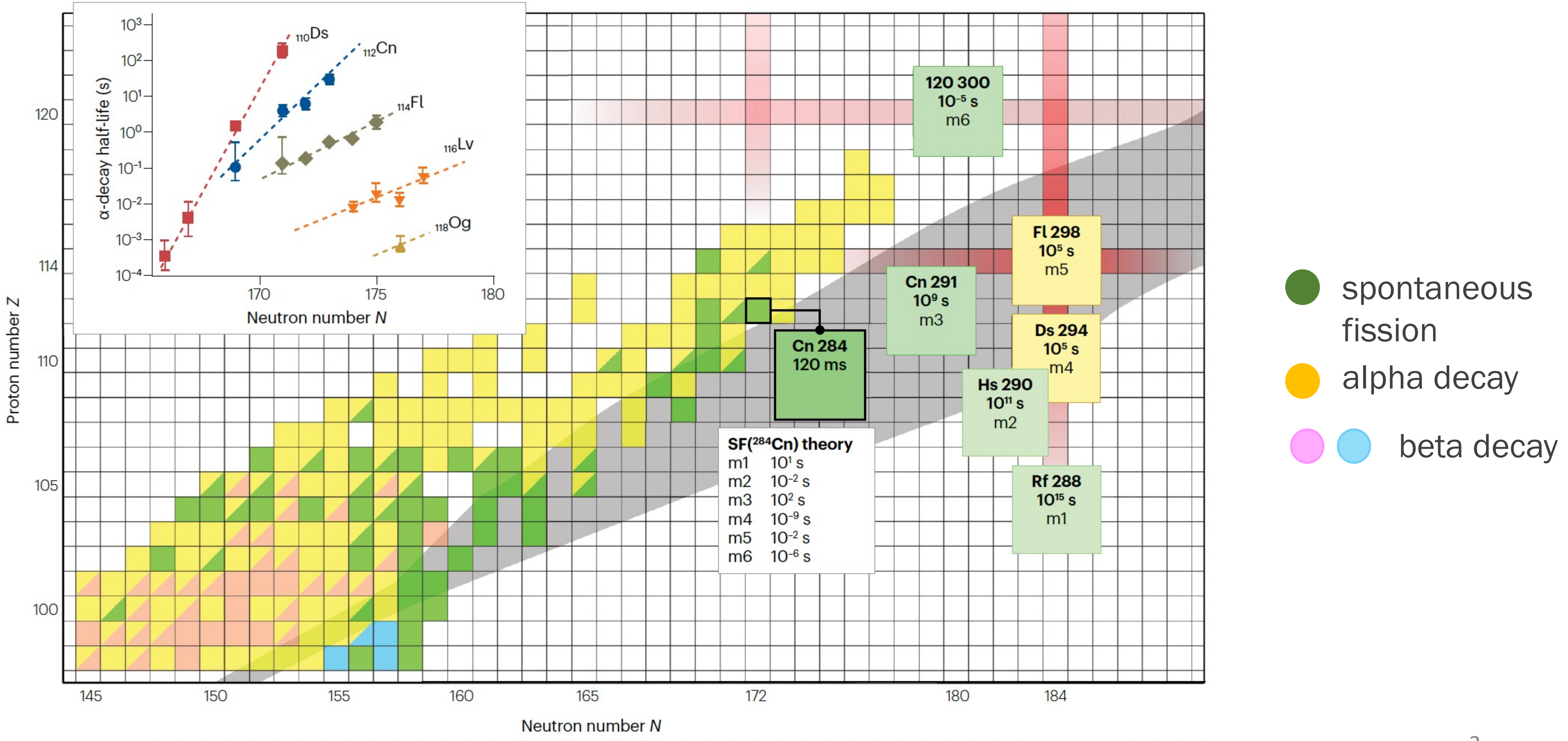
Putting nuclear Hamiltonians to the test: towards superheavy nuclei and real-time dynamics

FRANCESCA BONAITI, FRIB&ORNL

WORKSHOP ON "NUCLEAR HAMILTONIANS FOR ADVANCING NUCLEAR PHYSICS AND BEYOND" @ INT, SEATTLE, WA

MAY 13, 2026

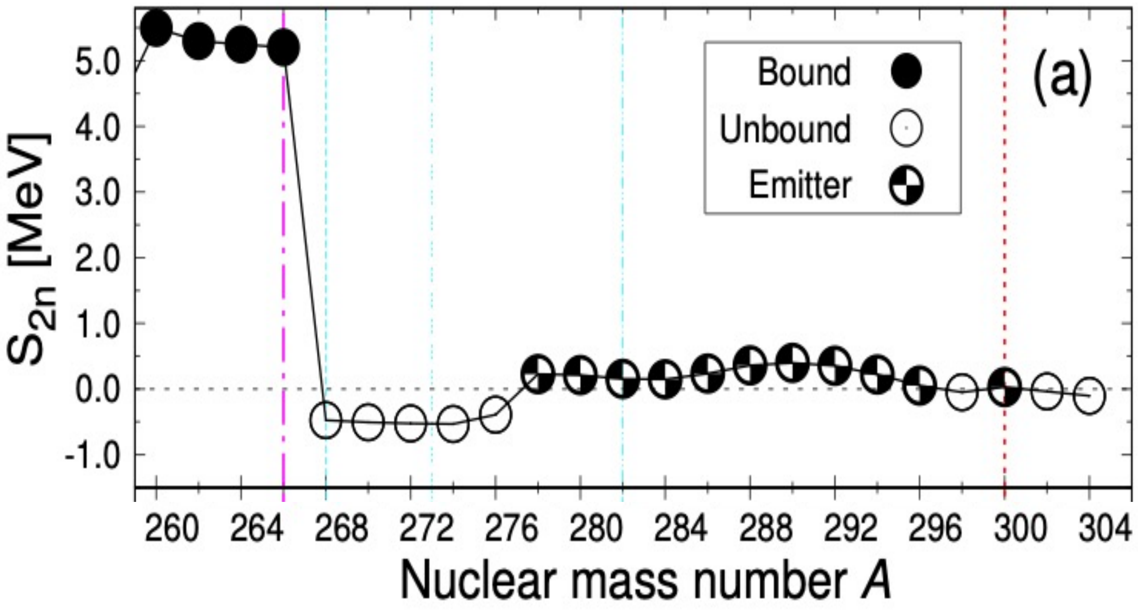
Searches for the "island of stability"



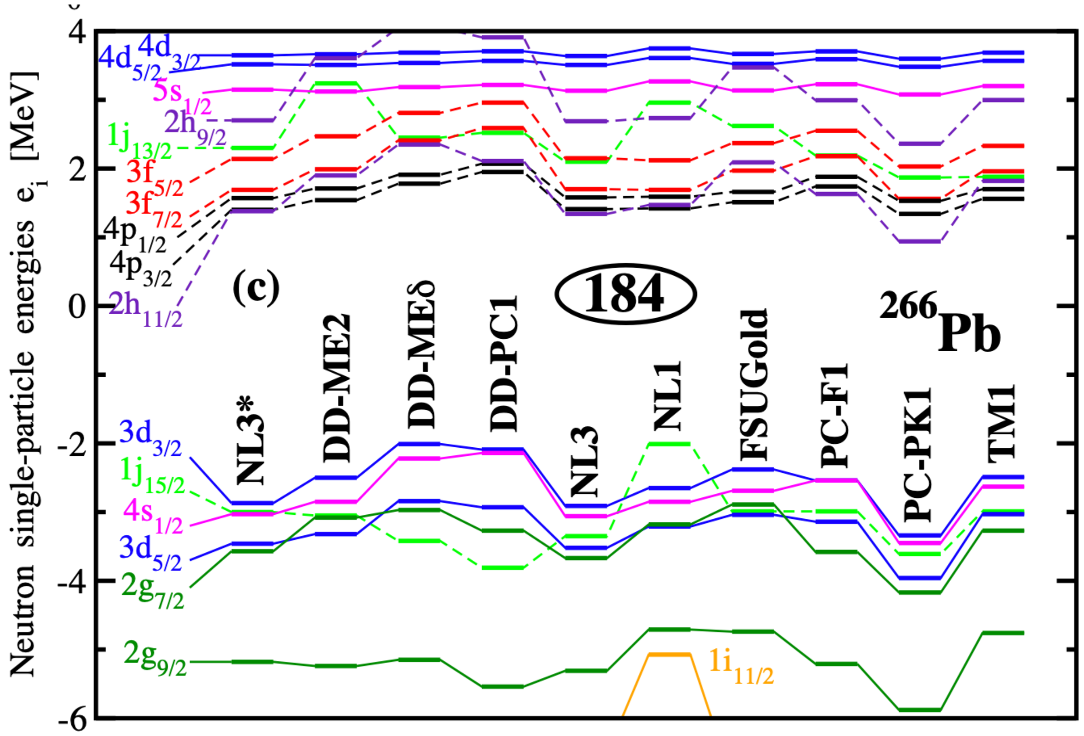
O. Smits et al, Nature Review Physics **6**, 86–98 (2024).

What is the next shell closure we find beyond ^{208}Pb?

A possible candidate: ^{266}Pb



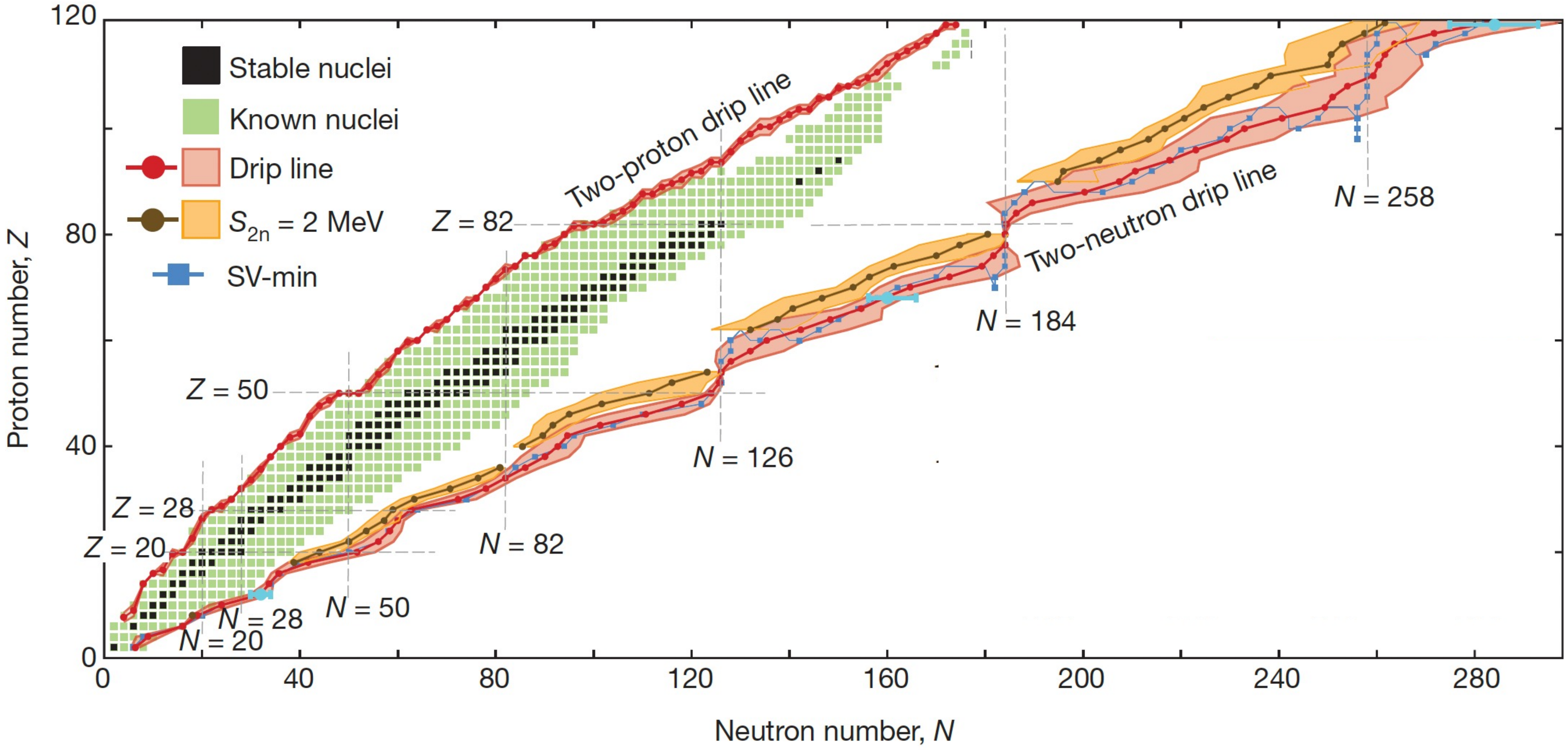
S. Kim et al, PRC 105, 034340 (2022).



