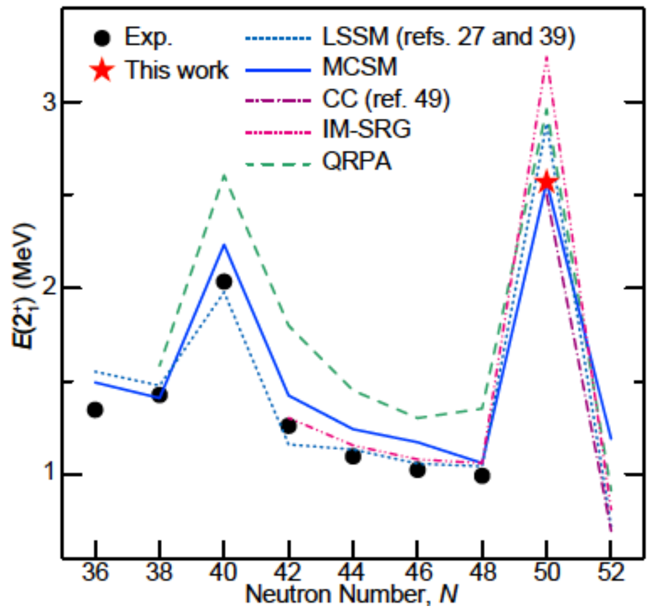
A few more success stories of ab initio computations of nuclei

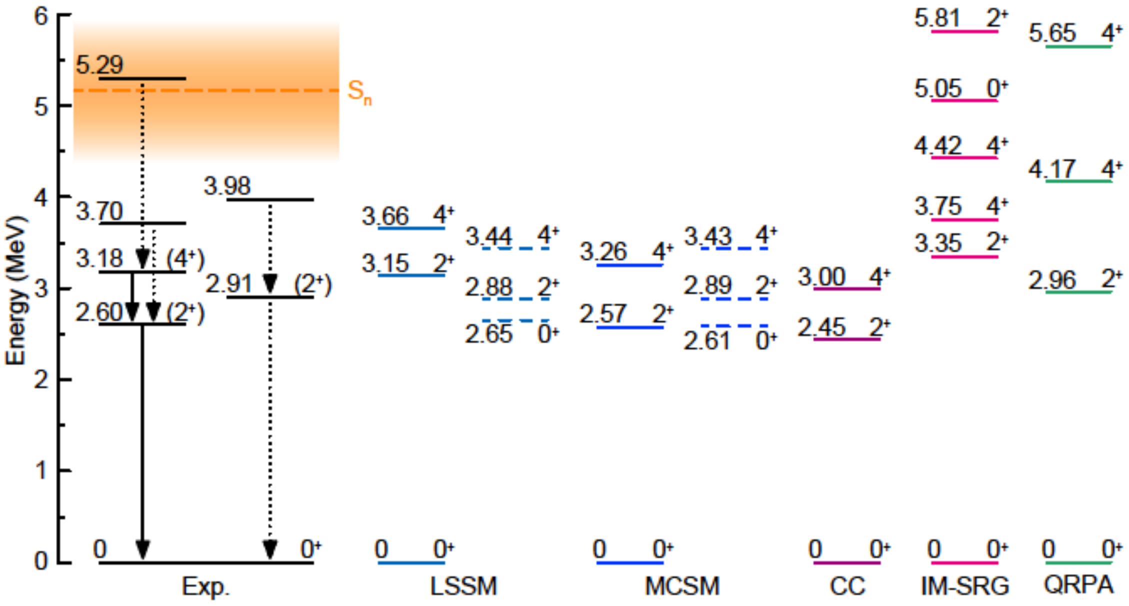
^{78}Ni (Z=28, N=50) is a neutron-rich doubly magic nucleus



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

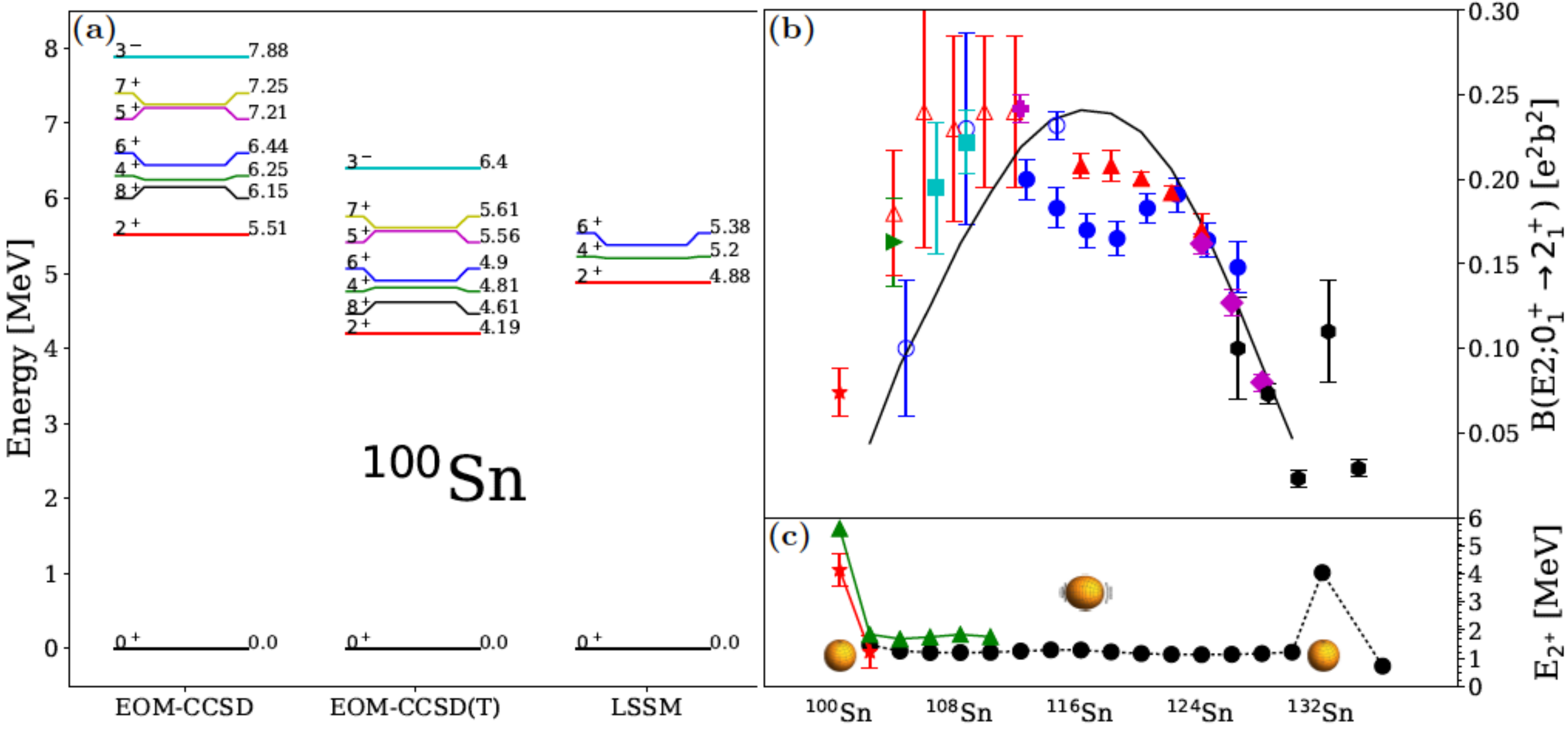




Predictions from 2016
LSSM: shell model
CC: EFT Hamiltonian, adjusted to 2,3,4 nucleons only

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



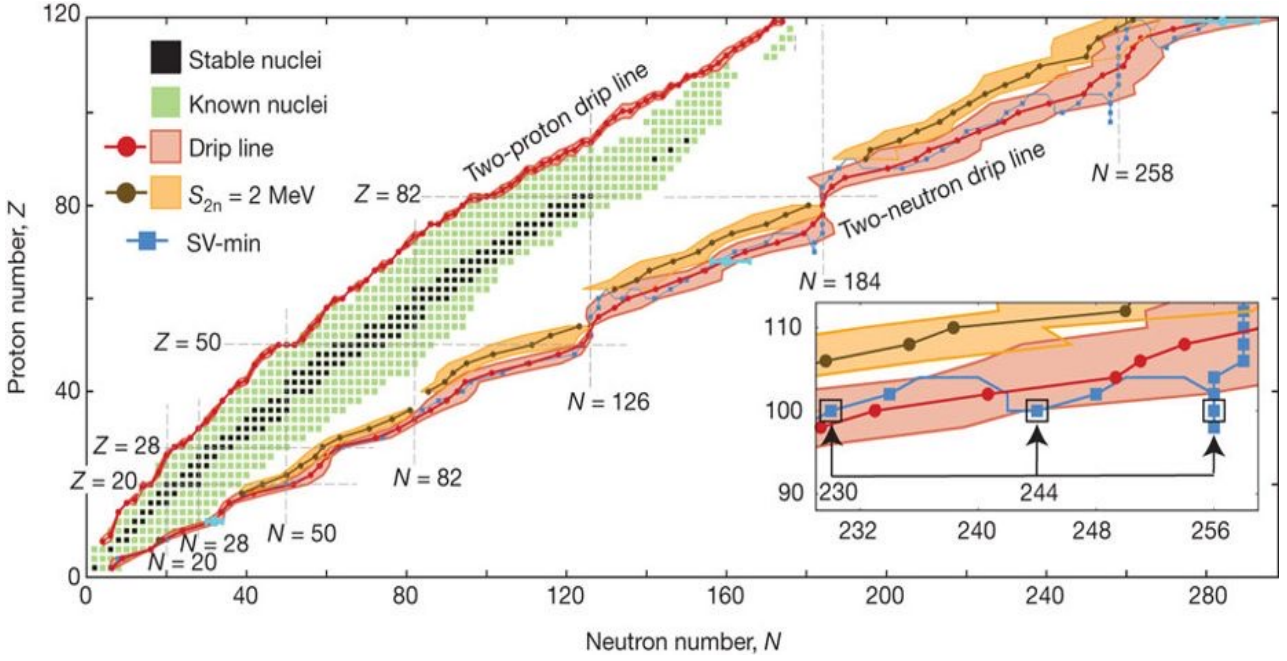
Coupled cluster based on interaction 1.8/2.0(EM); LSSM: Large Scale Shell Model [Faestermann, Gorska & Grawe (2013)]

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)

