Ab initio calculations at the superheavy frontier

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HIRSCHEGG 2026 – CHALLENGES IN EFFECTIVE FIELD THEORY DESCRIPTIONS OF NUCLEI

HIRSCHEGG, AUSTRIA

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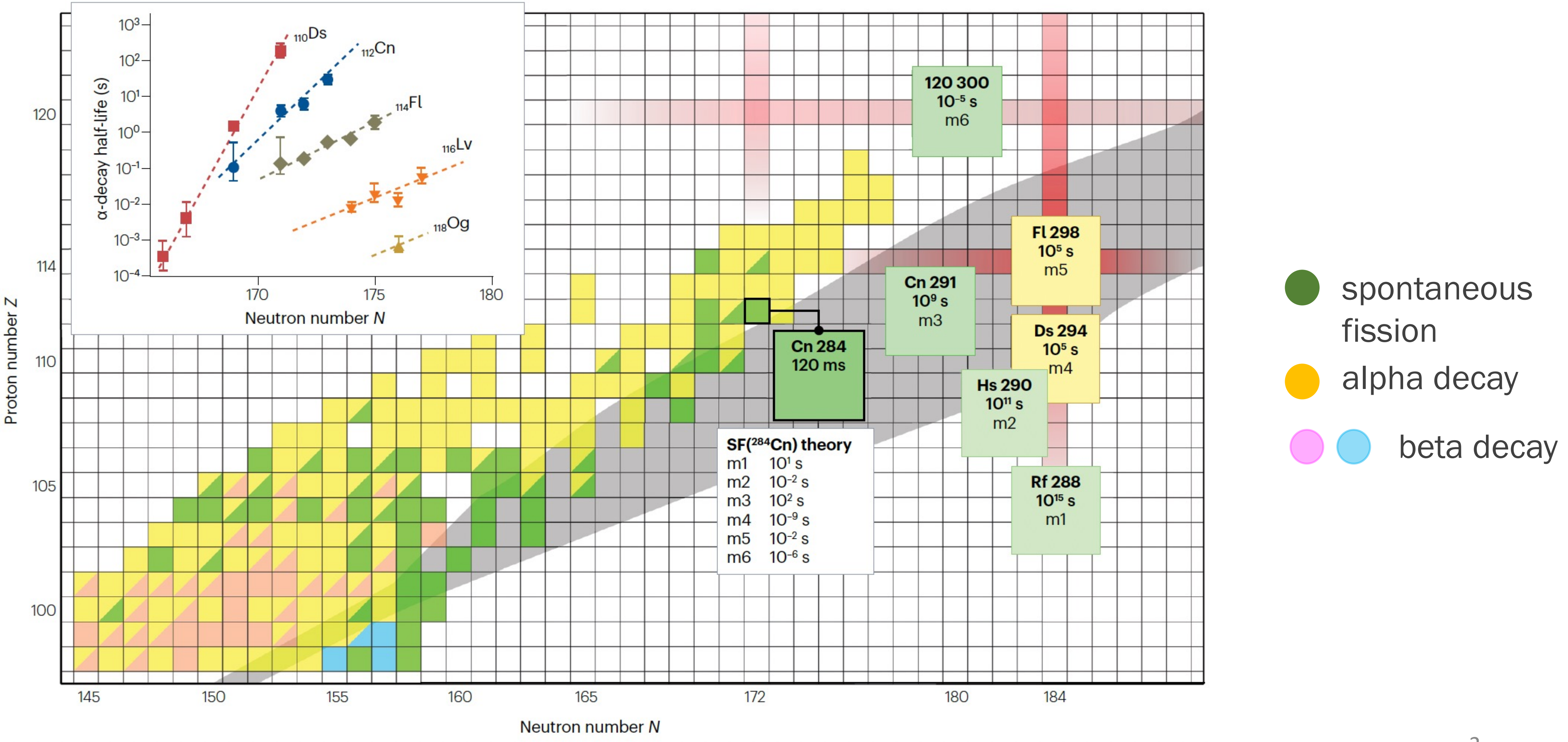
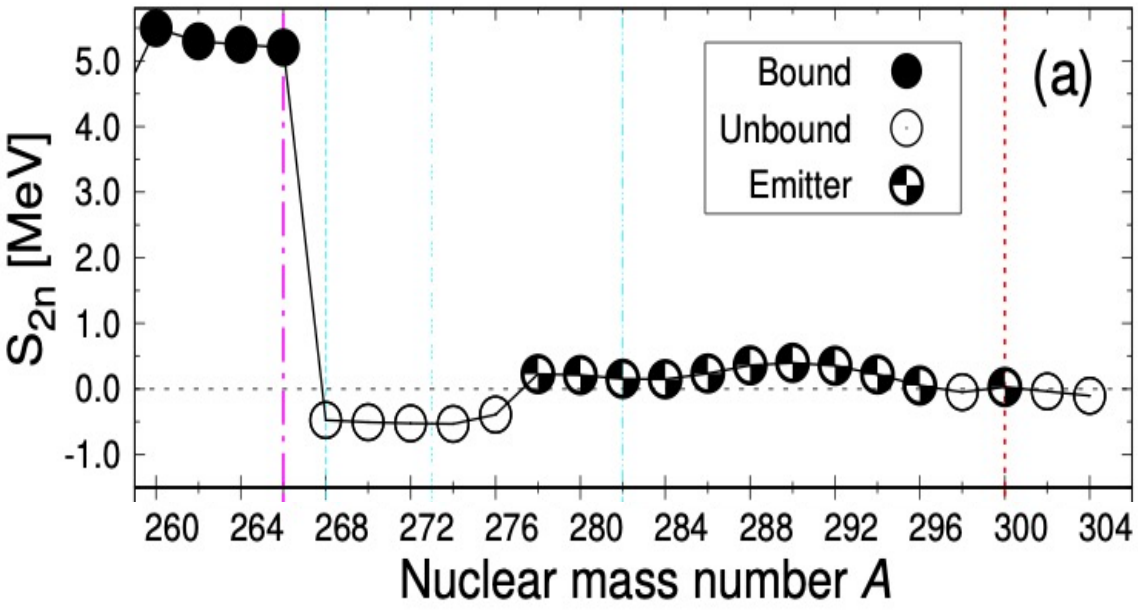
Searches for the "island of stability"