A. Afanasjev et al, PRC 91, 014324 (2015).

Separation energies and single-particle energies results from mean-field calculations indicate possible doubly-magic nature of ^{266}Pb.

^{266}Pb could be the last bound lead isotope

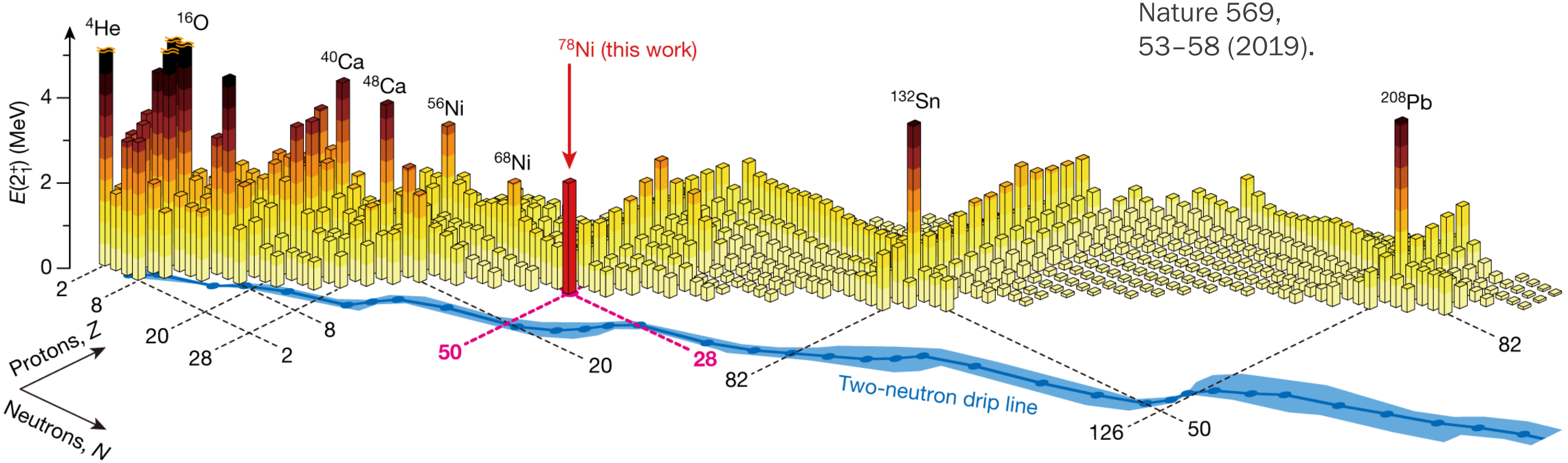


J. Erler et al, Nature 486, 1075–1079 (2024).

We can now tackle these questions from an *ab initio* perspective!

“Doubly magic” signatures: the first 2^+ state

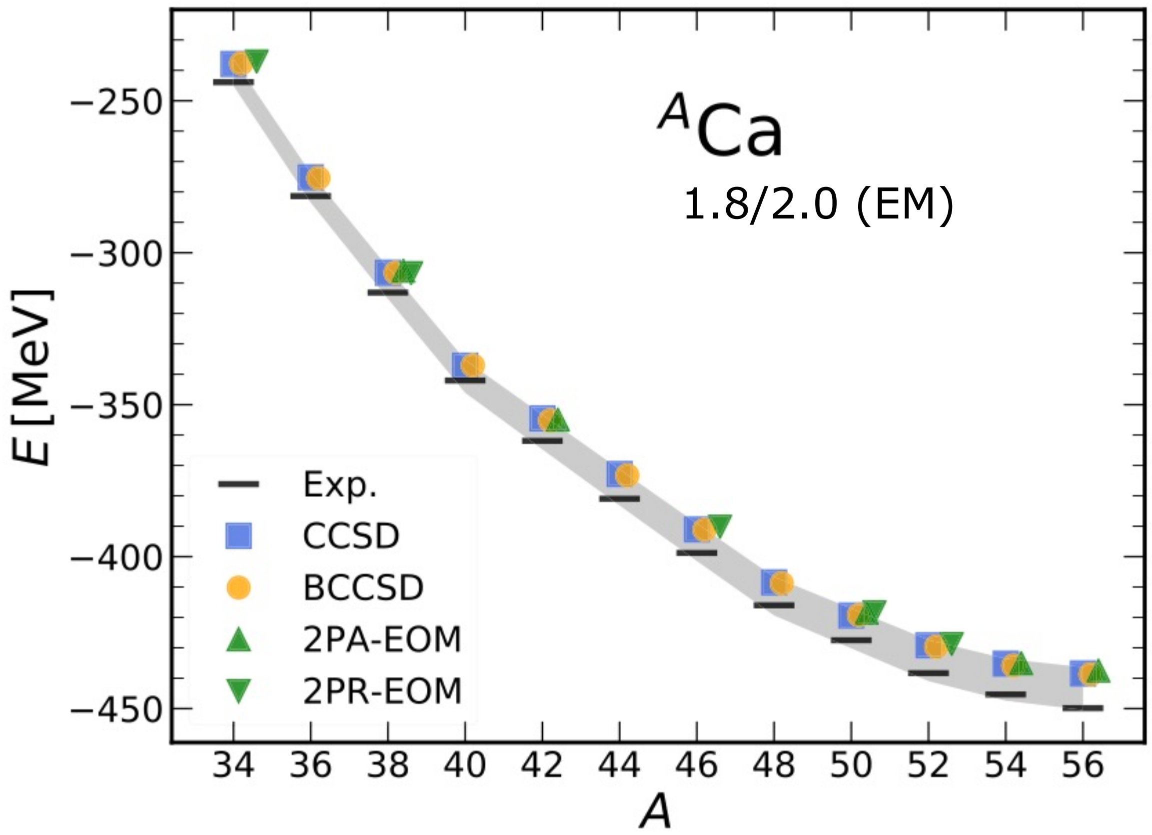
R. Taniuchi et al, Nature 569, 53–58 (2019).

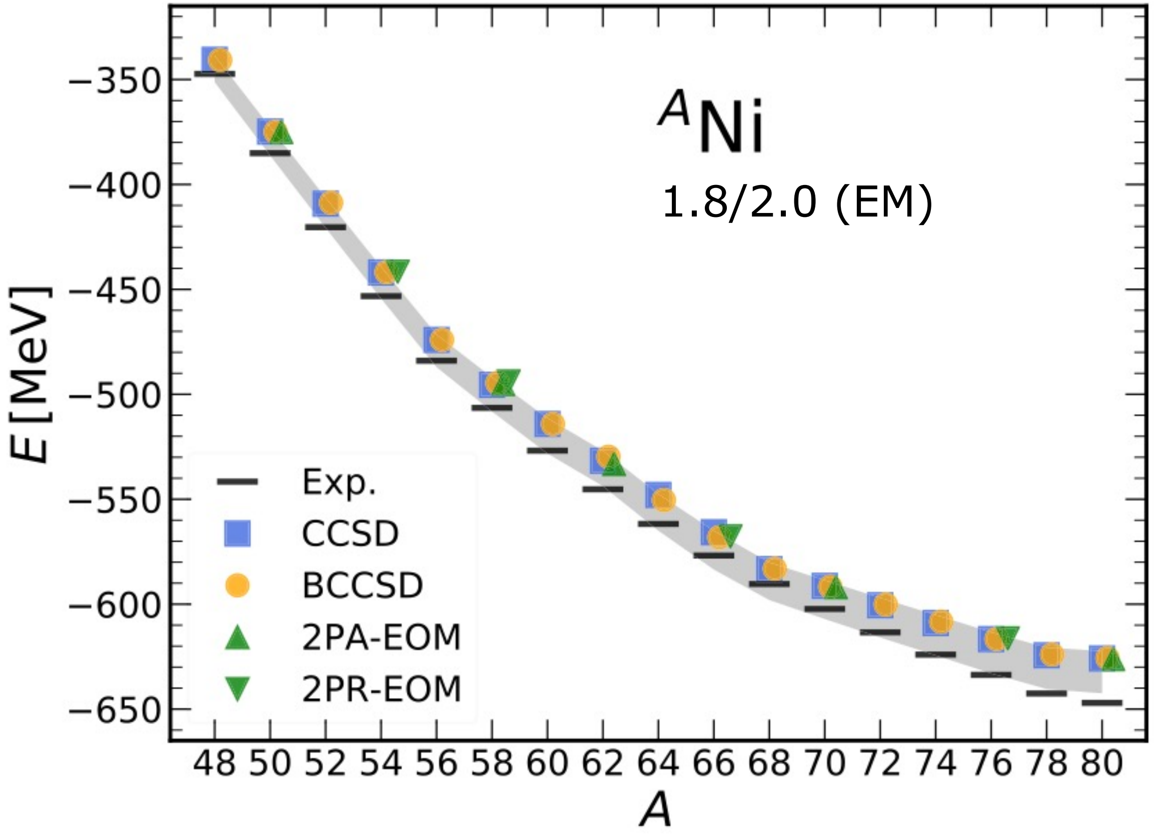


Goal: predicting the excited spectrum of ^{266}Pb using a nuclear Hamiltonian from chiral EFT and a systematically improvable many-body method (coupled-cluster theory).

A pragmatic choice

F. Marino, **FB,** et al, PRC 113, 044301 (2026).

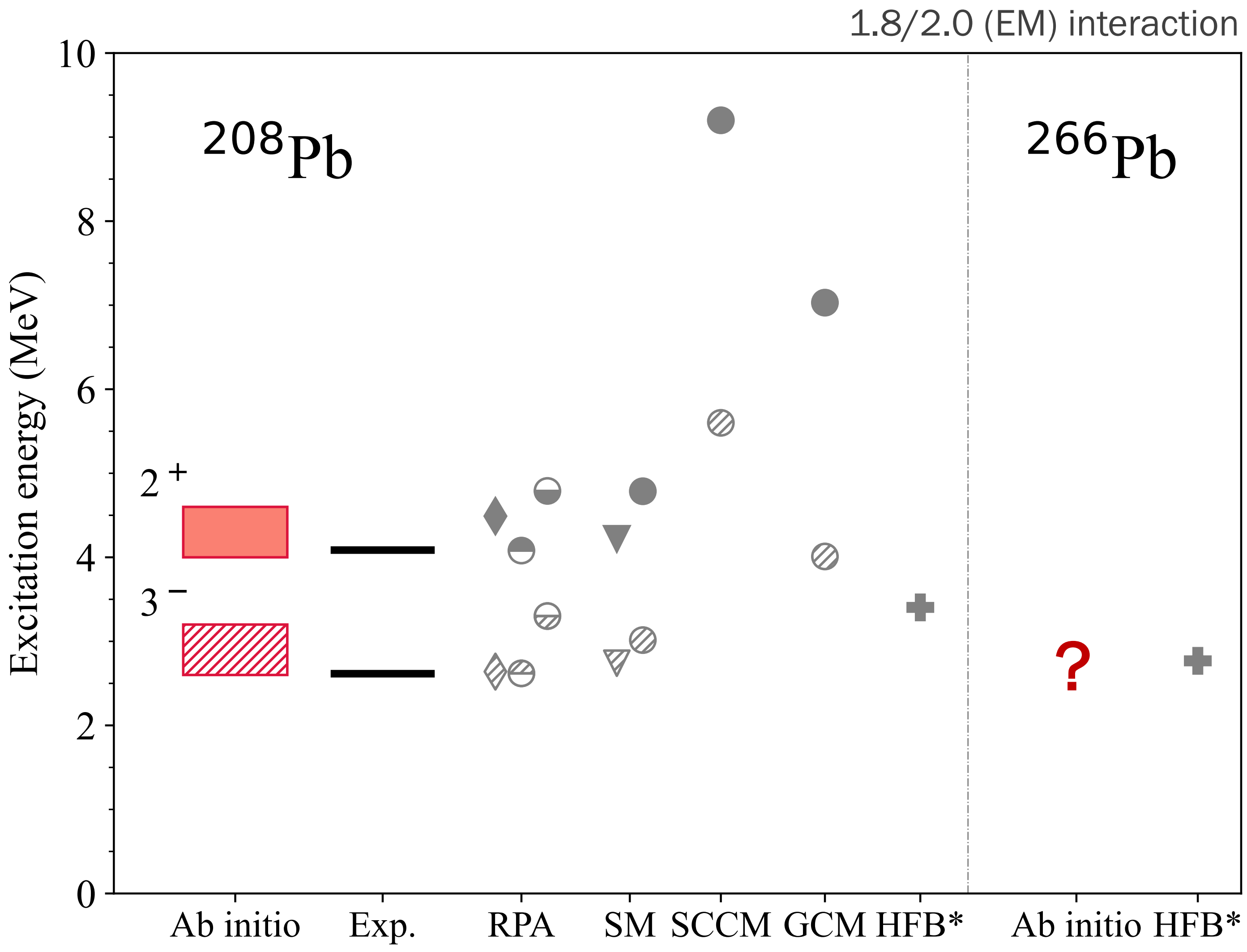




We choose the 1.8/2.0 (EM) interaction, which describes well ground-state energies and excited spectra in closed-shell nuclei, despite conceptual&UQ limitations.