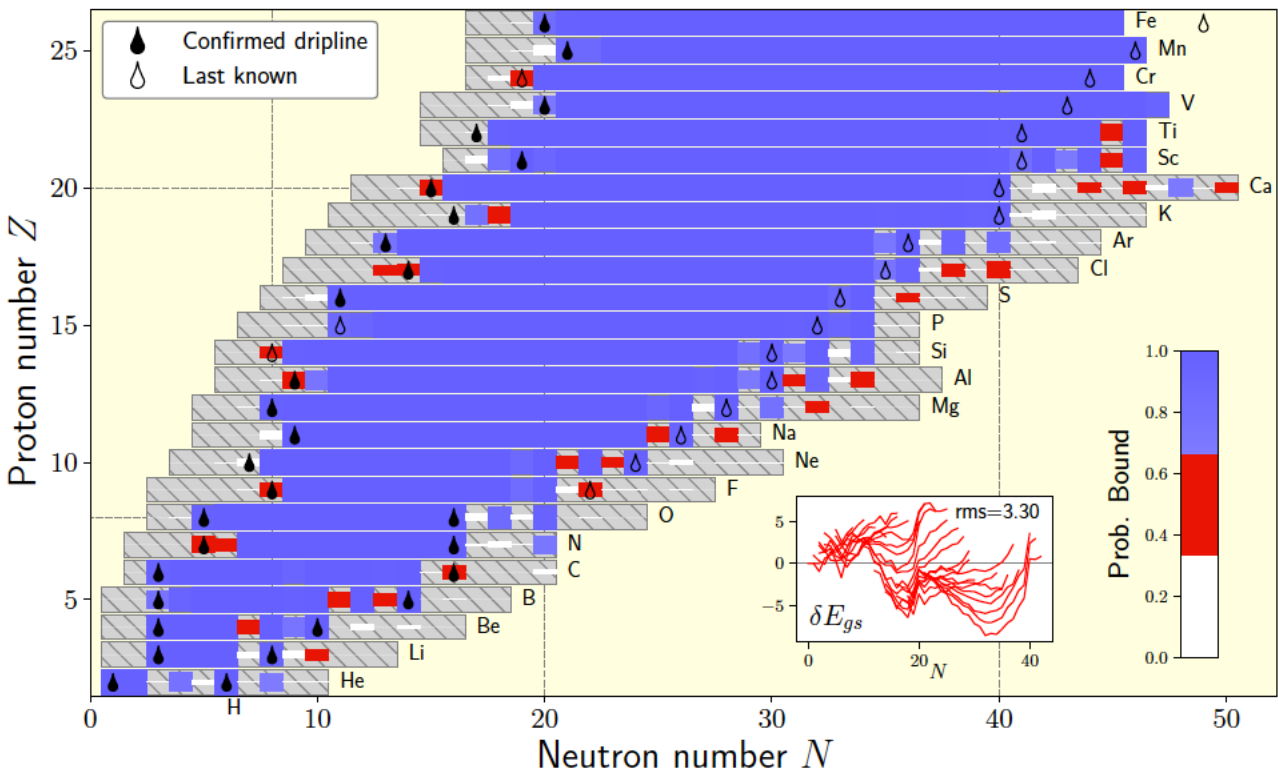
Limits of the nuclear landscape …
… coming within the limits of Hamiltonian-based methods

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

VOLUME 85, NUMBER 25 PHYSICAL REVIEW LETTERS 18 DECEMBER 2000

Neutron Radii in Nuclei and the Neutron Equation of State

B. Alex Brown

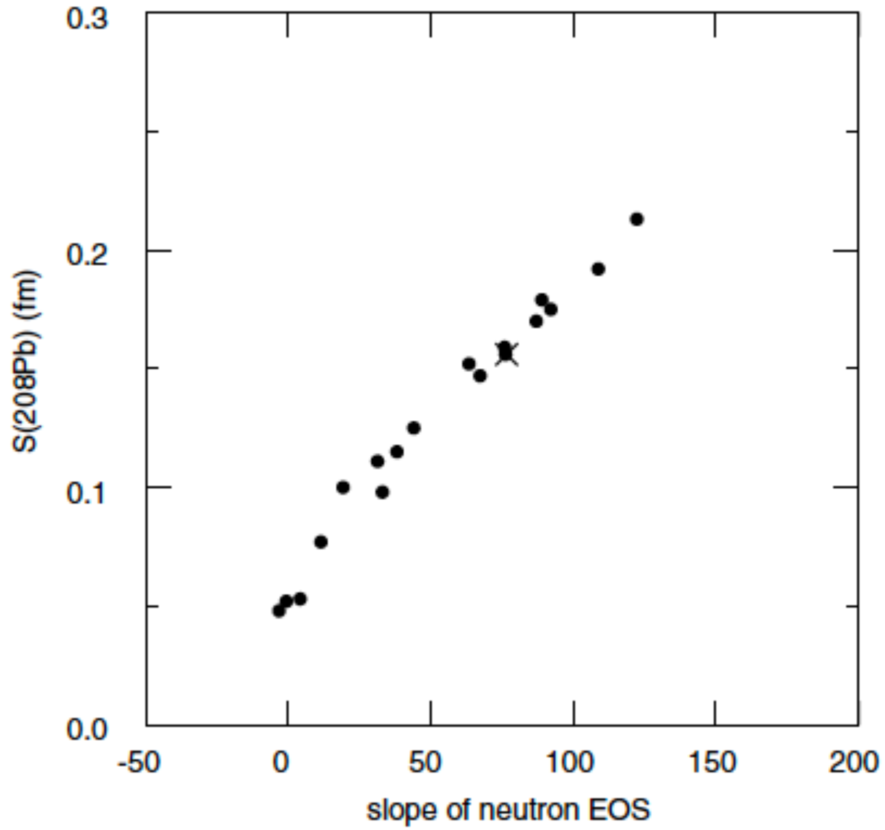
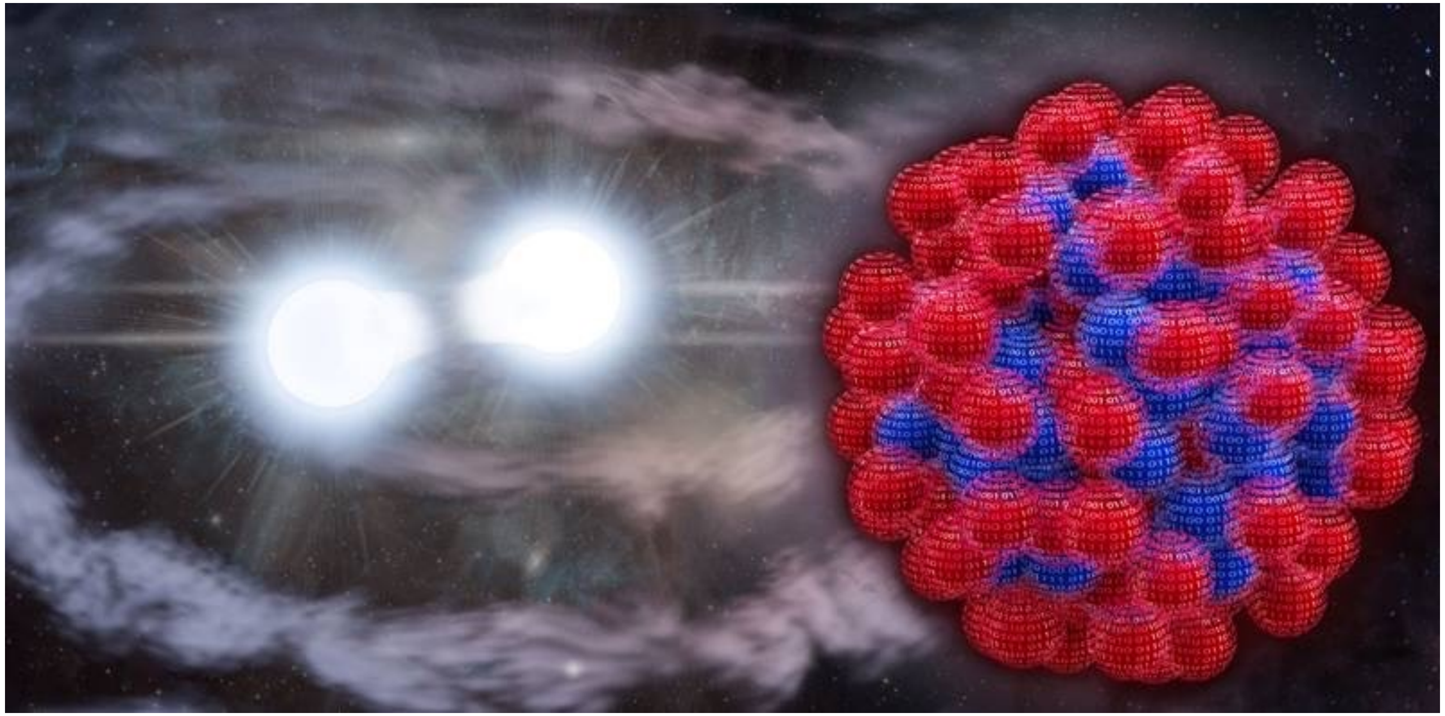
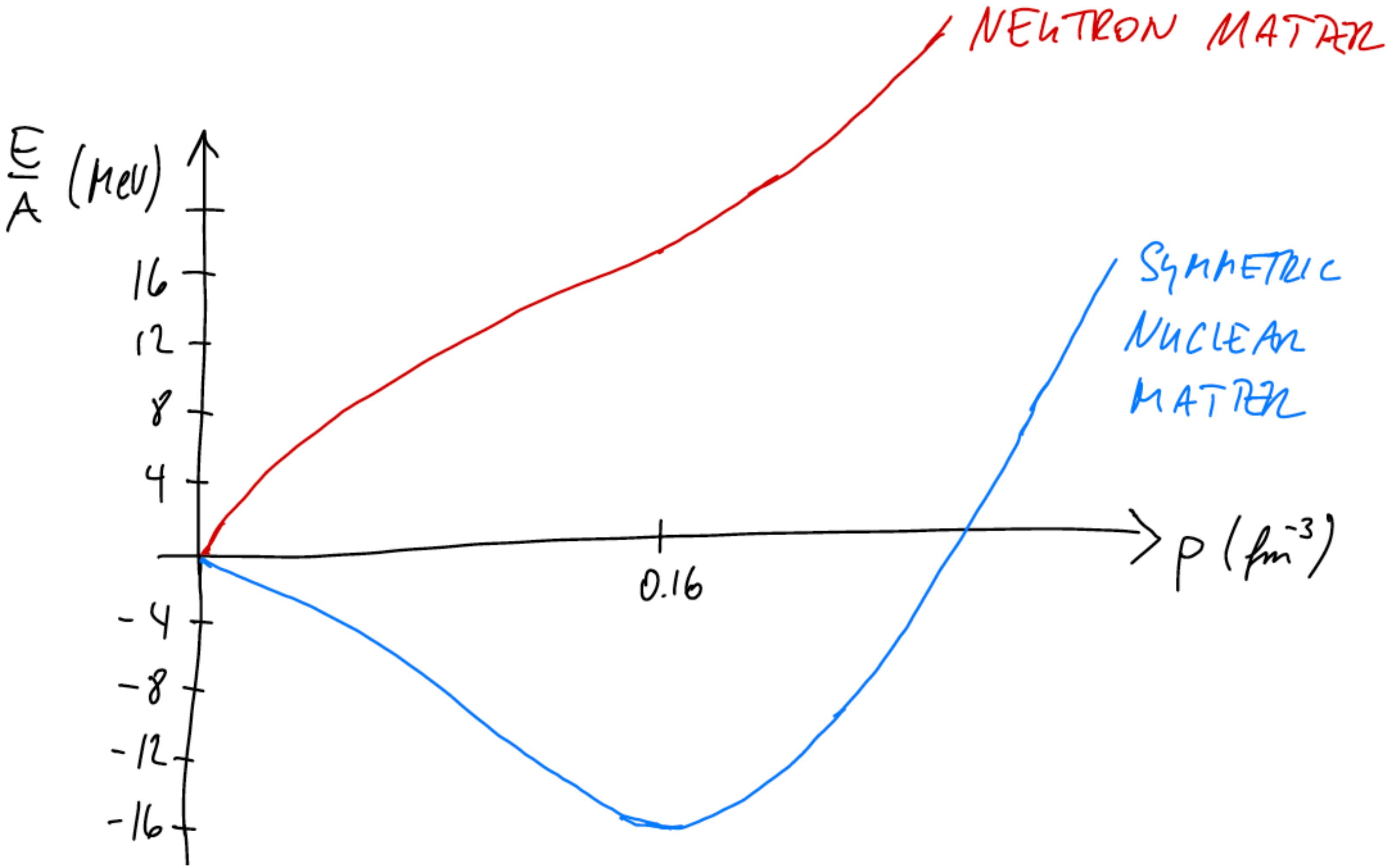