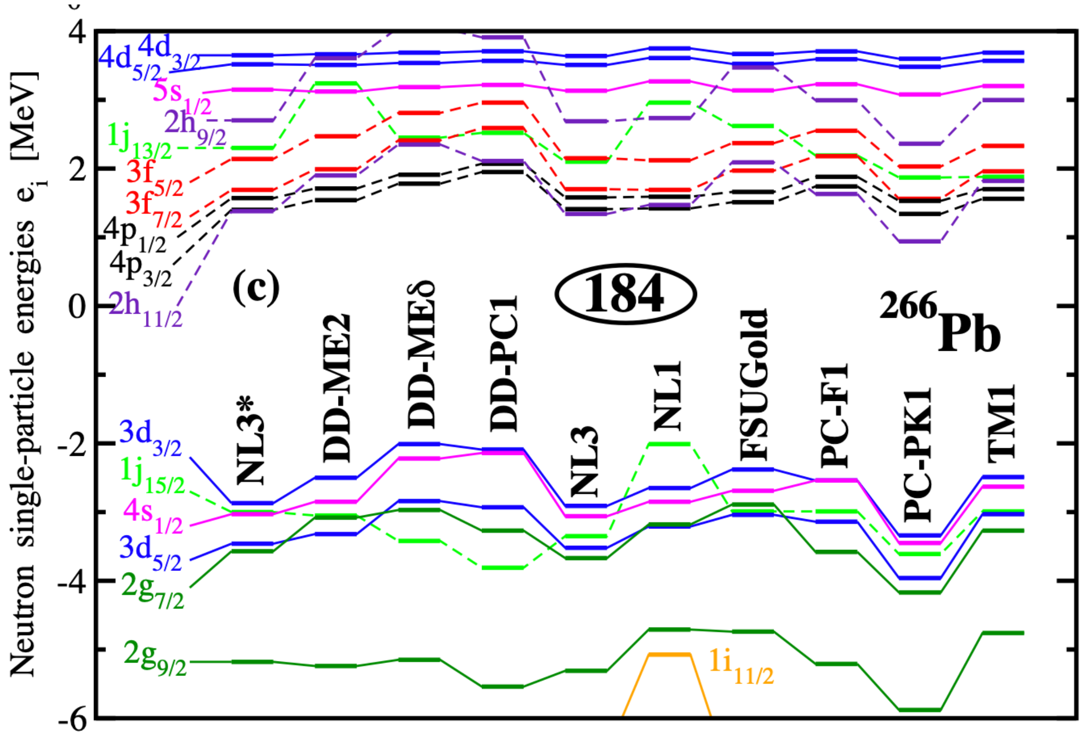


O. Smits et al, Nature Review Physics **6**, 86–98 (2024).