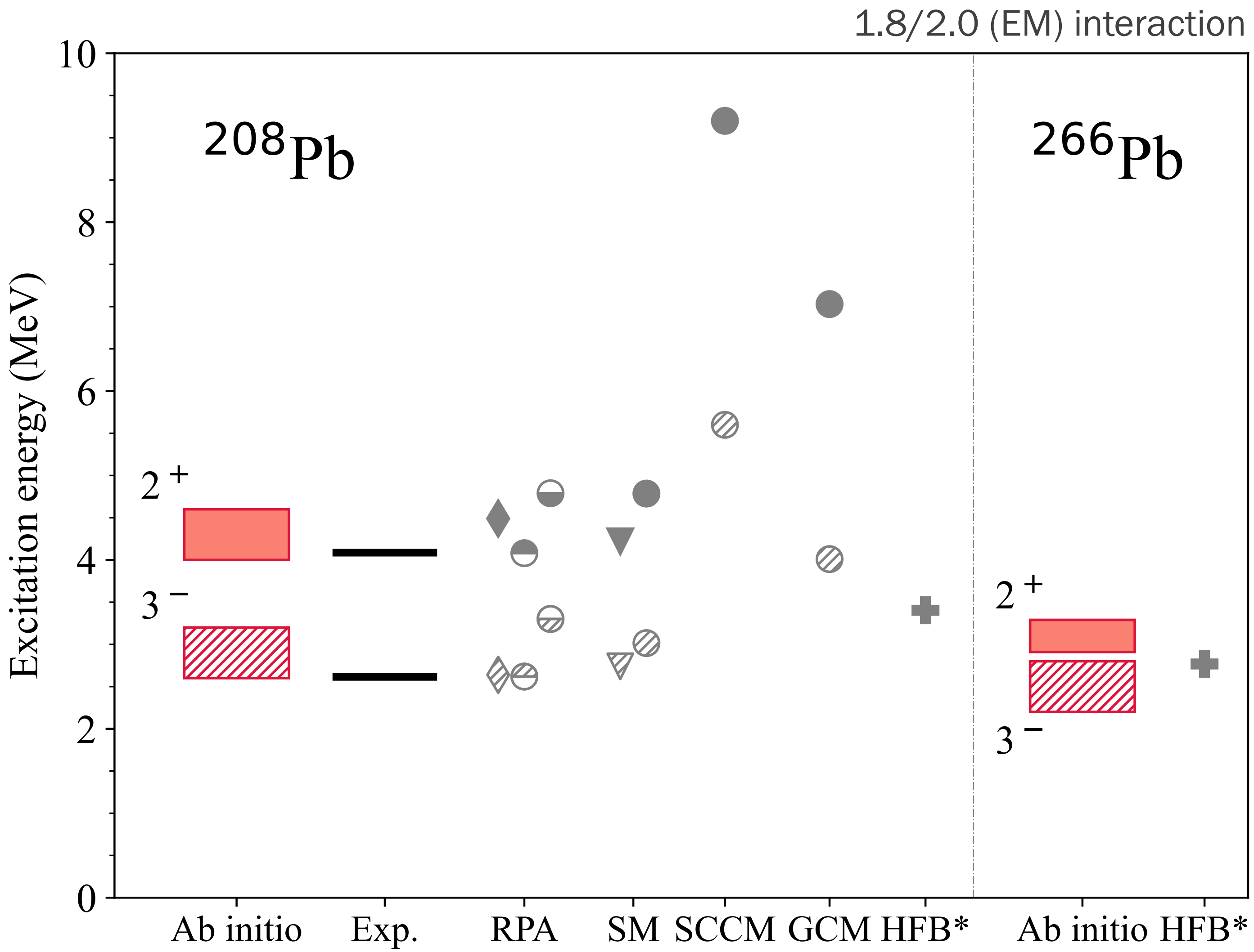
see Matthias Heinz's talk

Excited states in ^{208}Pb



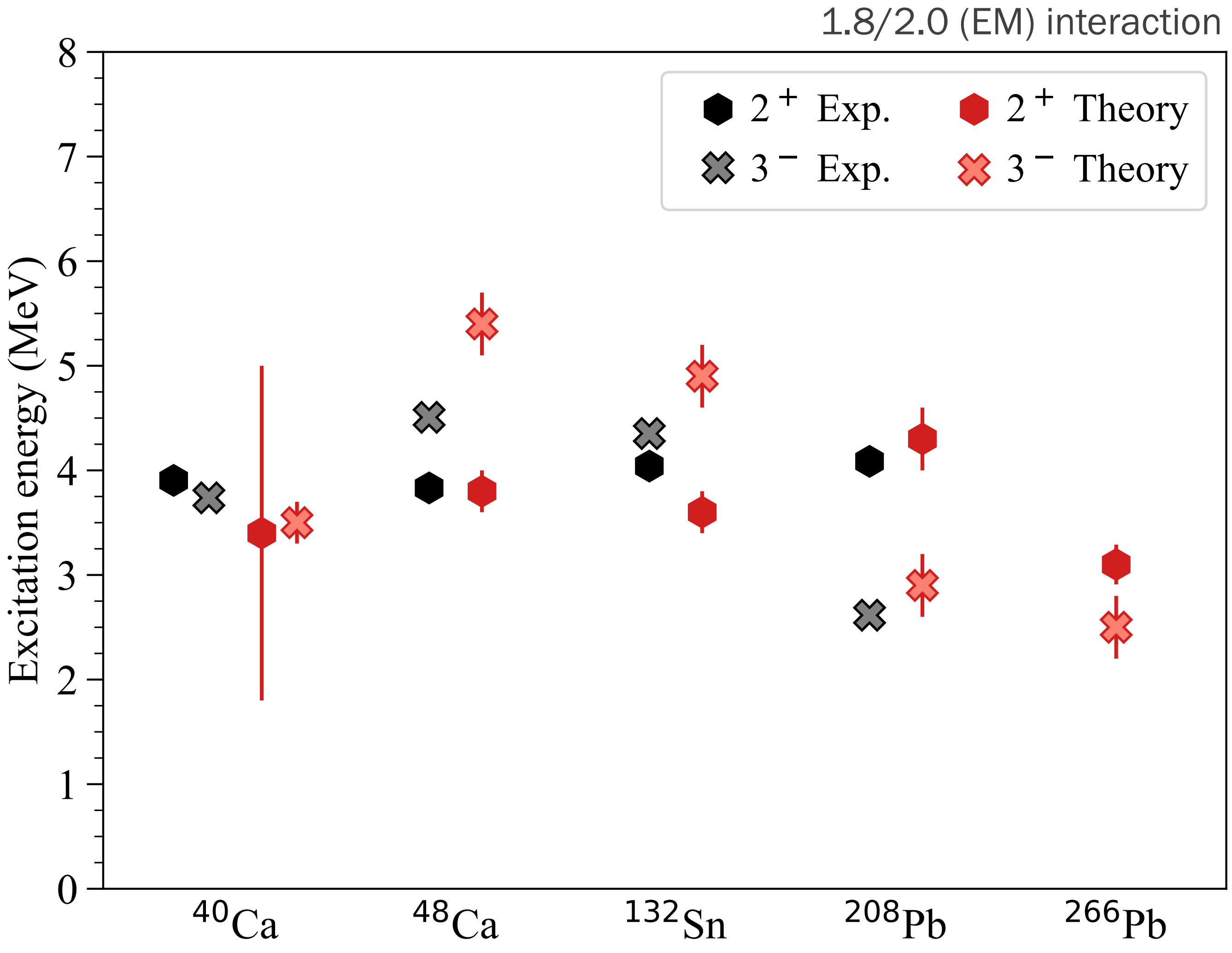
FB et al, arXiv:2508.14217 [nucl-th].

^{266}Pb is doubly magic



FB et al, arXiv:2508.14217 [nucl-th].

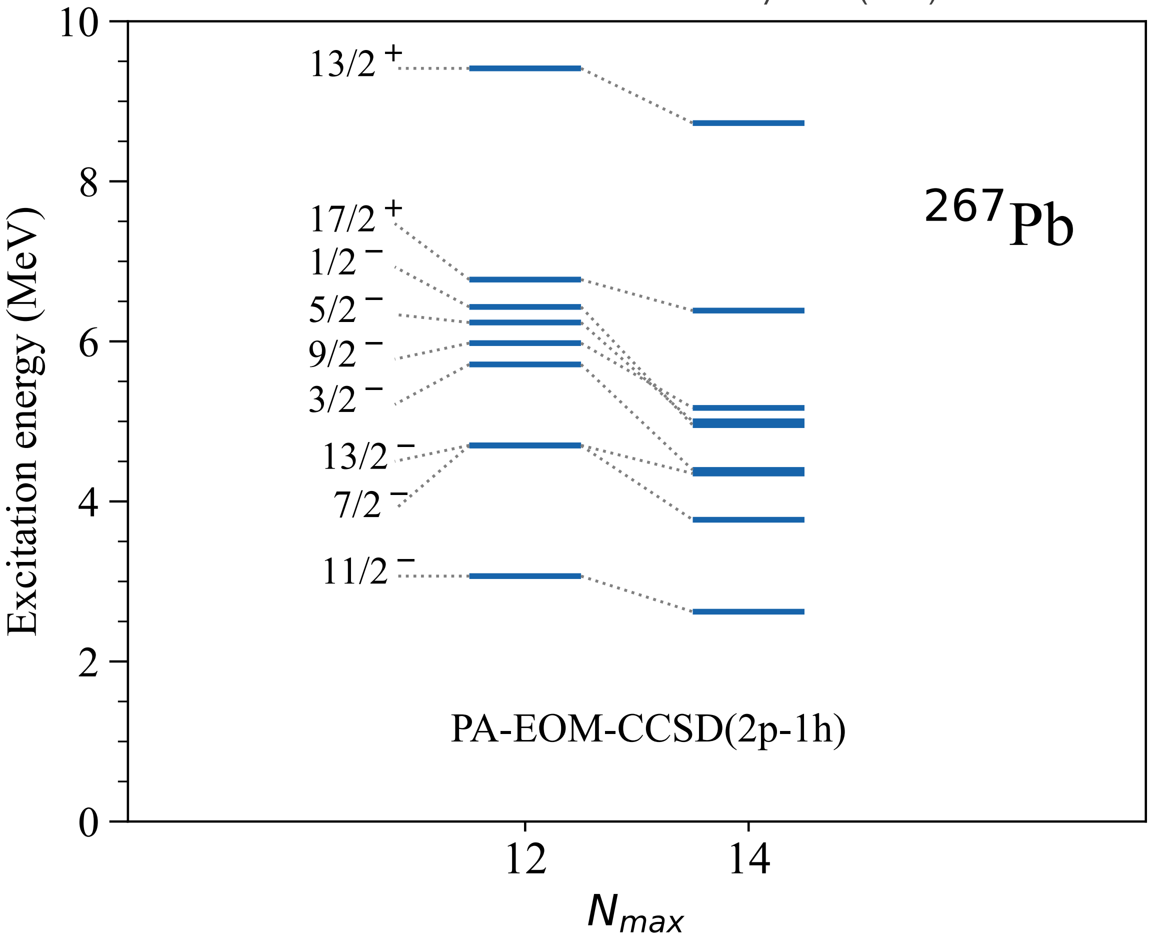
From light to heavy doubly magic nuclei



FB et al, arXiv:2508.14217 [nucl-th].