FIG. 3. The derivative of the neutron EOS at $\rho_n = 0.10$ neutron/fm^3 (in units of MeV fm^3/neutron) vs the S value in ^{208}Pb for 18 Skyrme parameter sets. The cross is SkX.



Credit: Andy Sproles, ORNL

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

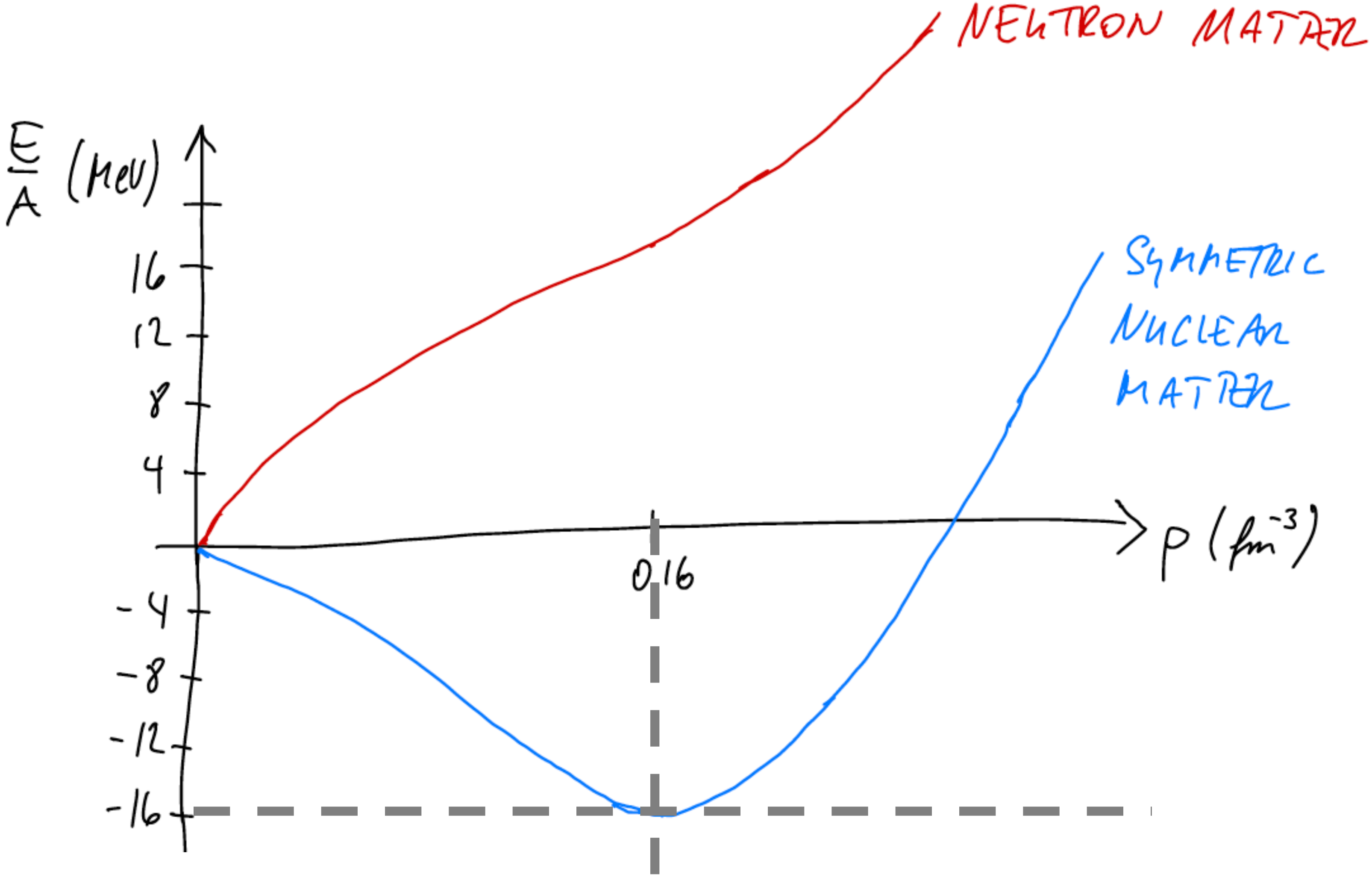


Pure neutron matter: $A = N$

Symmetric matter: $N = Z$

Note: Coulomb force neglected; electrons not included

Nuclear Equation of State



Pure neutron matter: $A = N$

Symmetric matter: $N = Z$

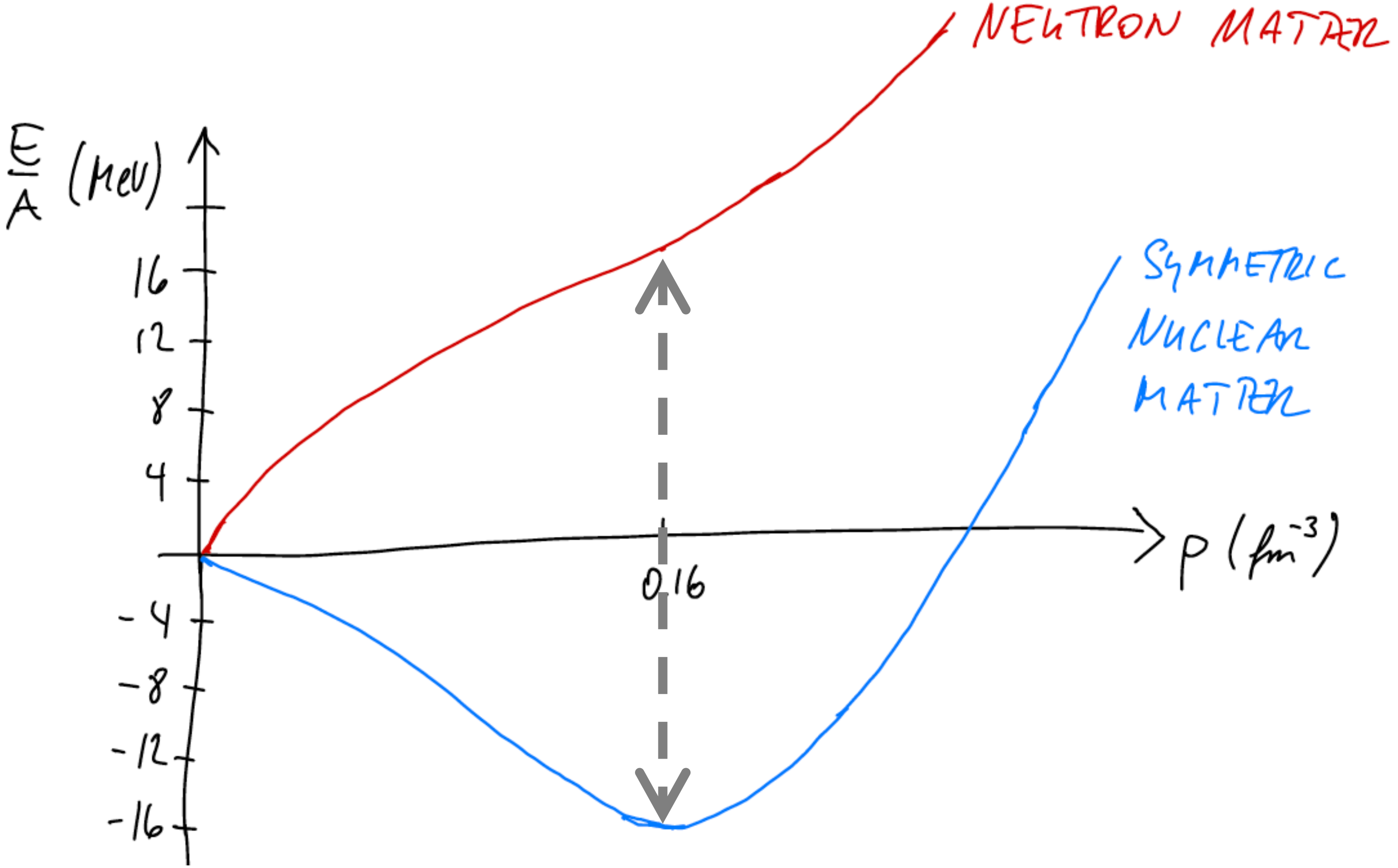
Note: Coulomb force neglected; electrons not included