A possible candidate: ^{266}Pb



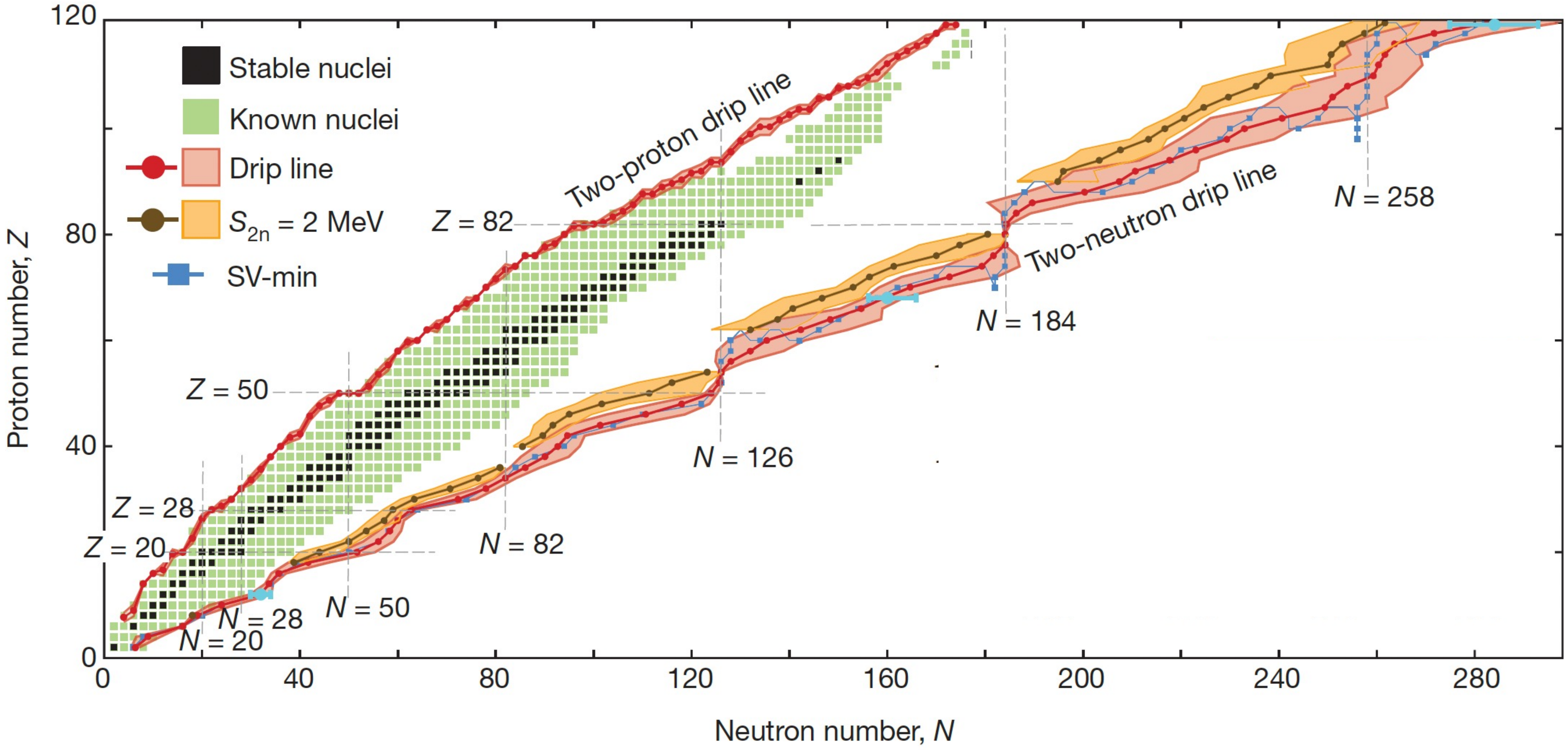
S. Kim et al, PRC 105, 034340 (2022).