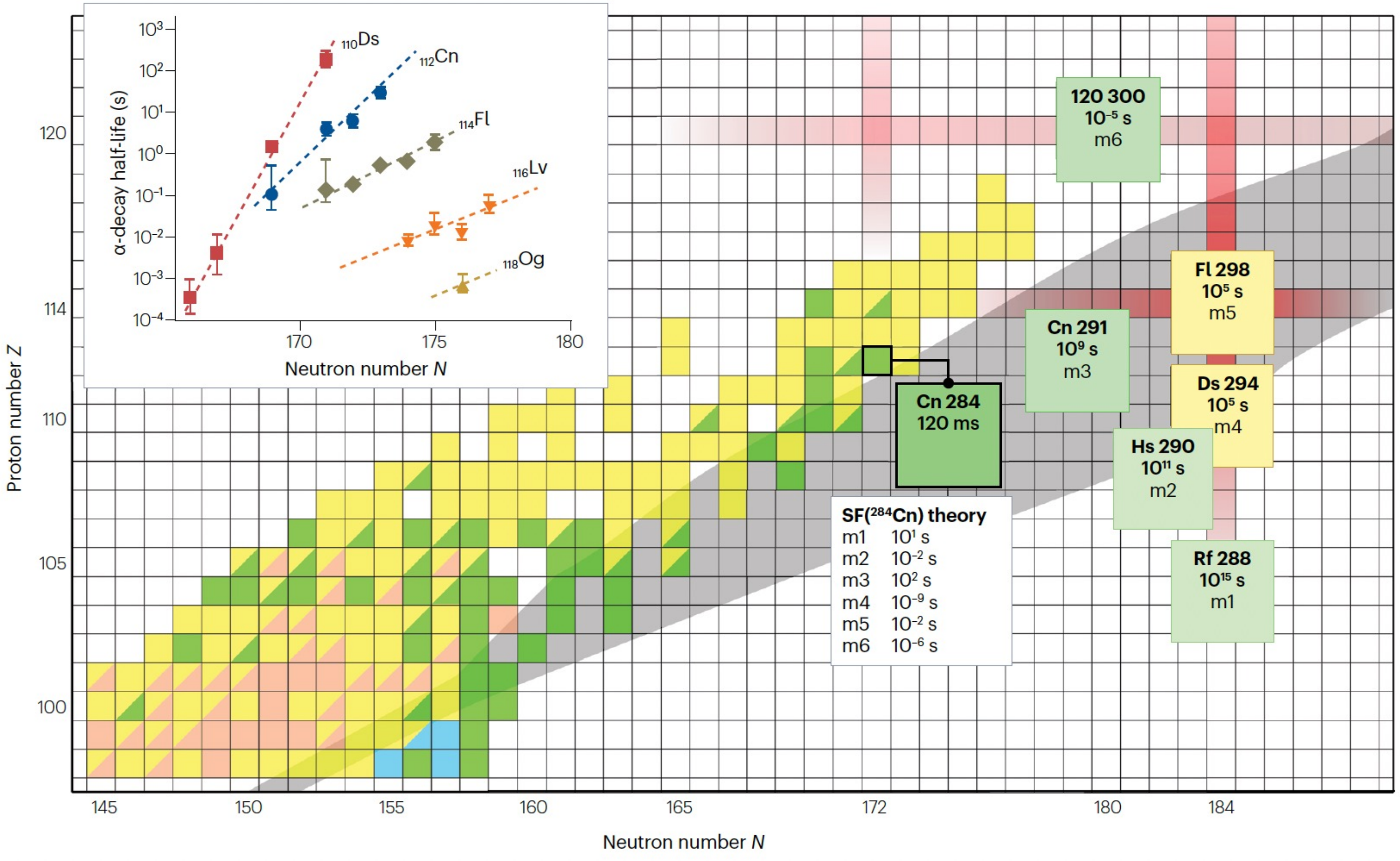
Is ^{266}Pb the last bound lead isotope?

1.8/2.0 (EM) interaction



FB et al, arXiv:2508.14217 [nucl-th].

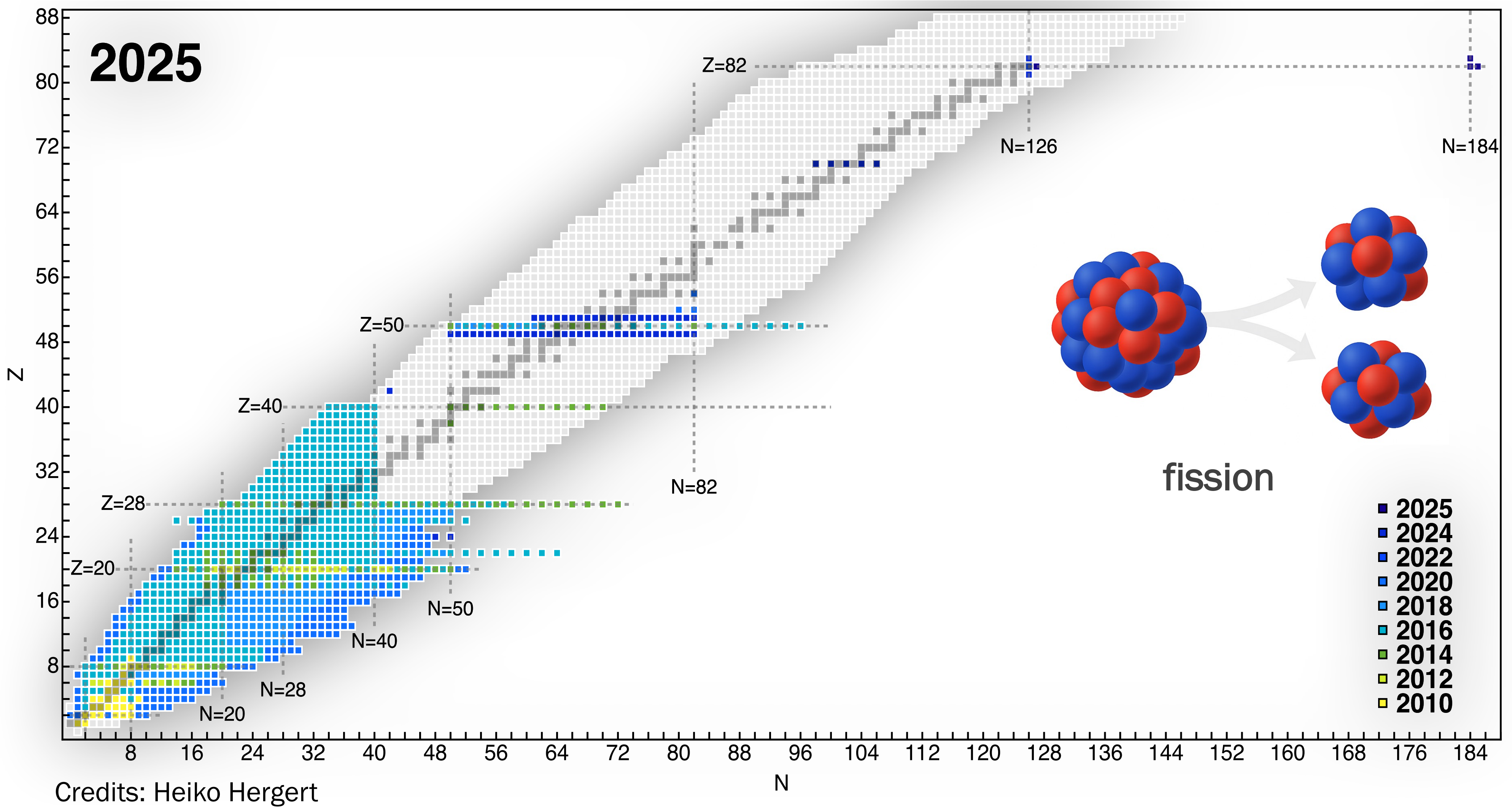
With an eye to the future



- In superheavy elements, one sees an **increased competition** between the **short-ranged nuclear force** and the **long-ranged electrostatic force**.
- This can yield e.g. to exotic density distributions, as shown by mean-field calculations.
- **Can such competition pose a challenge to chiral EFT?**

O. Smits et al, Nature Review Physics **6**, 86–98 (2024).

We pushed the ab initio boundaries, but there is some other interesting physics northeast…



Credits: Heiko Hergert

How to solve the time-dependent Schrödinger equation from a first-principles perspective?

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle$$

Coupled-cluster theory

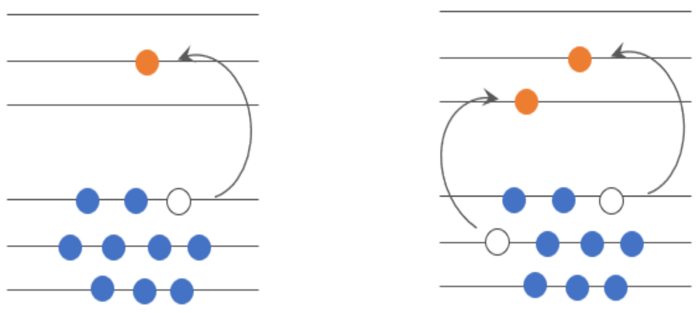
- Starting point: Hartree-Fock reference state $|\Phi_0\rangle$
- Add correlations via:

$$|\Psi(t)\rangle = e^{T(t)} |\Phi_0\rangle$$

with

$$T(t) = t_0(t) + \sum_{ia} t_i^a(t) a_a^\dagger a_i + \sum_{ijab} t_{ij}^{ab}(t) a_a^\dagger a_b^\dagger a_j a_i + \dots$$

singles and doubles (CCSD)



→ CC equations become ordinary differential eqs for the time-dependent amplitudes

D.A. Pigg, G. Hagen, H. Nam, T. Papenbrock, PRC 86, 014308 (2012).

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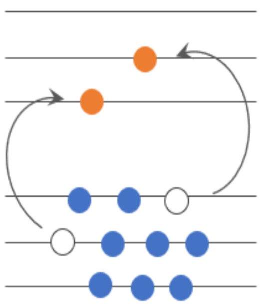
One can also only isolate **doubles (CCD)**



→ **CC equations** become **ordinary differential eqs** for the **time-dependent amplitudes**

D.A. Pigg, G. Hagen, H. Nam, T. Papenbrock, PRC 86, 014308 (2012).

Time evolution from the mean-field

- ❑ Fission typically modeled within mean-field approaches (time-dependent Hartree-Fock).
- ❑ Do we need to add correlations and go beyond this description?
- ❑ To evaluate this, we introduce correlation dynamically and look at time evolution of the system starting from HF reference.

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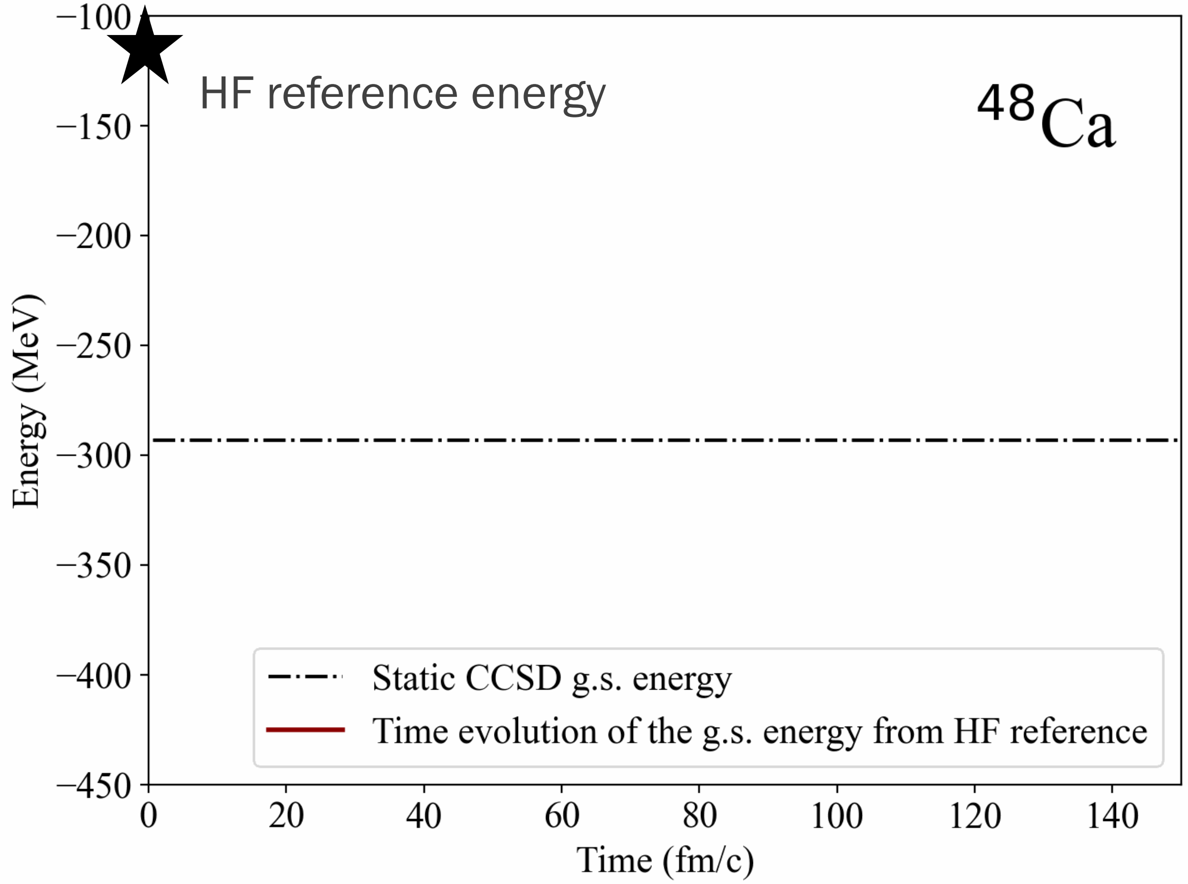