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: $A = N$

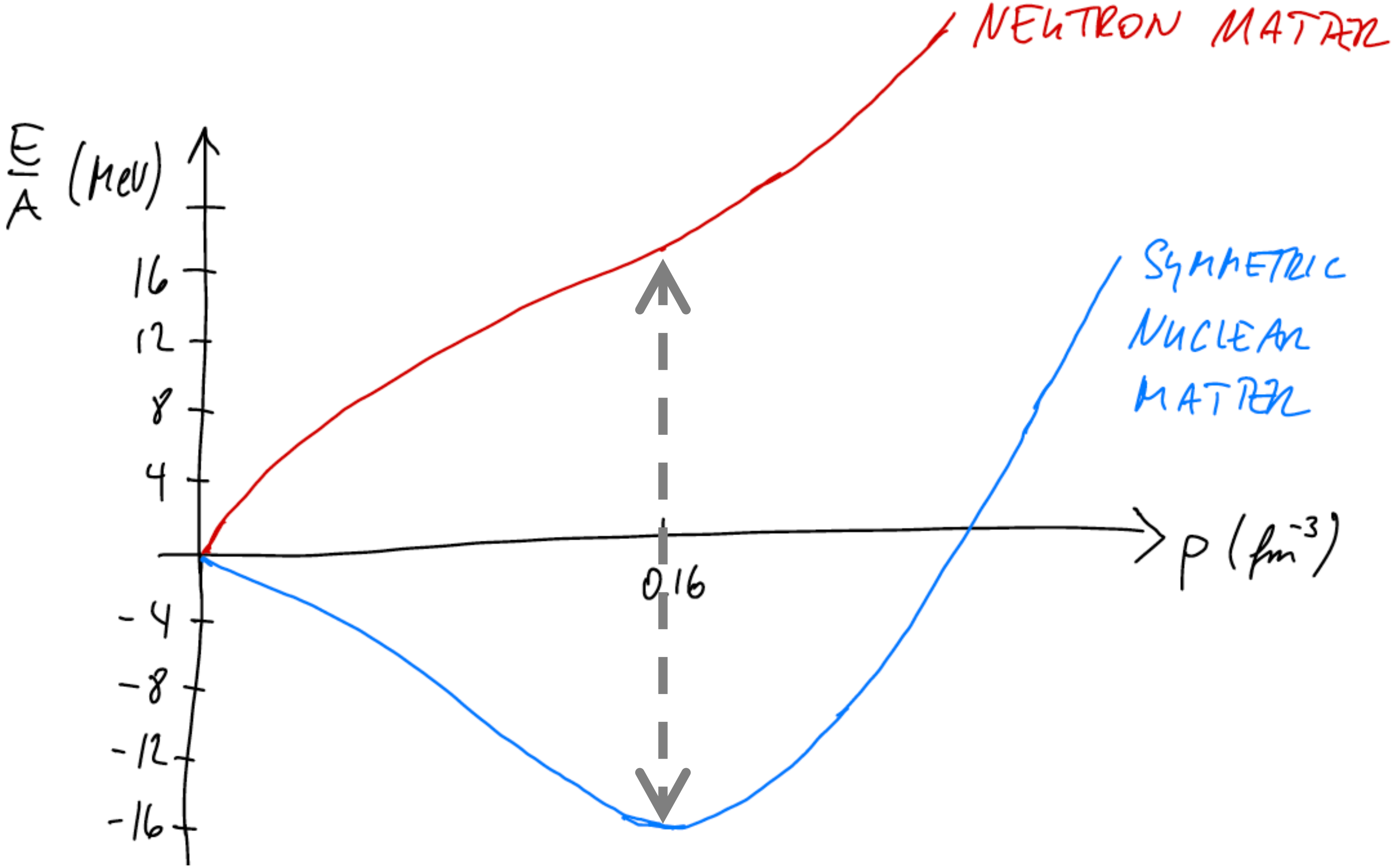
Symmetric matter: $N = Z$

Note: Coulomb force neglected; electrons not included

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

$E_{sym} \approx 32$ MeV

Nuclear Equation of State



Pure neutron matter: $A = N$

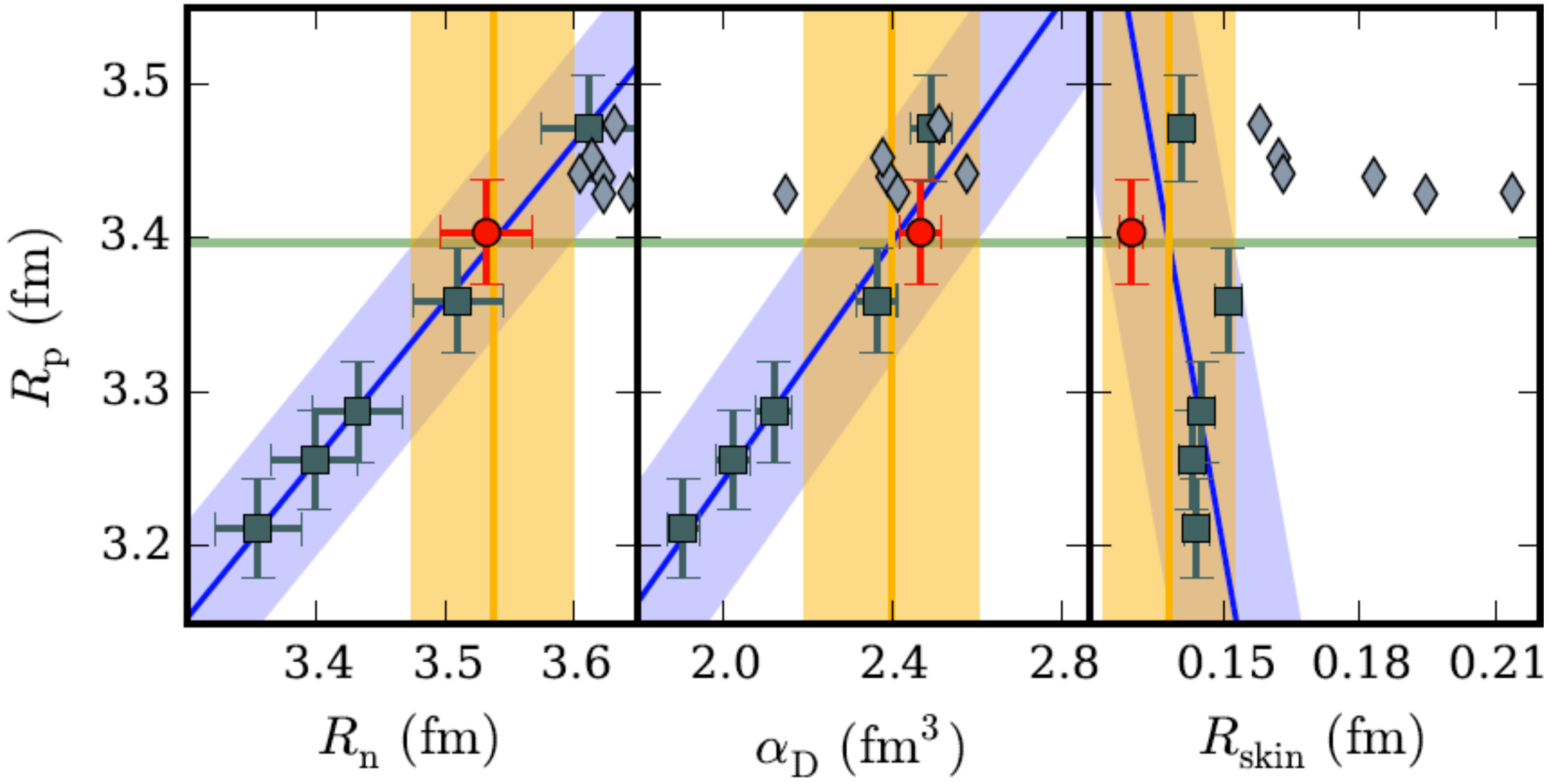
Symmetric matter: $N = Z$

Note: Coulomb force neglected; electrons not included

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

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

Neutron skin in ^{48}Ca

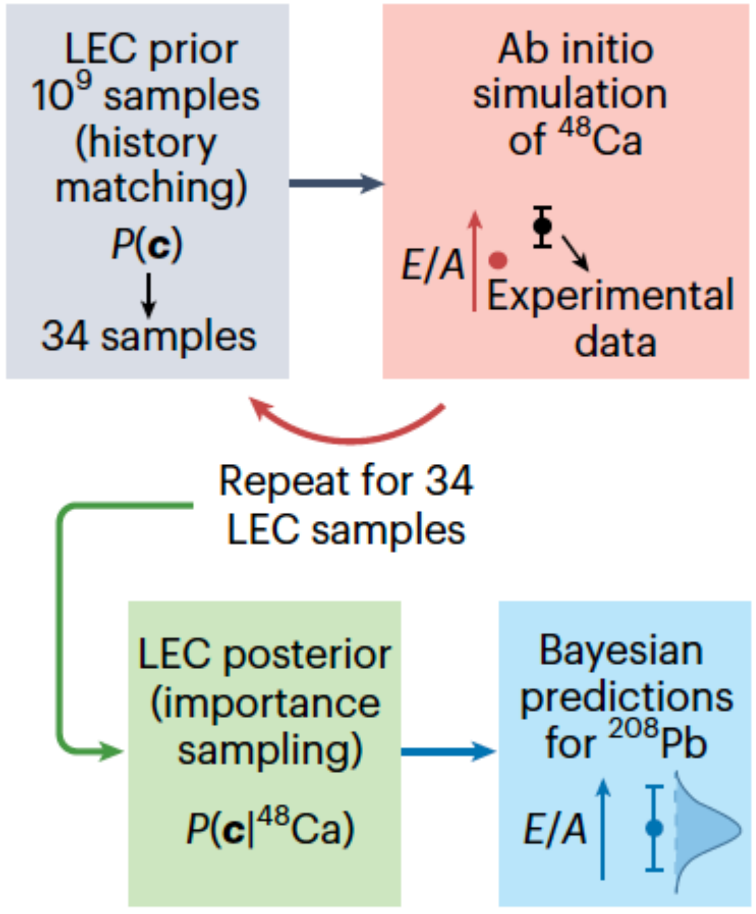


Uncertainty estimates from family of chiral interactions
[$NNLO_{sat}$, potentials by Hebeler *et al*. (2011), and DFT].