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.

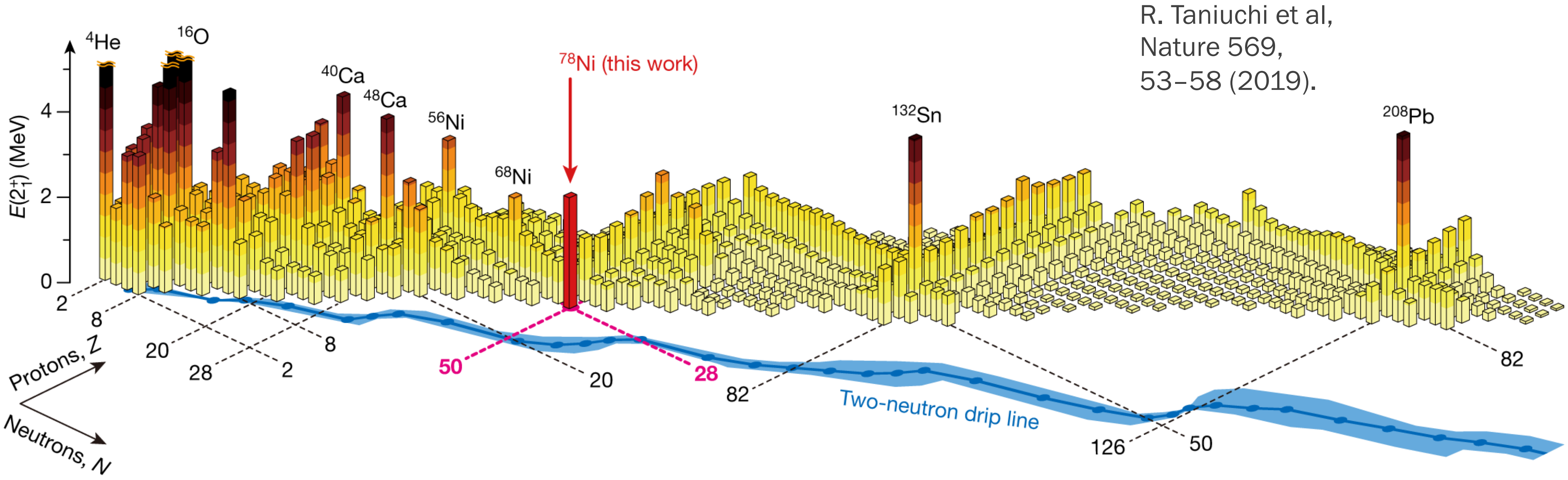
^{266}Pb could be the last bound lead isotope