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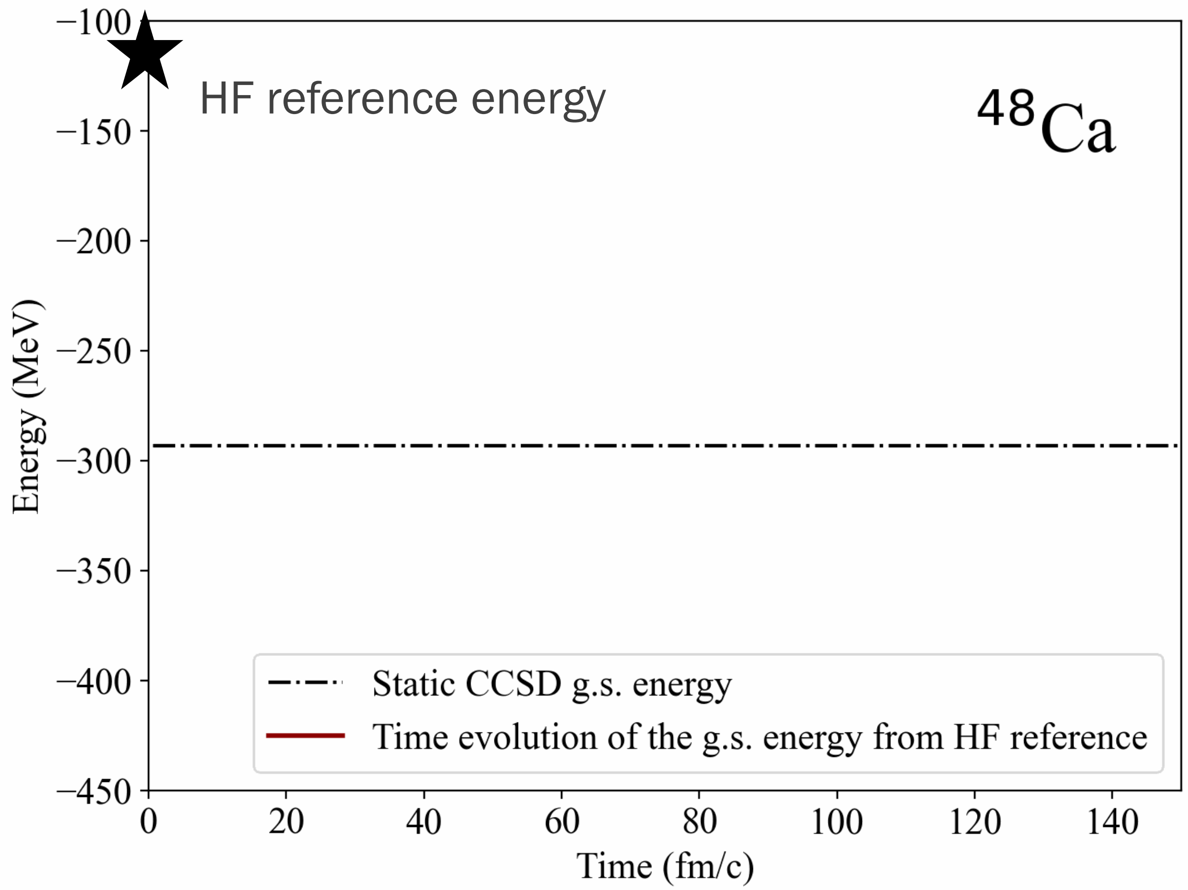
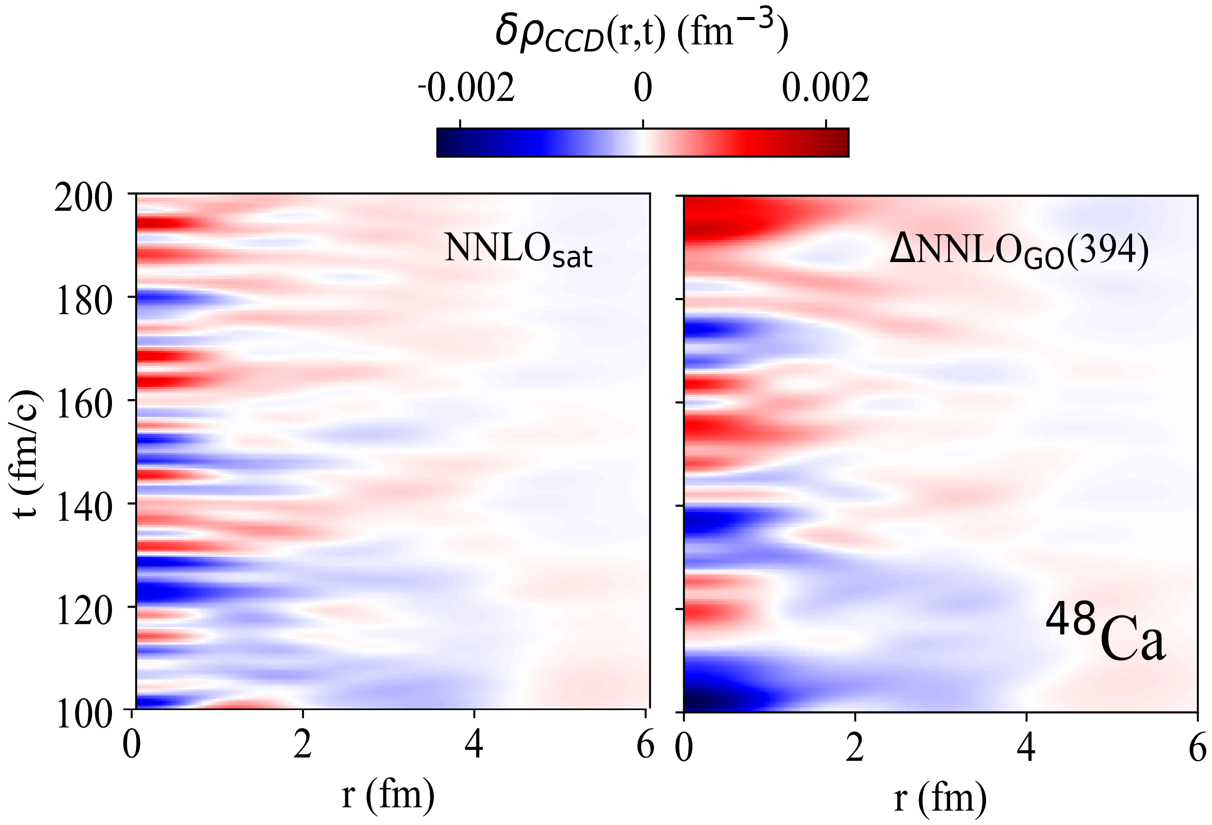


We can look at the **typical time scales and amplitudes** of **nuclear density fluctuations**.

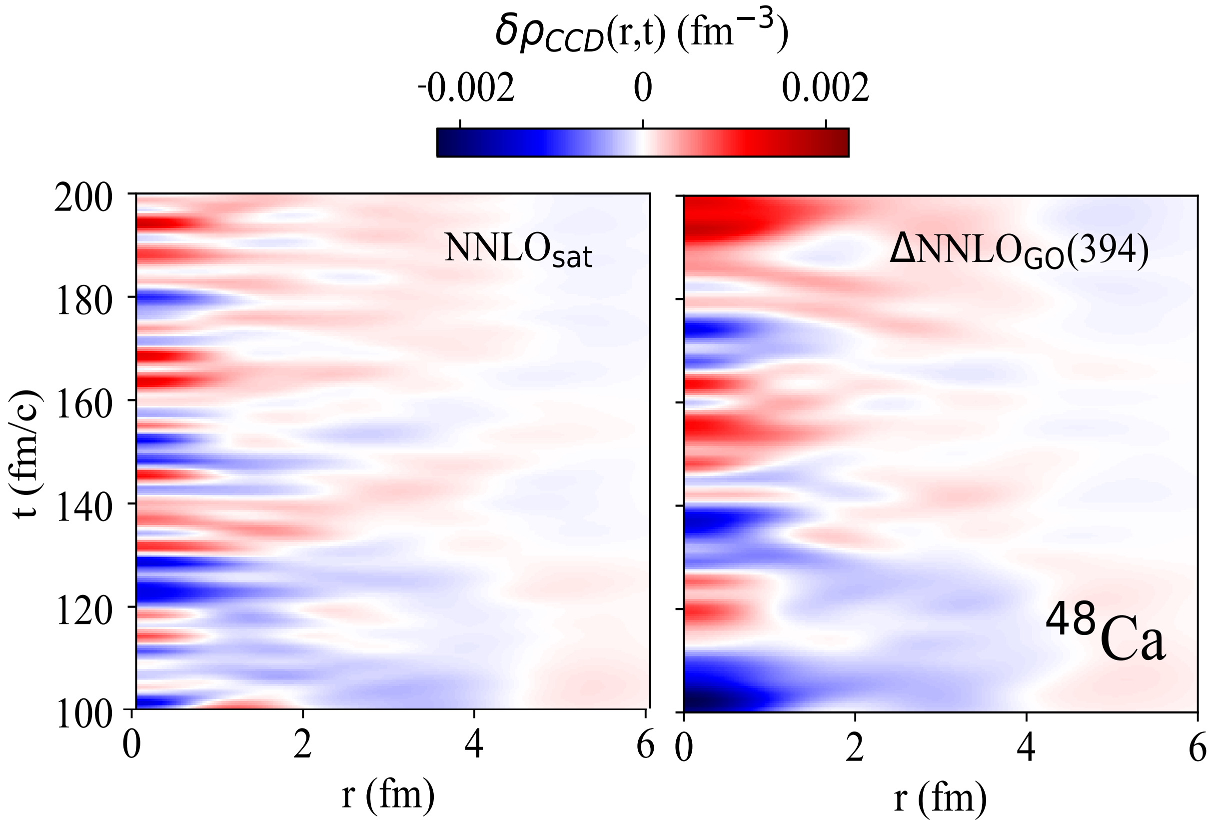
Nuclear density fluctuations: ^{48}Ca



- ❑ We isolate effect of 2p-2h correlations by considering a CCD calculation.
- ❑ We calculate the density fluctuation with respect to its average over time.

FB et al, arXiv:2604.12089 [nucl-th].

Nuclear density fluctuations: ^{48}Ca



- We isolate effect of **2p-2h correlations** by considering a **CCD calculation**.
- We calculate the **density fluctuation** with respect to its **average over time.**
- We find **short-range fluctuations**, **one order of magnitude** shorter than **typical equilibration times in nuclear reactions**.