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

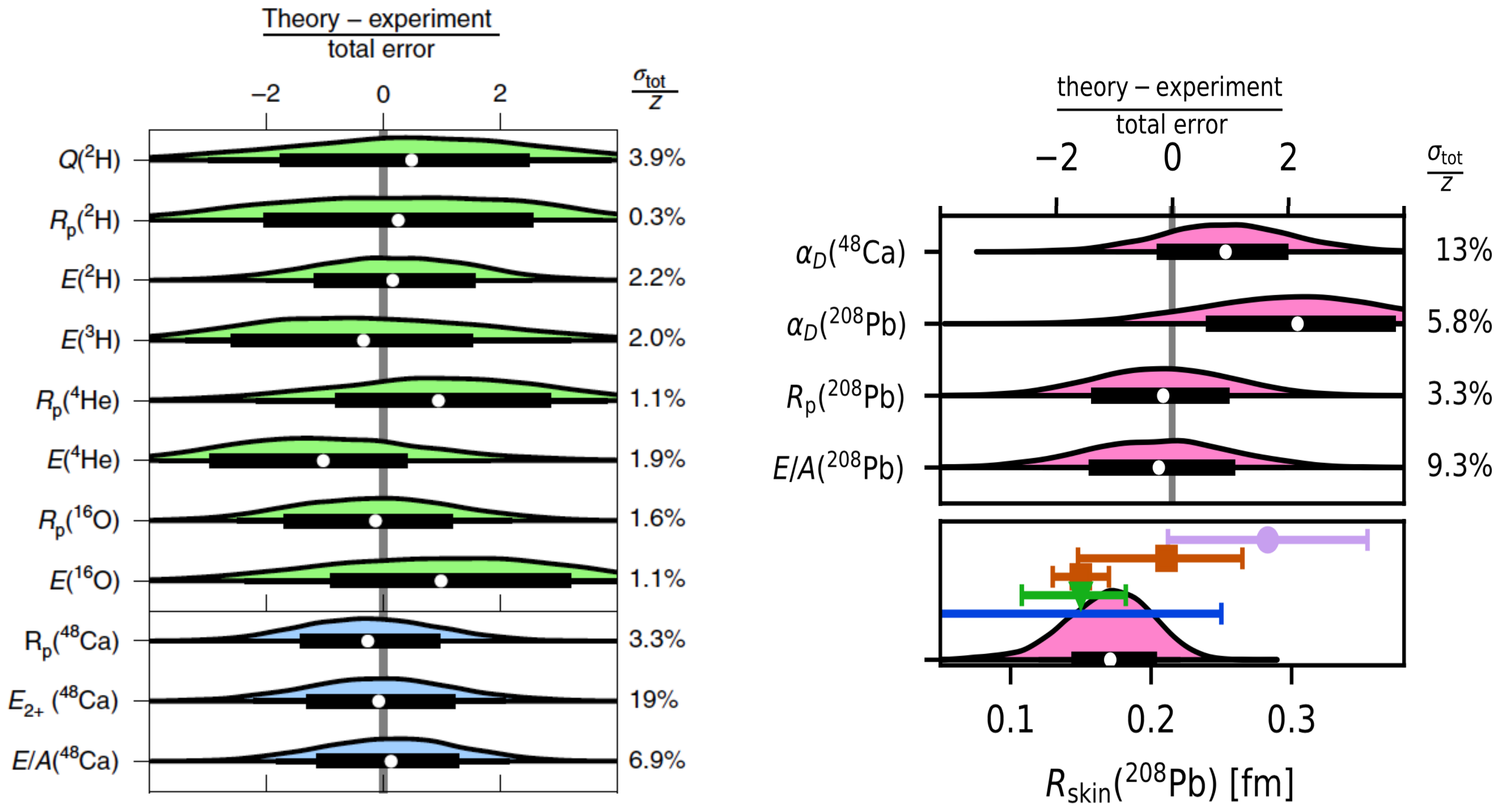
CREX, PREX, nuclear structure, and neutron stars

Uncertainty estimation in this work



Arnau Rios, Nature News & Views 2022

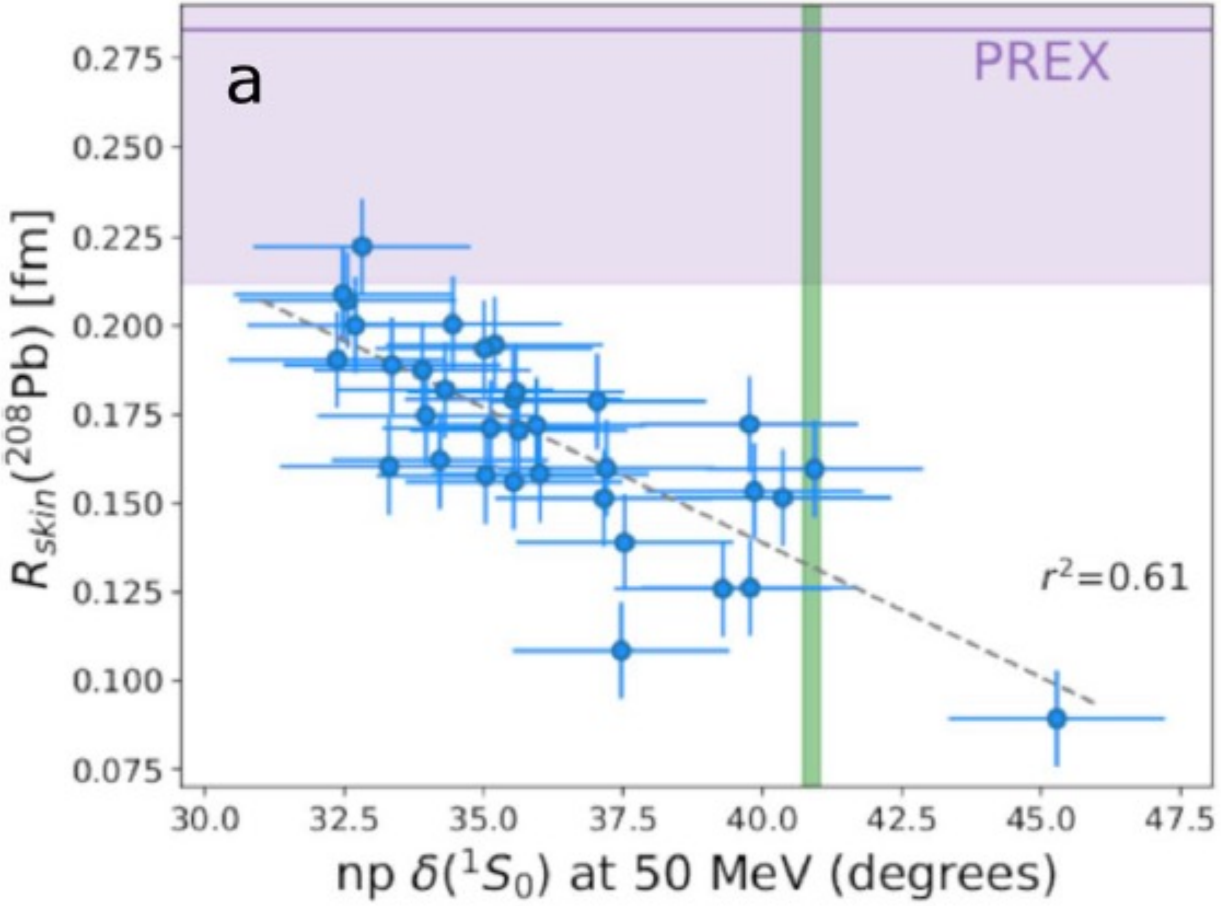
Emulators sieved through 10^8 EFT interactions; 34 non-implausible forces yield $R_{skin}(^{208}\text{Pb}) = 0.14 - 0.20$ fm



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…

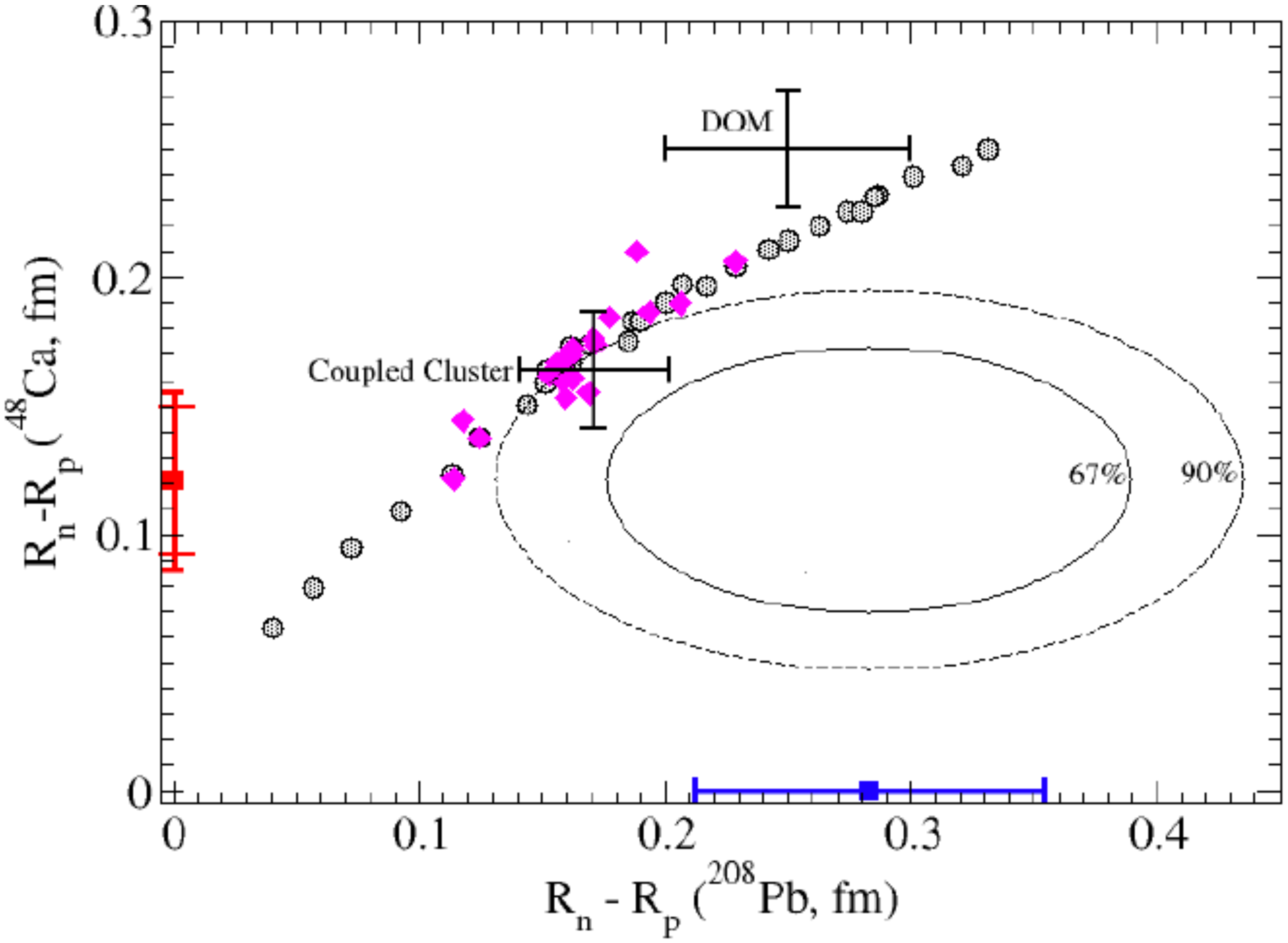
NN scattering precludes large neutron skins