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

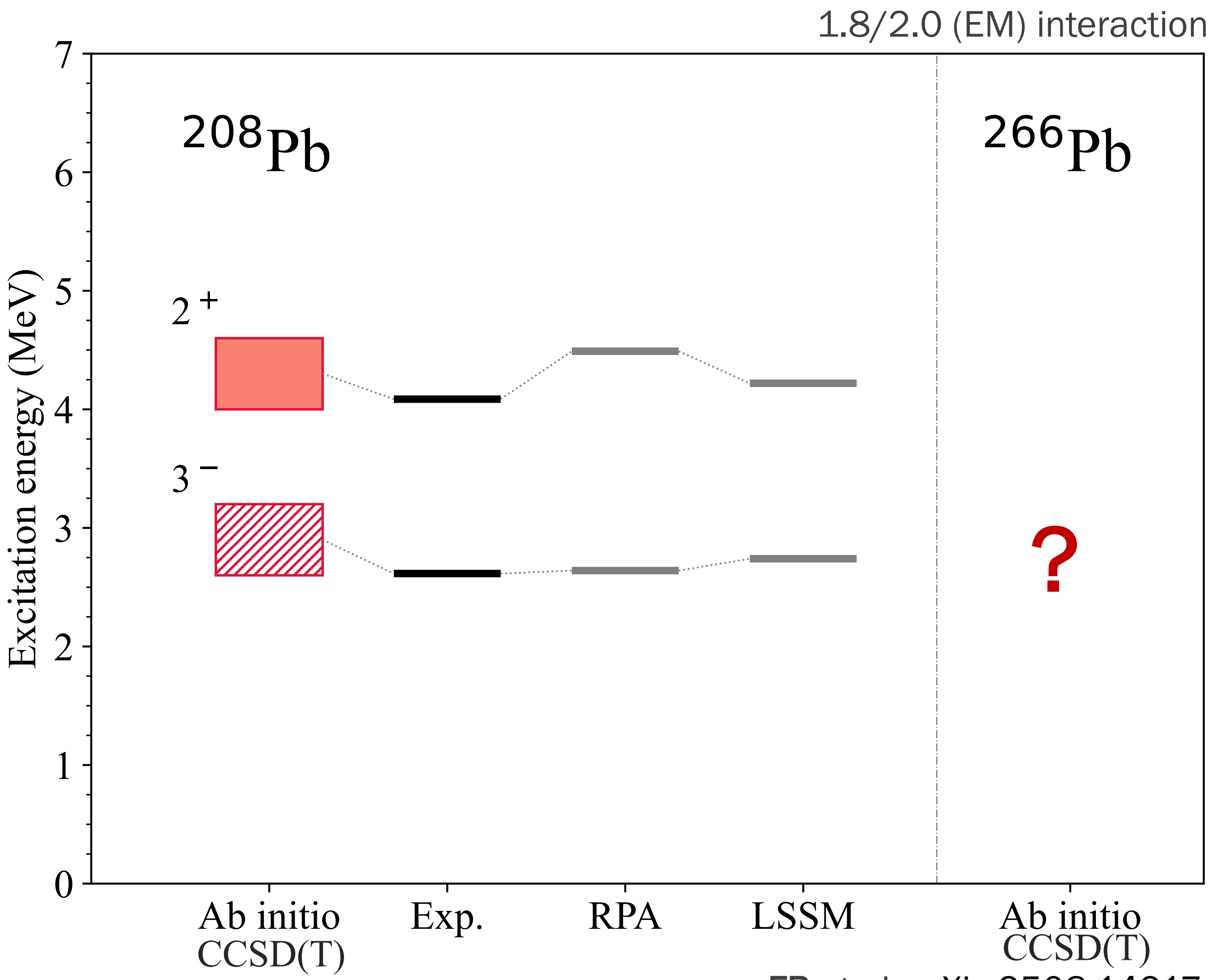
What can we say on ^{266}Pb from a first principles perspective?

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



Goal: get to the excited spectrum of ^{266}Pb from first principles.
We use the 1.8/2.0 (EM) interaction and coupled-cluster theory.