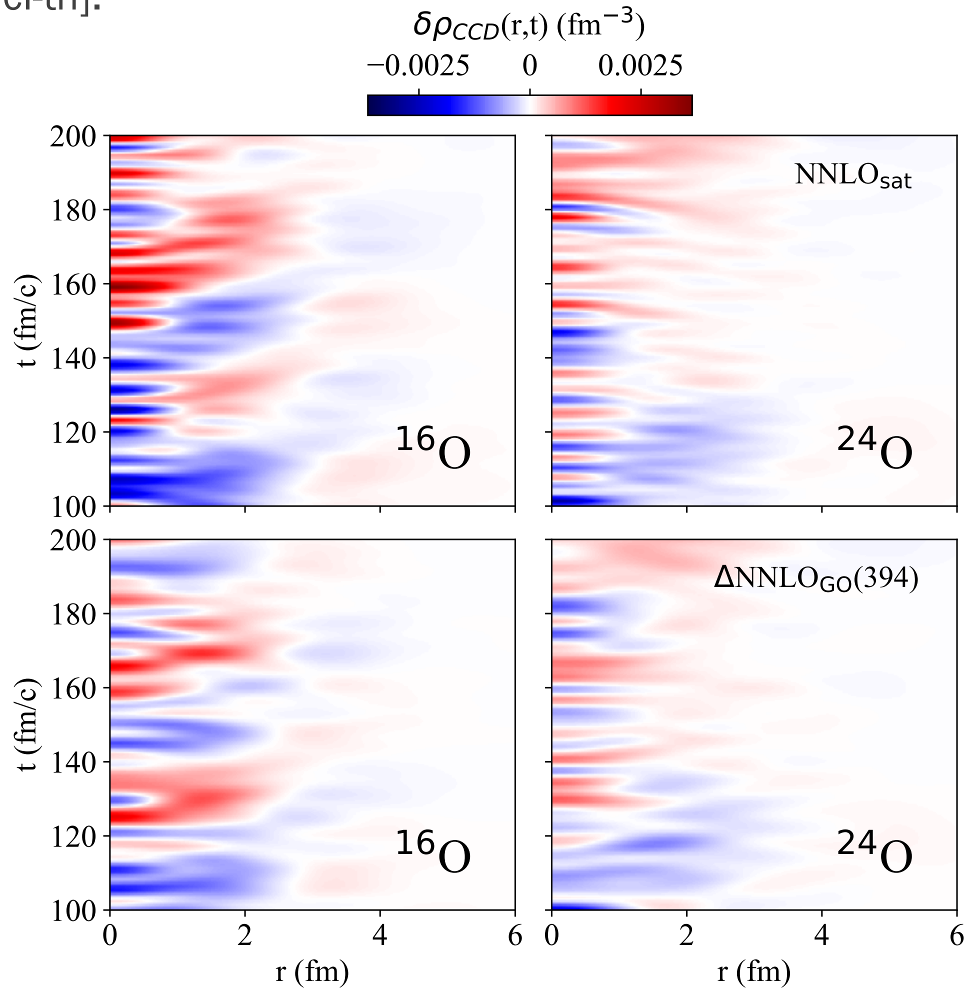
Jedele et al, PRL 118, 062501 (2017).

This is a pure **beyond-mean-field** effect!

FB et al, arXiv:2604.12089 [nucl-th].

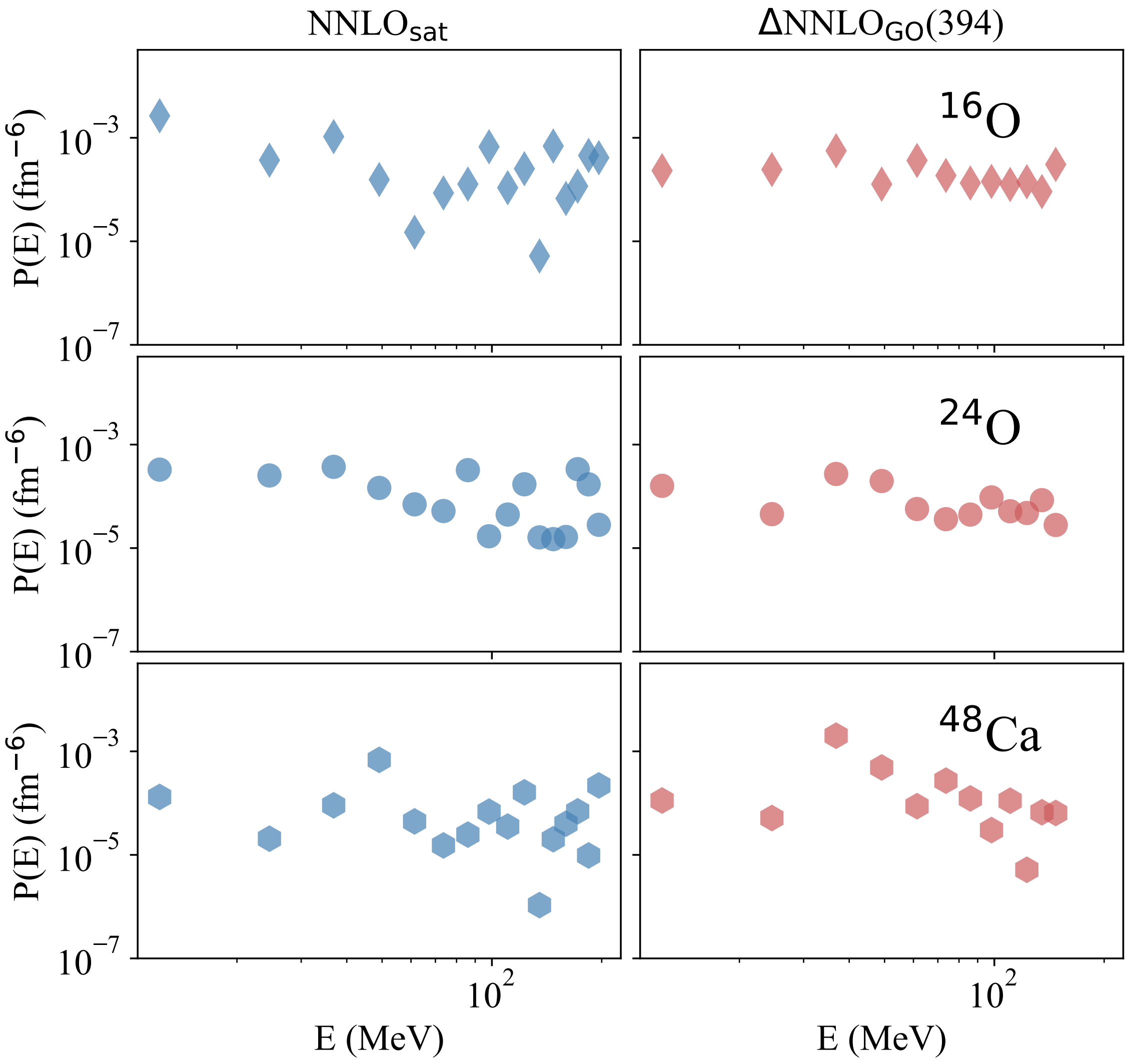
Nuclear density fluctuations: ^{16,24}O

FB et al, arXiv:2604.12089 [nucl-th].



Short-time, short-range fluctuations are model-dependent yet universal:
they do not depend on the mass number.

Short-range fluctuations are stochastic!

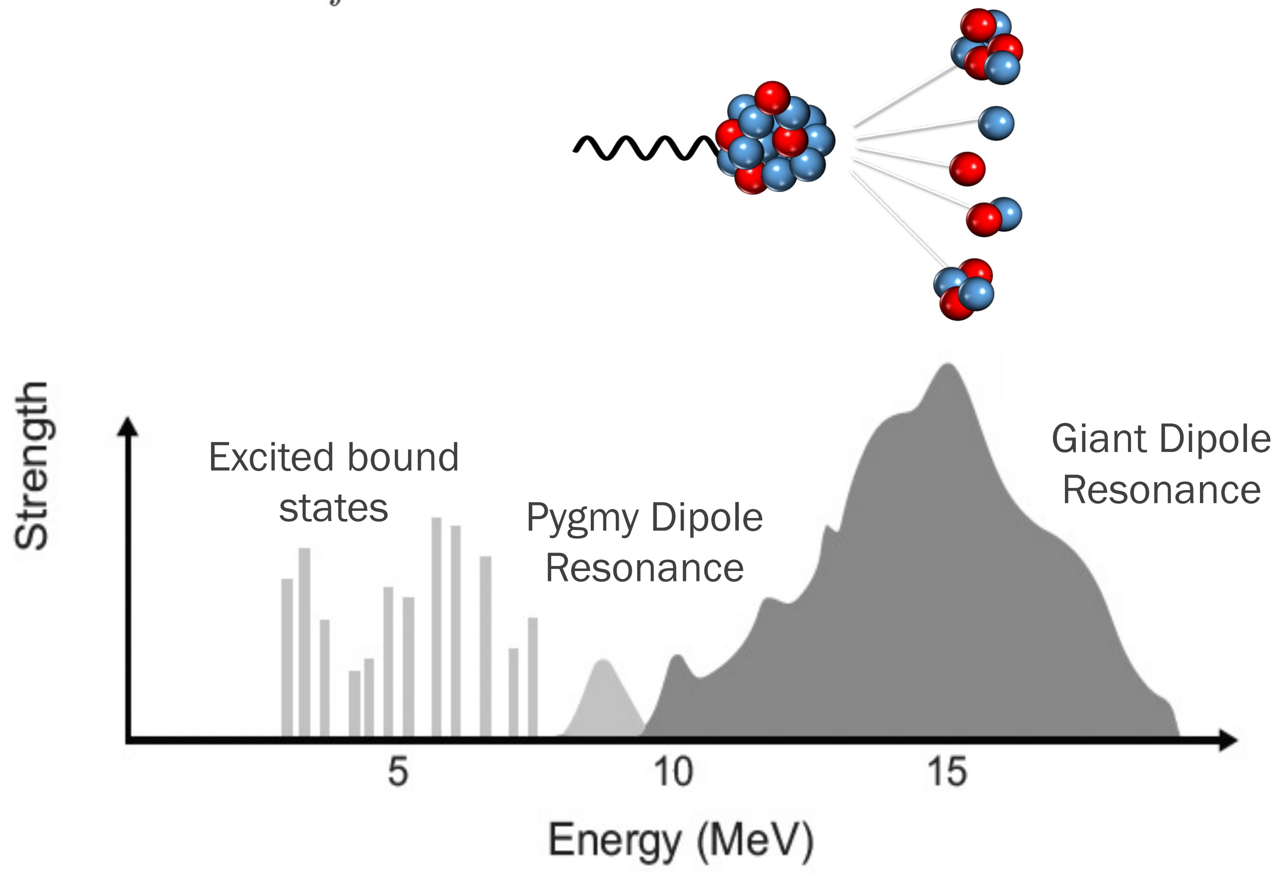


FB et al, arXiv:2604.12089 [nucl-th].

A simple physics case: nuclear response functions from a time-dependent perspective

Nuclear response functions

$$R(\omega) = \sum\!\!\!\!\!\!\int_f |\langle \Psi_f | \Theta | \Psi_0 \rangle|^2 \delta(E_f - E_0 - \omega)$$



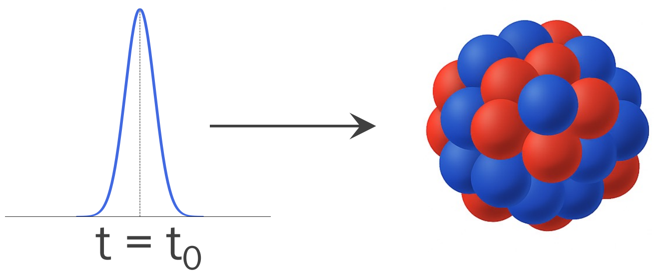
Responses in a time-dependent approach

Goal: solving

$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle$$

with

$$\hat{H}(t) = \hat{H}_0 + \epsilon f(t) \hat{D}$$



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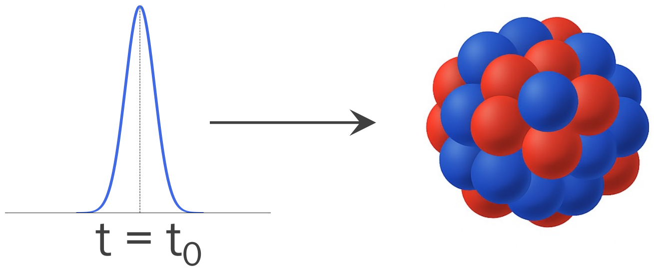

with

$$\hat{H}(t) = \hat{H}_0 + \epsilon f(t) \hat{D}$$

For small ε, first-order time-dependent perturbation theory yields:

$$D(t) = \langle \Psi(t) | \hat{D} | \Psi(t) \rangle$$

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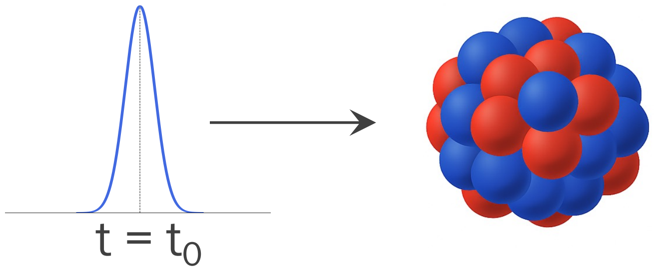