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



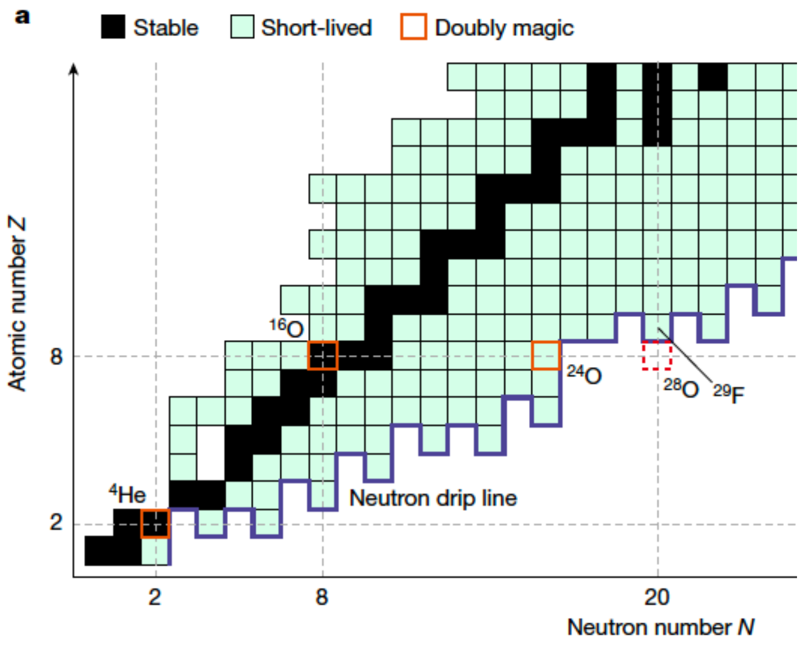
Adhikari et al., Phys. Rev. Lett. 129, 042501 (2022)

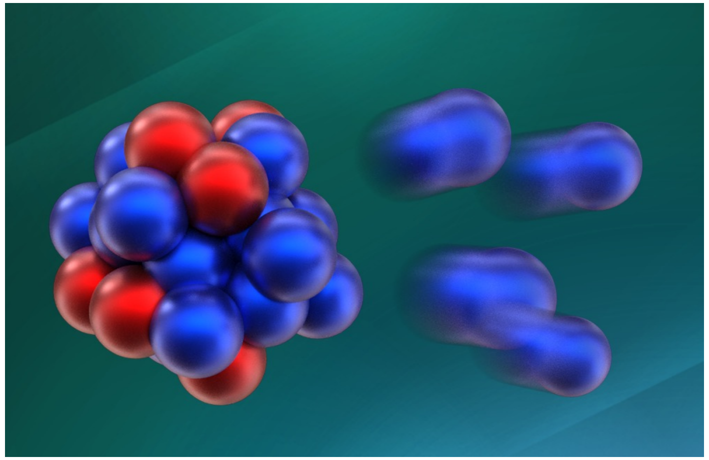
First observation of ^{28}O

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

A: It is not!

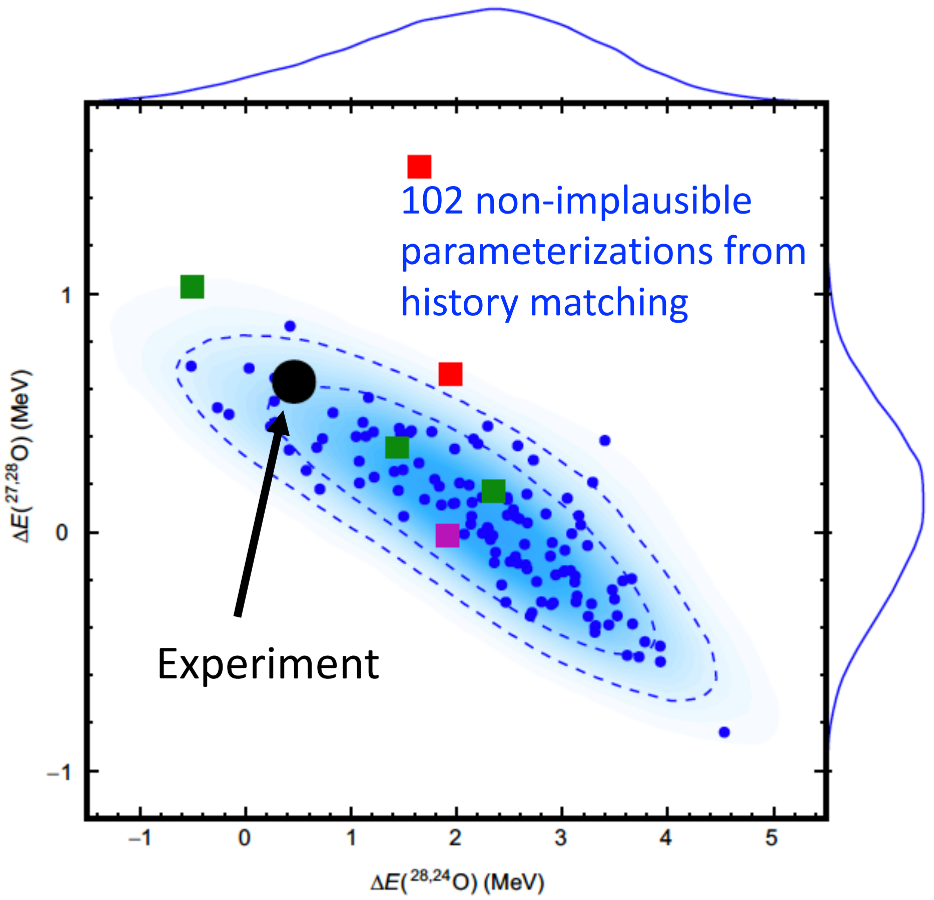
Kondo *et al*, Nature **620**, 965 (2023)





Credit: Andy Sproles, ORNL

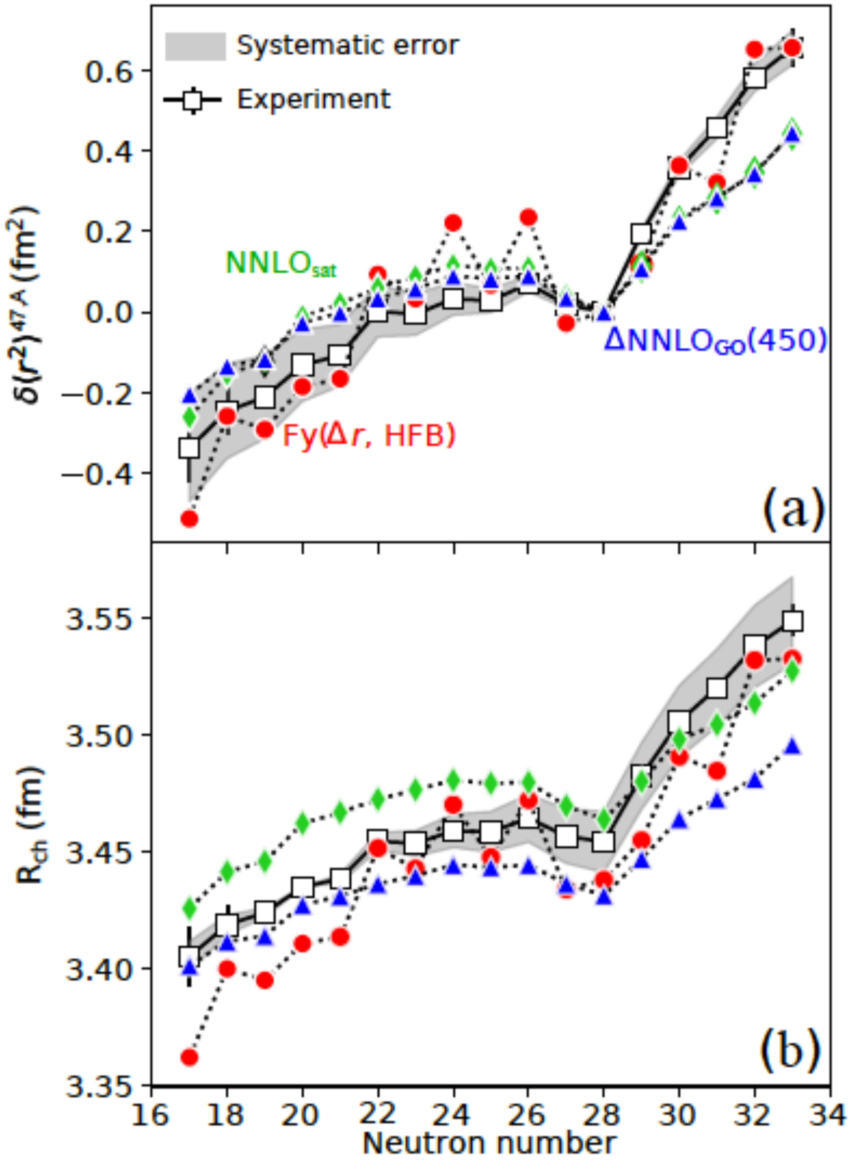
Interactions from chiral effective field theory show that ^{28}O is believed to be unbound with 98%.