Excited states in ^{208}Pb

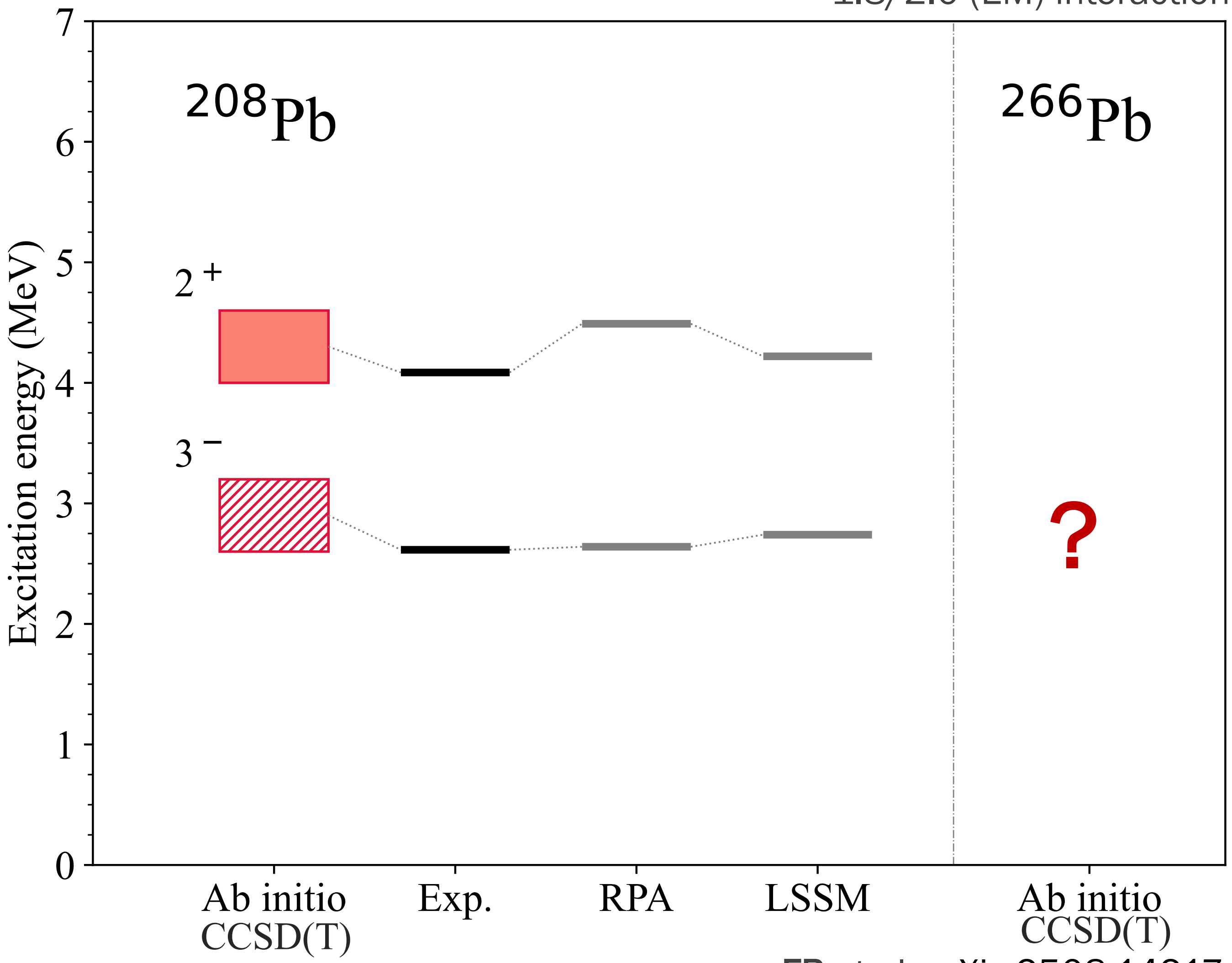


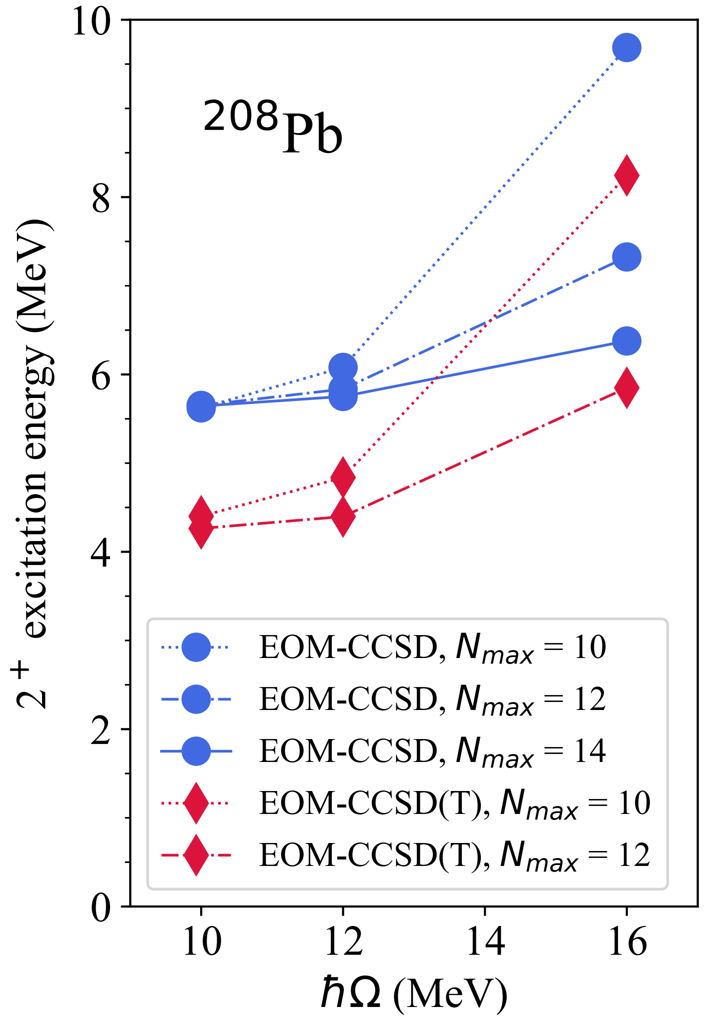
FB et al, arXiv:2508.14217 [nucl-th].