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For small ε, first-order time-dependent perturbation theory yields:

$$D(t) = \langle\Psi(t)|\hat{D}|\Psi(t)\rangle \longrightarrow \tilde{D}(\omega)$$

Fourier transform

Responses in a time-dependent approach

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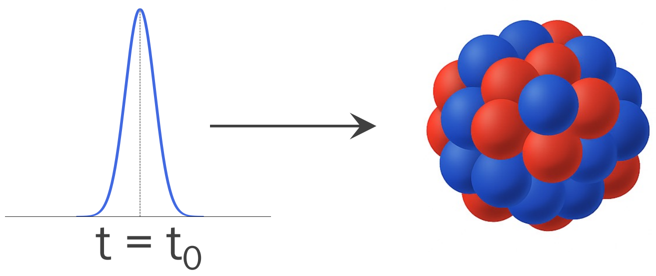
$$i\hbar \frac{d}{dt} |\Psi(t)\rangle = \hat{H}(t) |\Psi(t)\rangle$$



with

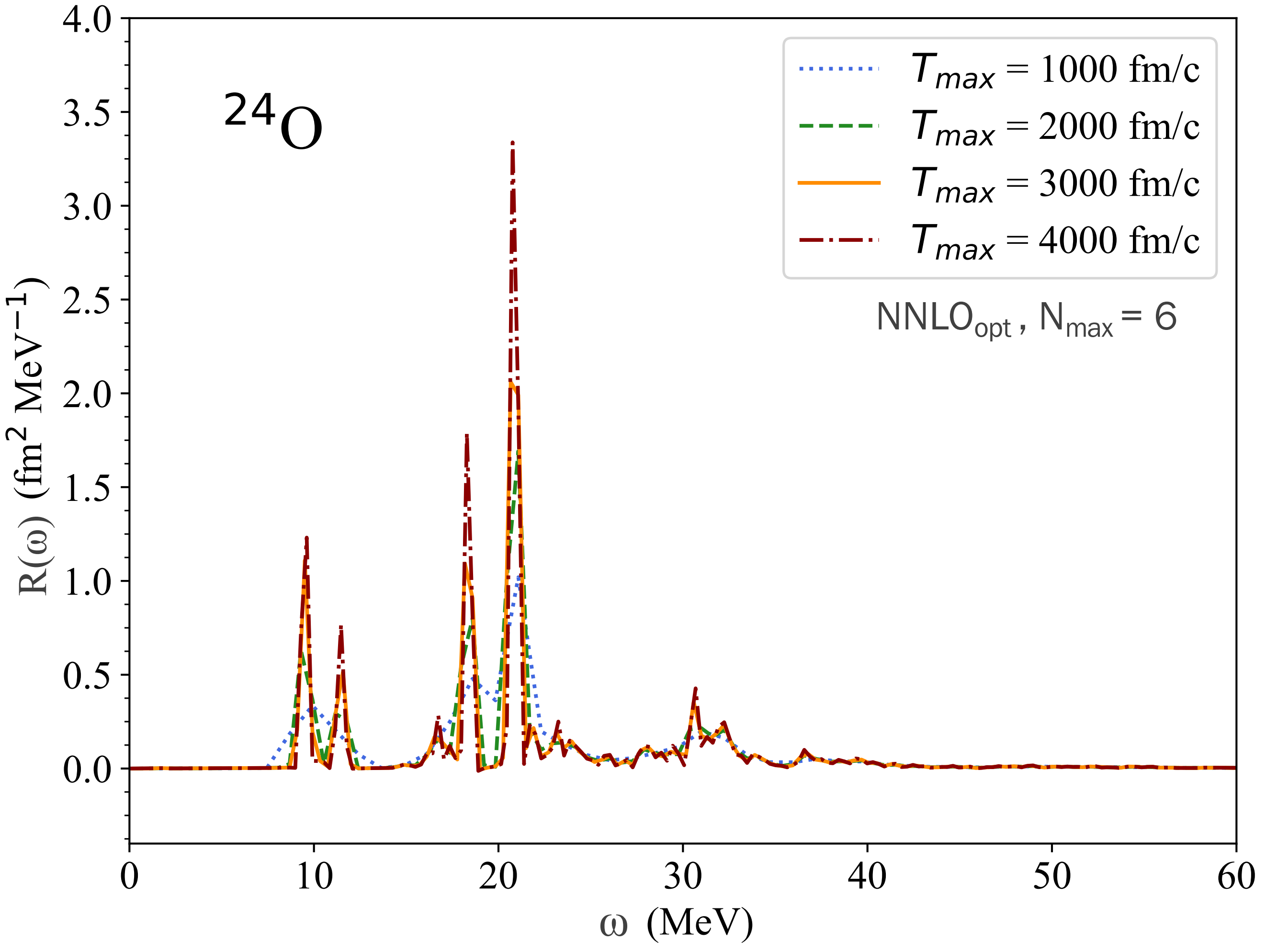
$$\hat{H}(t) = \hat{H}_0 + \epsilon f(t) \hat{D}$$

For small ε, first-order time-dependent perturbation theory yields:

$$D(t) = \langle \Psi(t) | \hat{D} | \Psi(t) \rangle \longrightarrow \tilde{D}(\omega) \longrightarrow R(\omega) = \mathrm{Im} \left(\frac{\tilde{D}(\omega)}{\epsilon \tilde{f}(\omega)} \right)$$

Fourier transform

Simulation time and resolution



Resolution

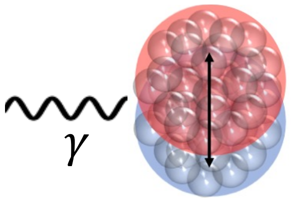
$$\Delta\omega = \frac{2\pi\hbar c}{t_{max}}$$

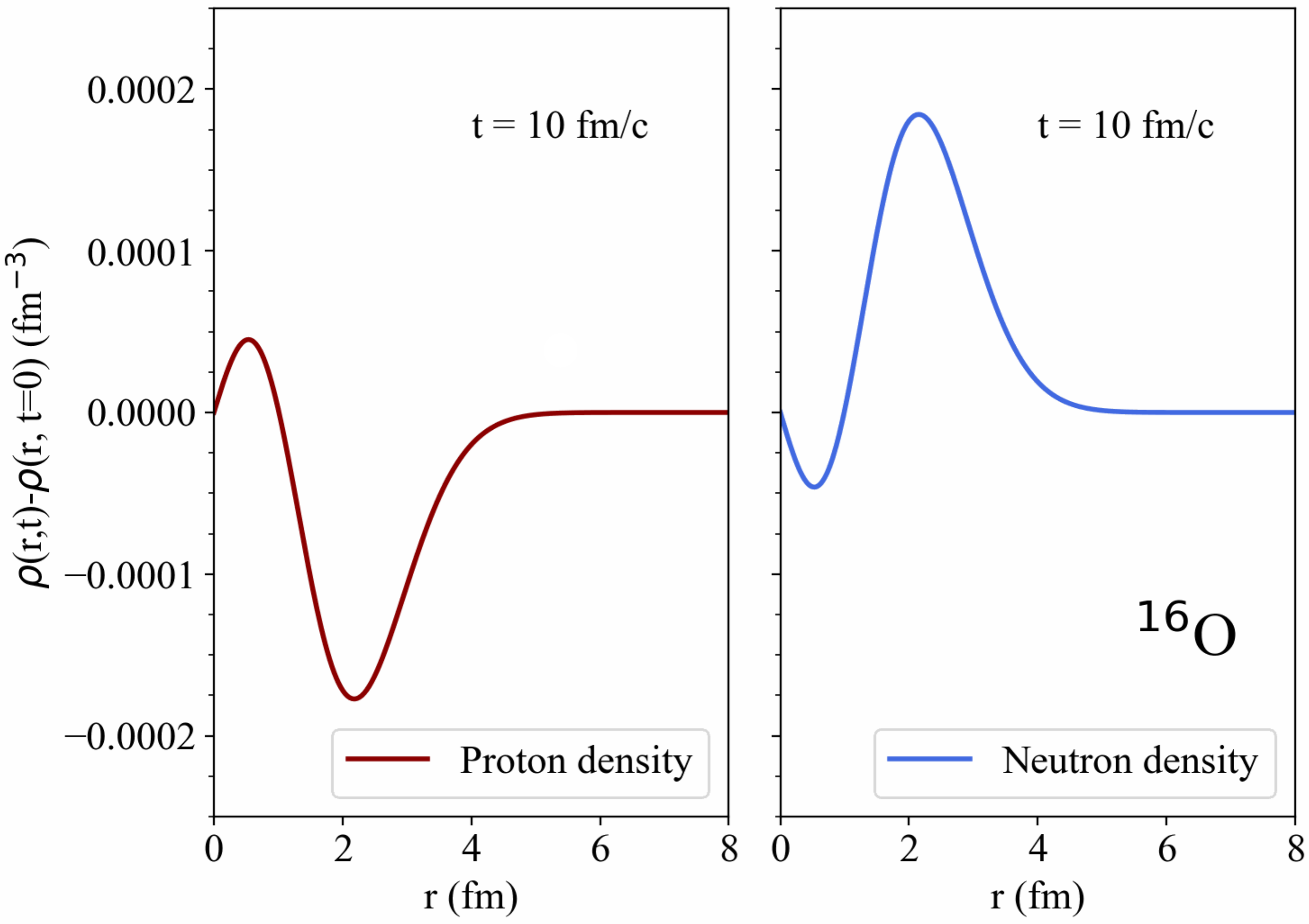
Maximum simulation time

FB et al, PRC **113**, 024312 (2026).

Collective oscillations in real time

^{16}O



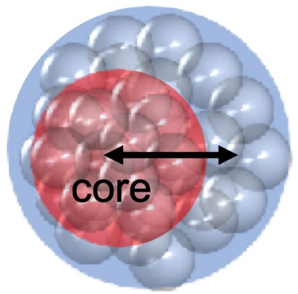


$NNLO_{opt}$, $N_{max} = 6$

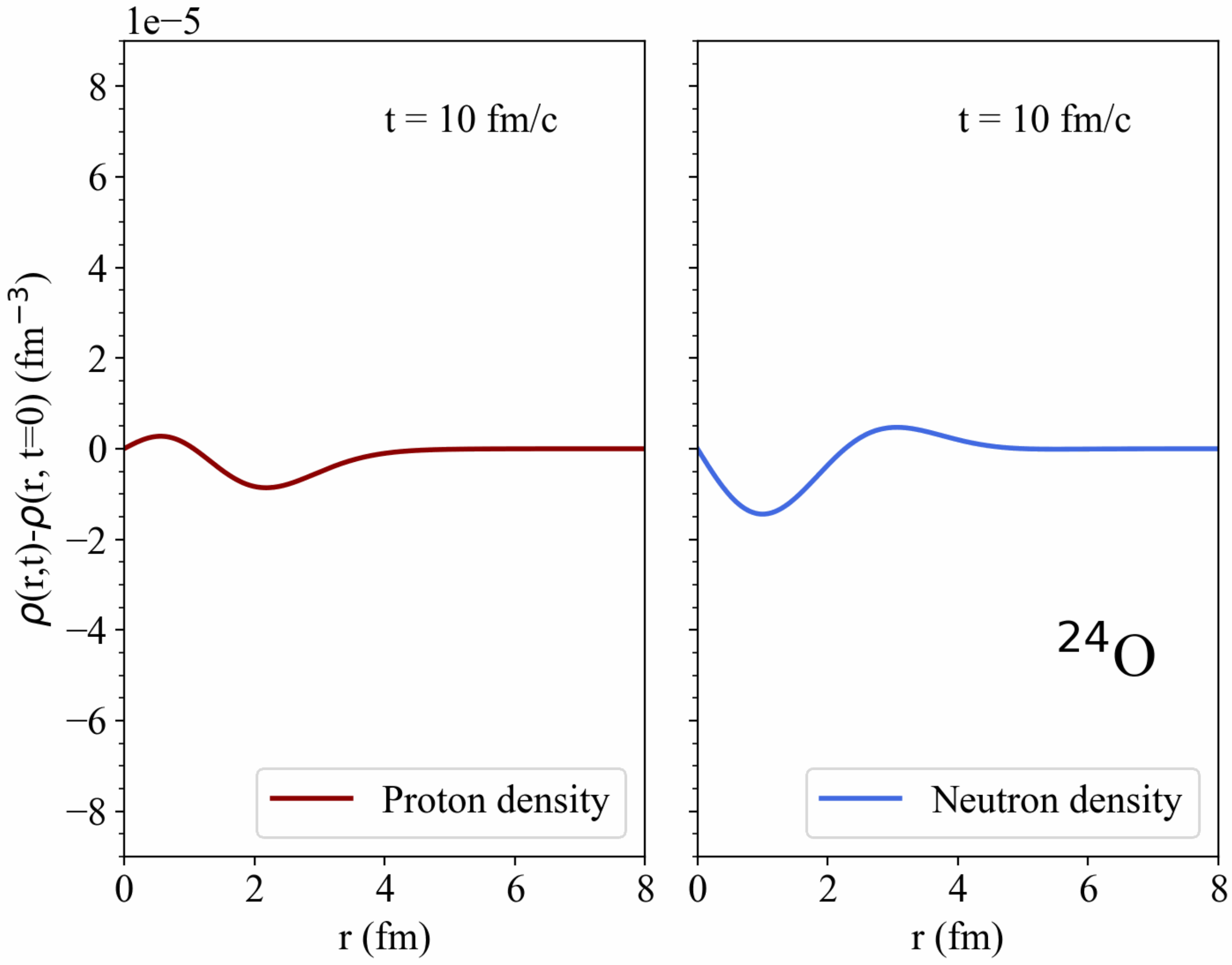
FB et al, PRC **113**, 024312 (2026).