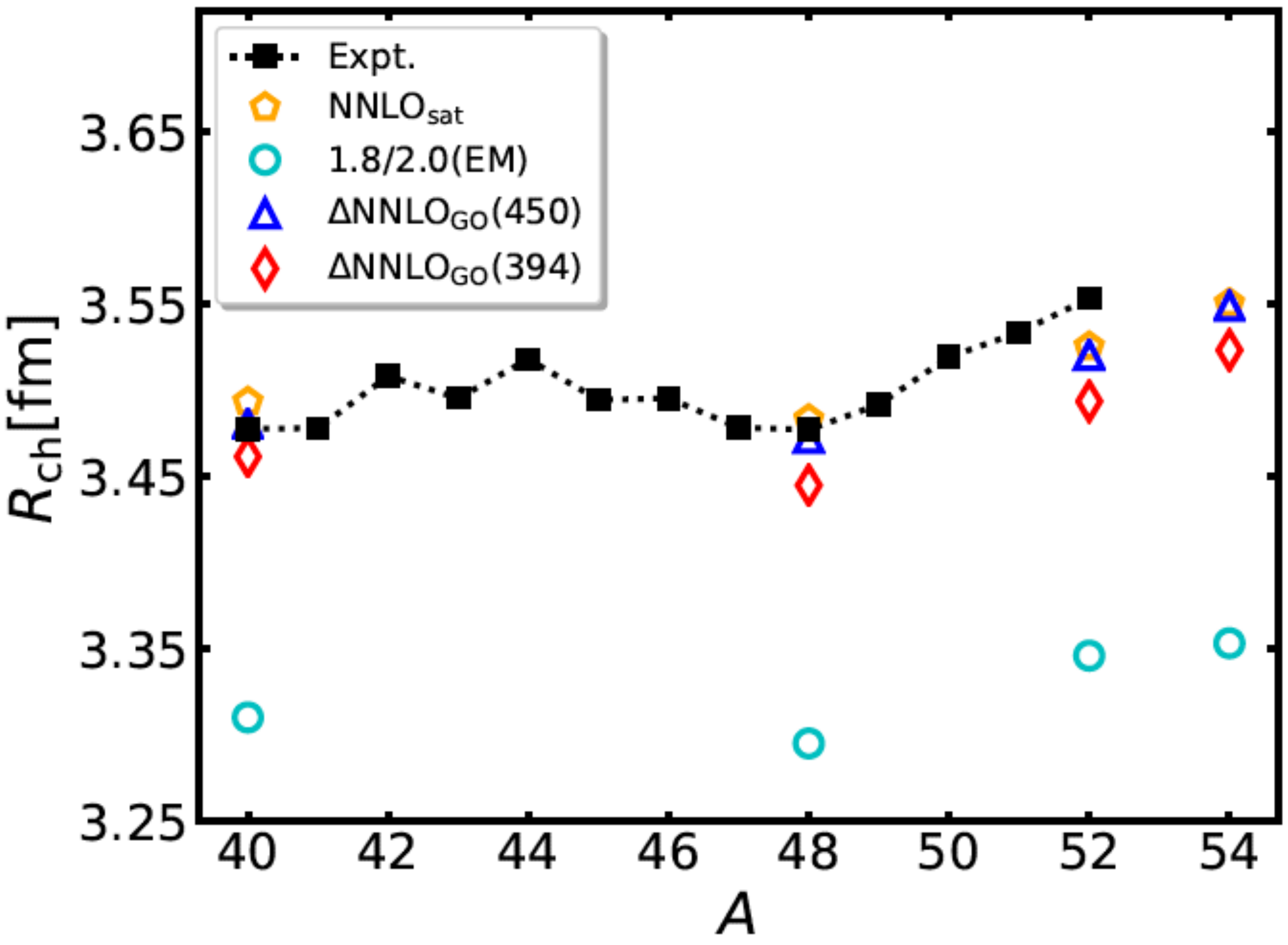


Challenges and open problems

(You might contribute to solving these ☺)

Challenges: Charge radii challenge nuclear theory





W.G. Jiang et al, arXiv:2006.16774

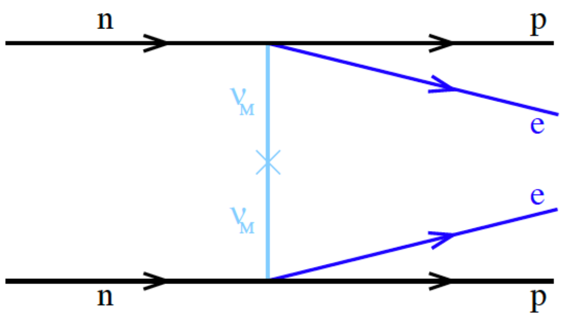
Sharp increase beyond N=28 not reproduced by EFT Hamiltonians

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

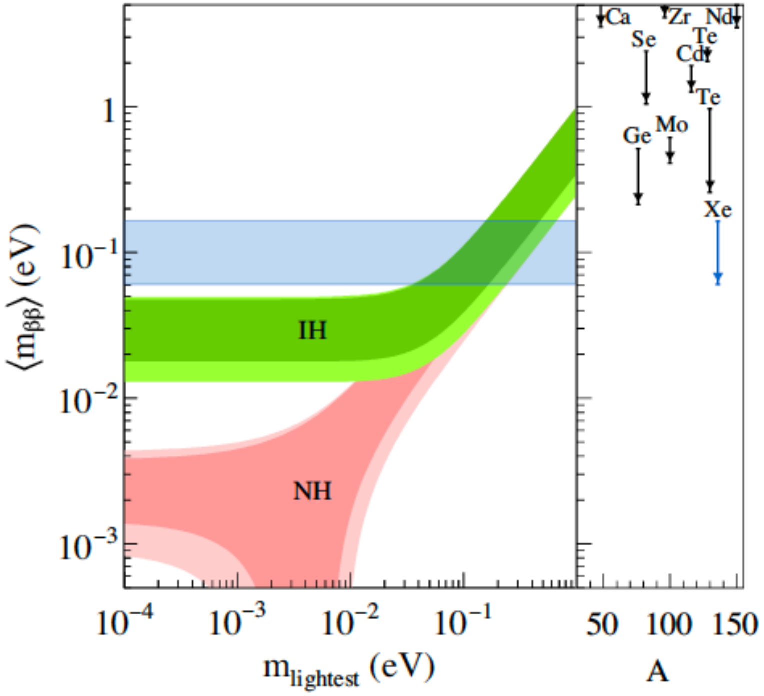
Challenges: Nuclear matrix element for neutrinoless $\beta\beta$ decay

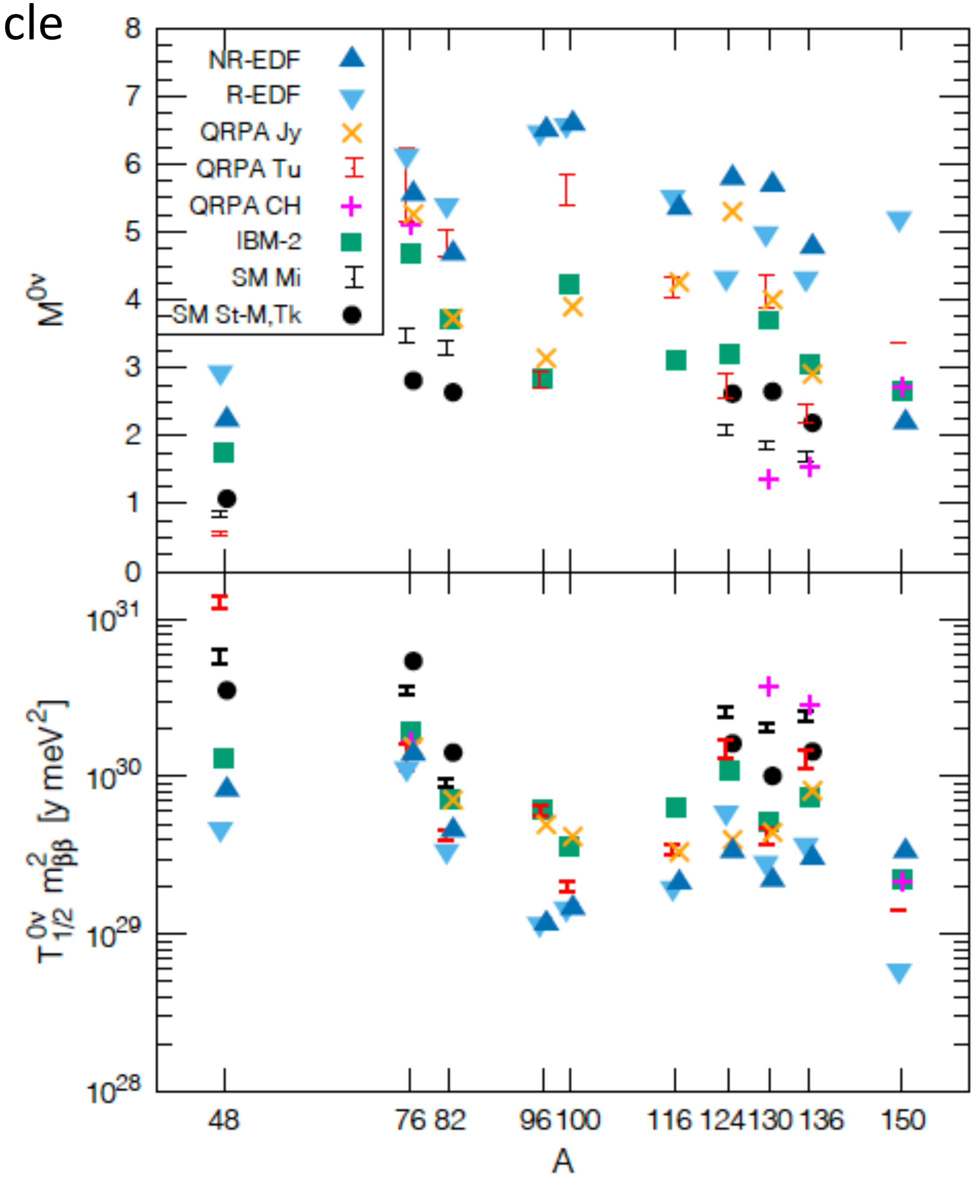
Hypothesis: The neutrino is a Majorana fermion, i.e. its own antiparticle
→ Search for neutrinoless $\beta\beta$ decay
Interest: Next-generation experiments will probe inverted hierarchy
Need: Nuclear matrix element to relate lifetime (if observed) to neutrino mass scale

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



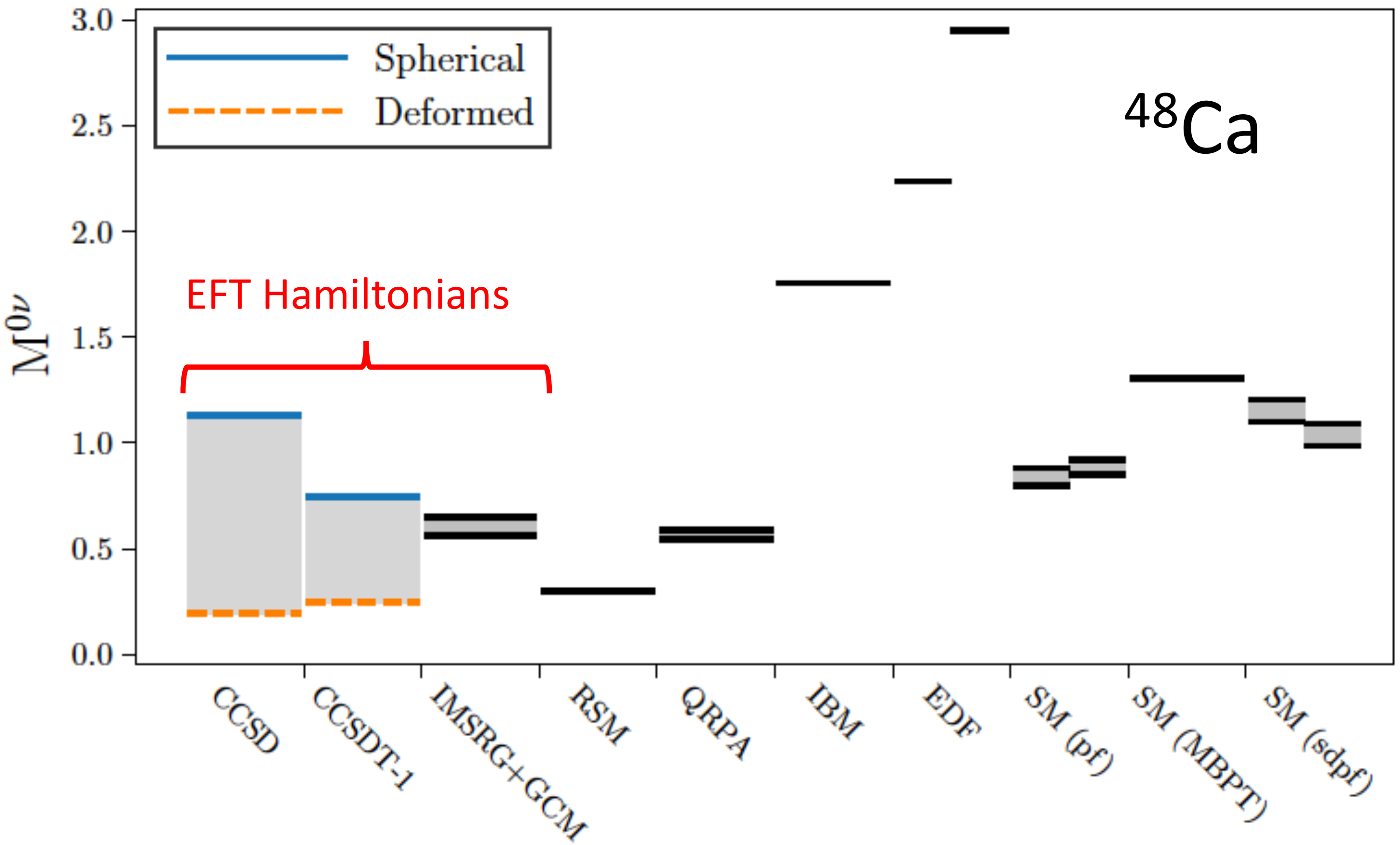
IH inverted hierarchy
NH normal hierarchy





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

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

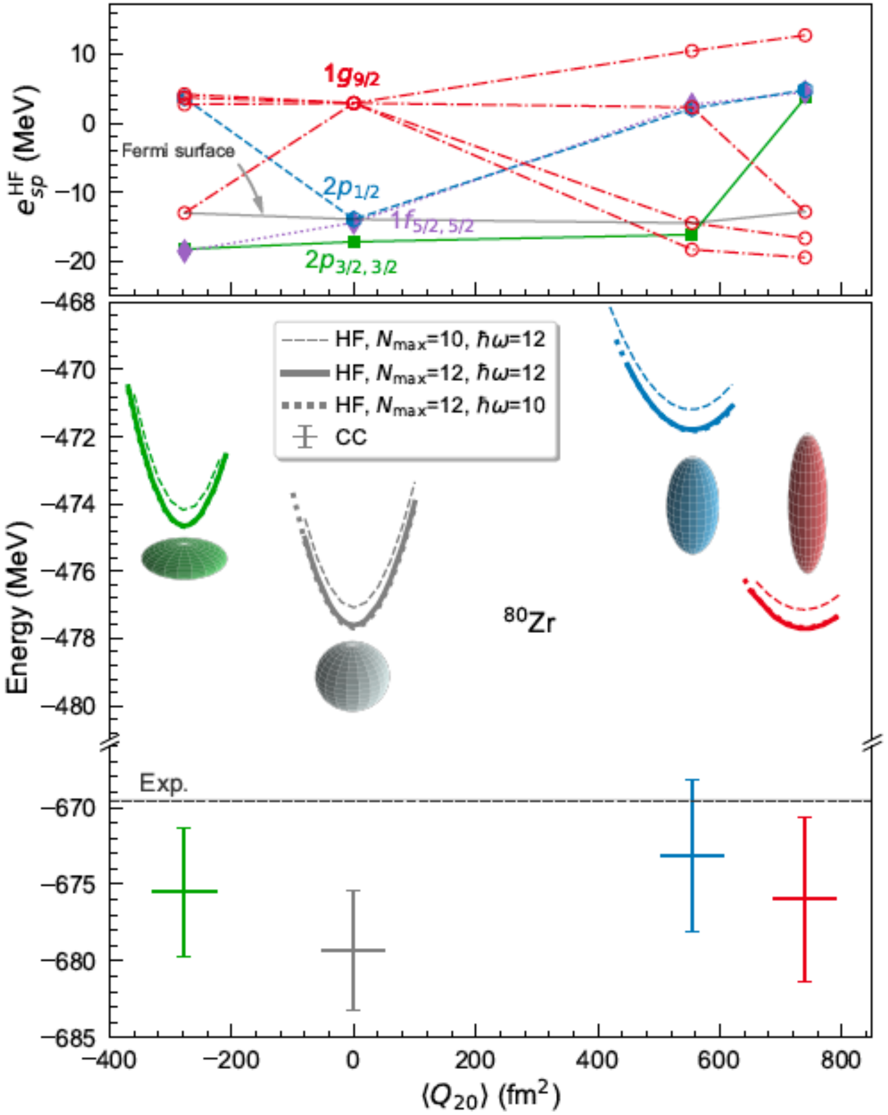


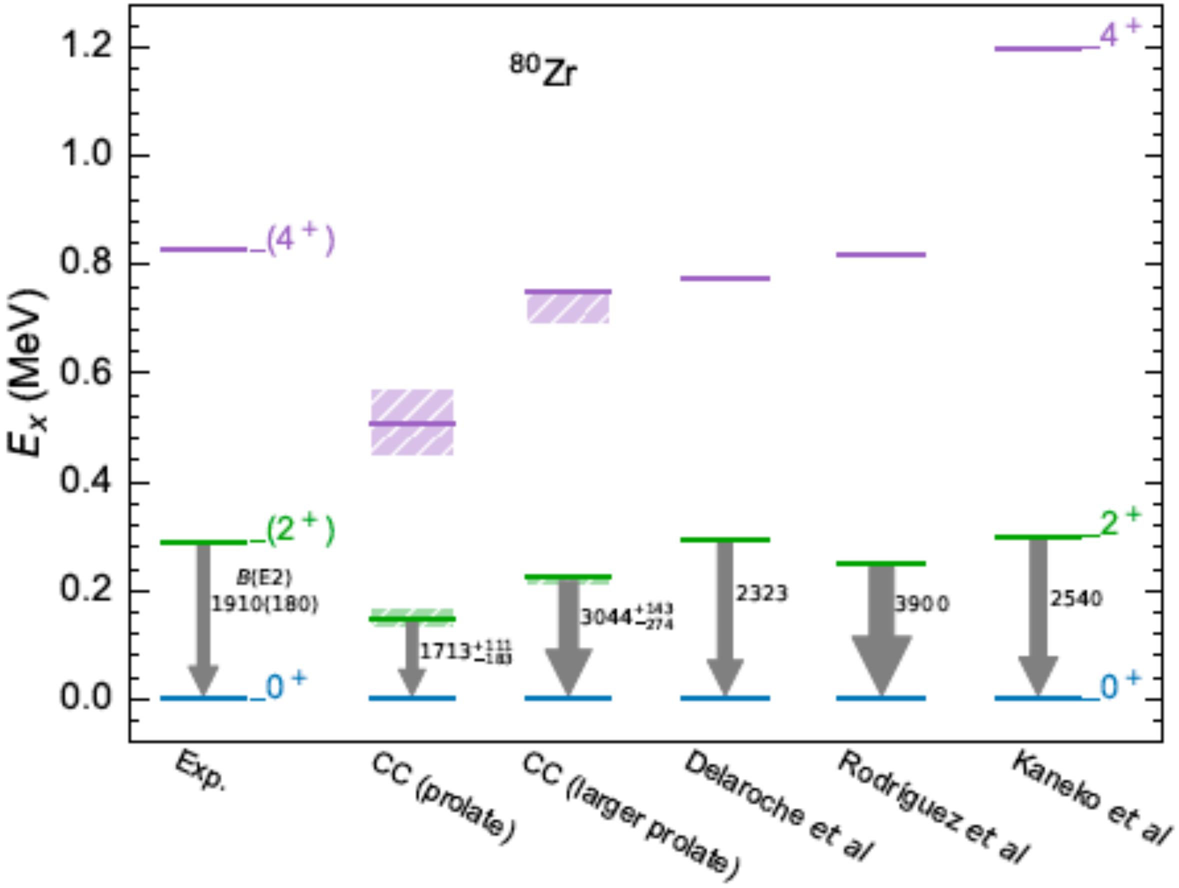
J. M. Yao et al., Phys. Rev. Lett. 124, 232501 (2020); arXiv:1908.05424.
S. J. Novario et al., Phys. Rev. Lett. 126, 182502 (2021); arXiv:2008.09696

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]

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!