Collective oscillations in real time

^{24}O



isolating
lowest-lying dipole-excited
state at low-energy



$NNLO_{opt}$,
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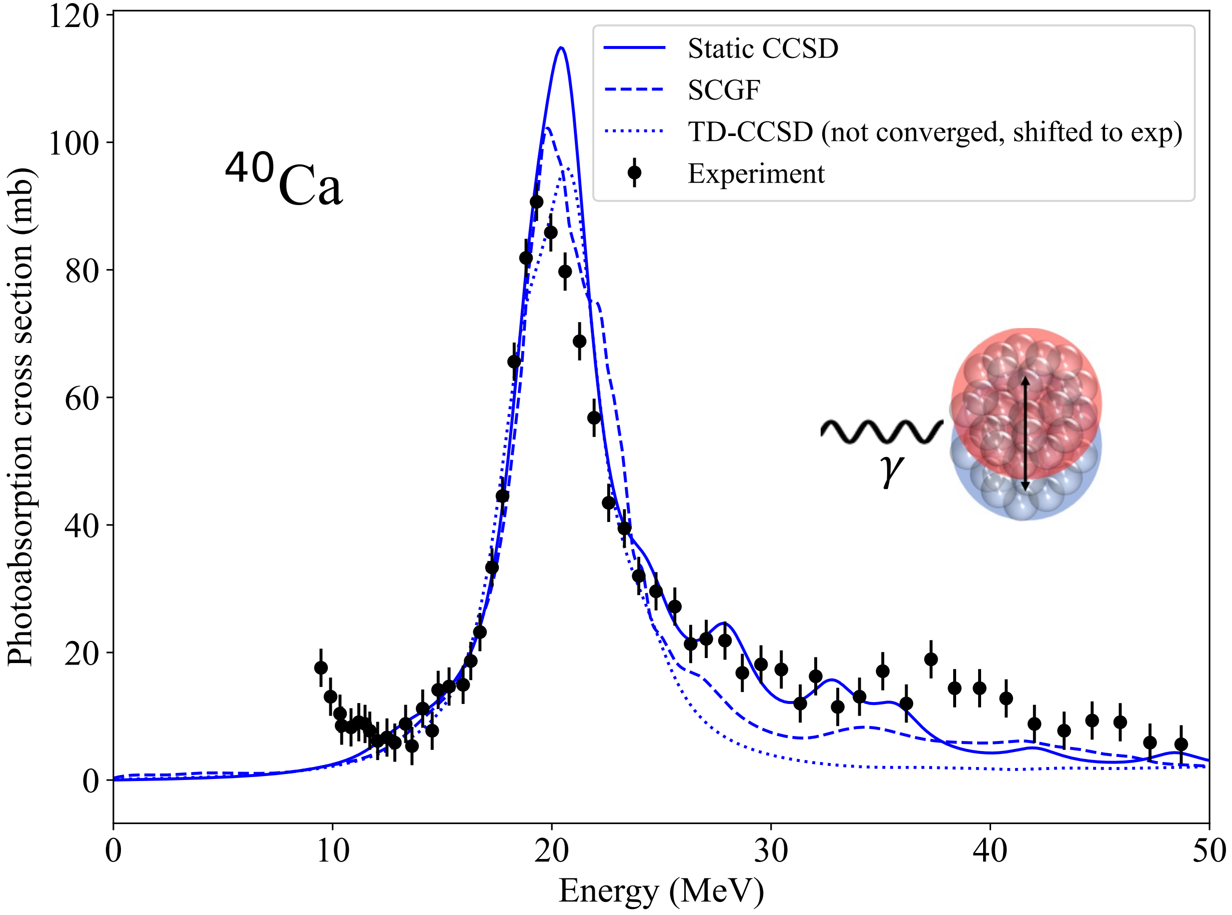
FB et al, PRC **113**, 024312 (2026).

Collective modes as fit observables?



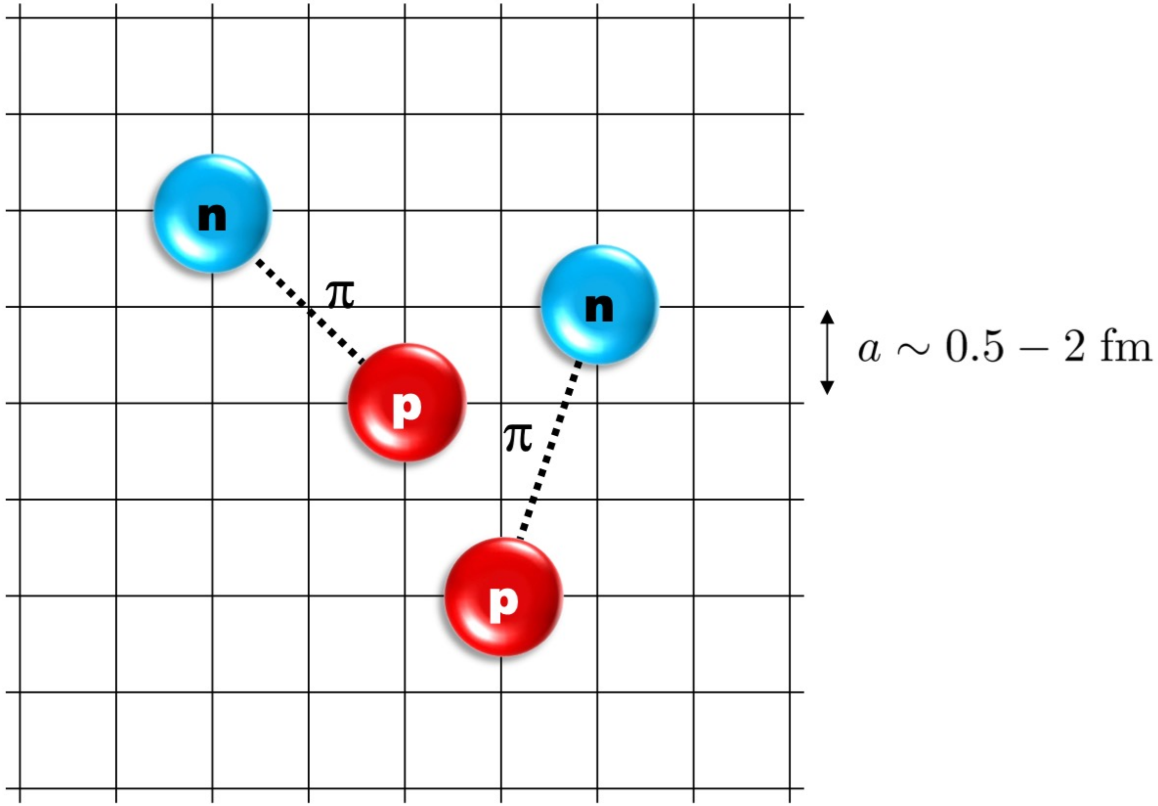
from S.Bacca et al, arXiv:2604.07229 [nucl-th] + my TDCC result

- We are now able to see **collective modes** emerging from **chiral forces** (from both a static and time-dependent perspective).
- Can they be a **useful input** for the **optimization/calibration** of **nuclear Hamiltonians**?

How do we go from this to a microscopic description of nuclear reactions?

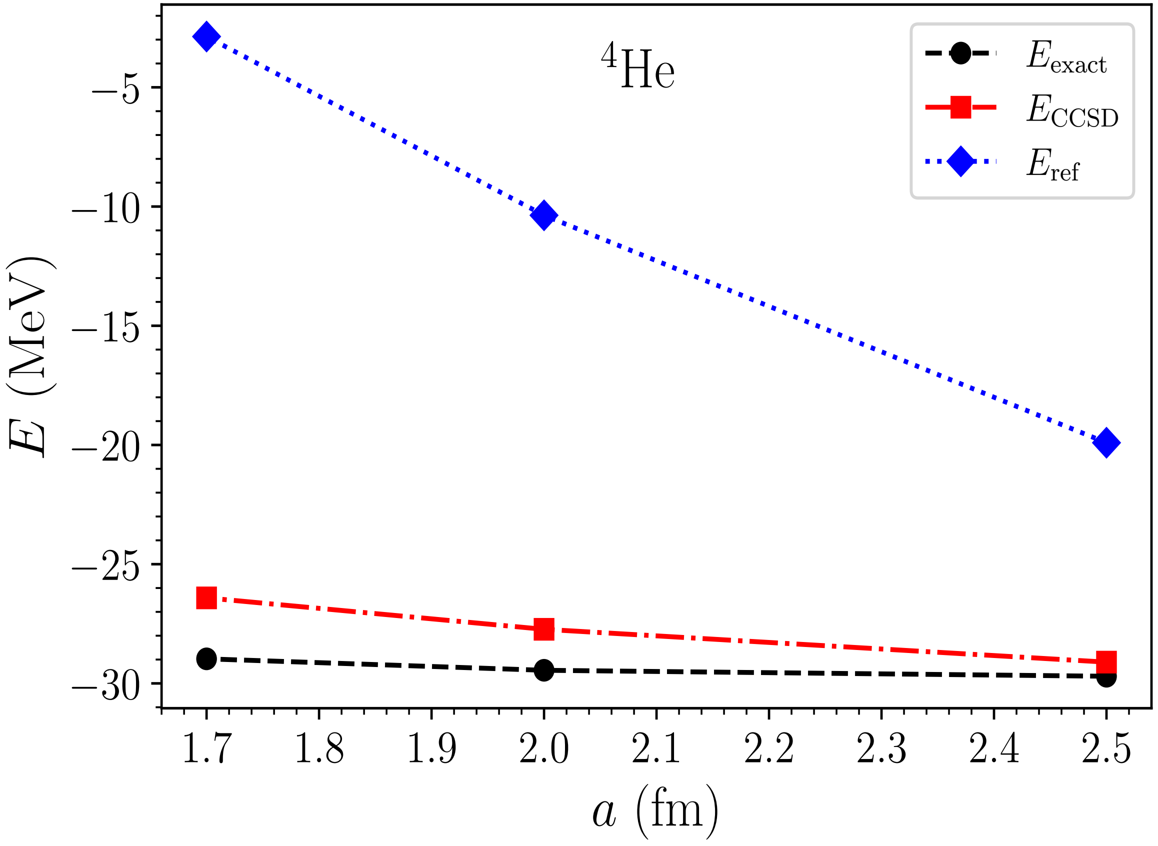
A natural framework: nuclei on the lattice

- We can exploit the short-range nature of the nuclear force! Correlations are only between neighbours.
- Computational cost scales with volume → problem becomes sparse!
- How far can we go with coupled-cluster on the lattice?



D. Lee, Prog. Part. Nucl. Phys. 63 117-154 (2009).

First steps on the lattice: ^{4}He



M. Rothman, B. Johnson-Toth, **FB**, G. Hagen, M. Heinz, T. Papenbrock, PRC 112, L051301 (2025).

Some open questions

- ❑ How to deal with increasing competition of nuclear and Coulomb force in superheavy nuclei?
- ❑ Can optimizing nuclear Hamiltonians on many-body dynamical observables be useful?
- ❑ How to further develop lattice Hamiltonians and link lattice and configuration-basis view of nuclei?

see Thomas Papenbrock's and Matthias Heinz's talks

Thanks to my collaborators&co-authors on the works I presented:

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@JGU Mainz: Sonia Bacca, Francesco Marino
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FRIB Theory Alliance

and to you for your attention!