Excited states in ^{208}Pb

EOM-CCS

1.8/2.0 (EM) interaction

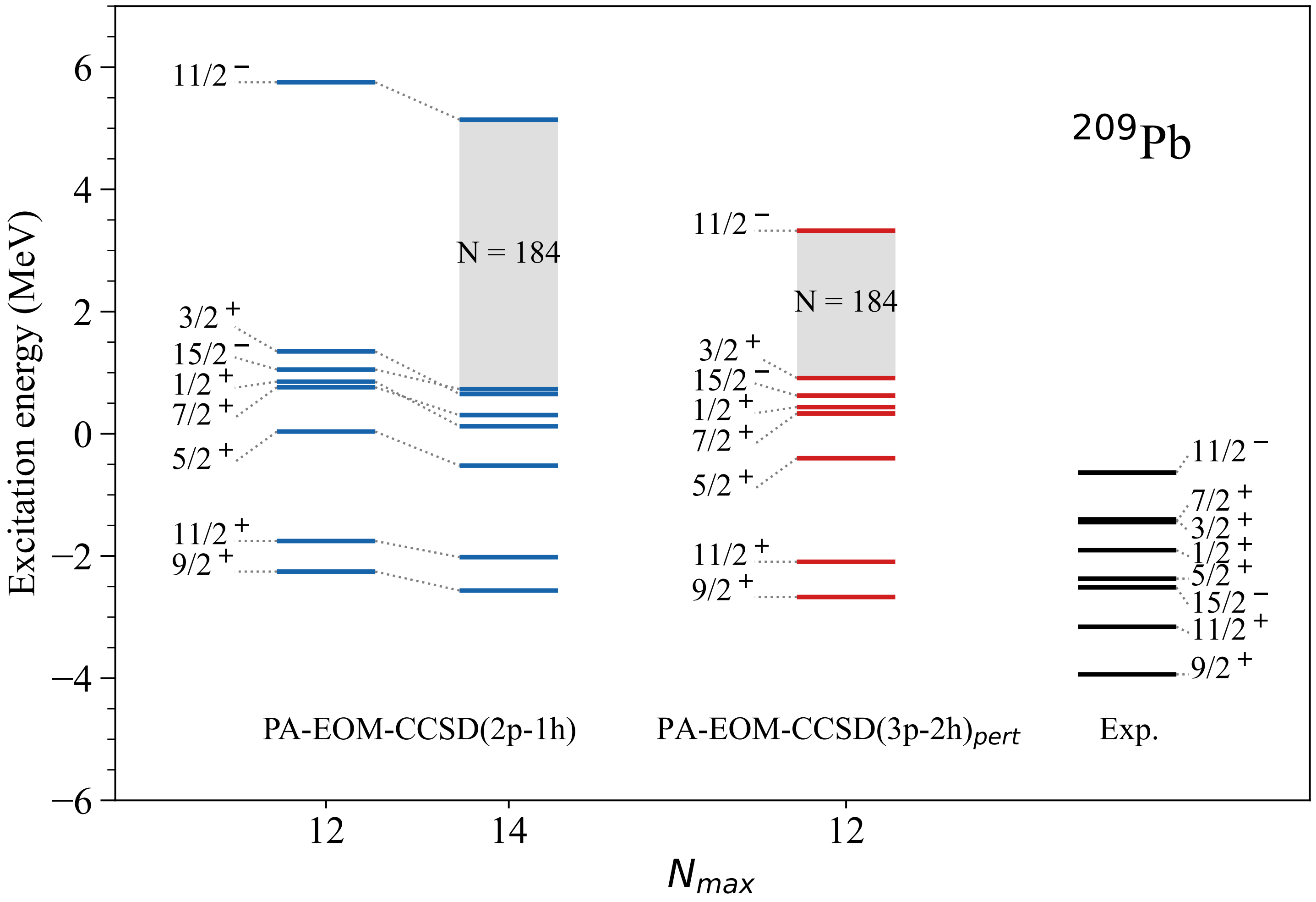




FB et al, arXiv:2508.14217 [nucl-th].

Excited states of ^{209}Pb

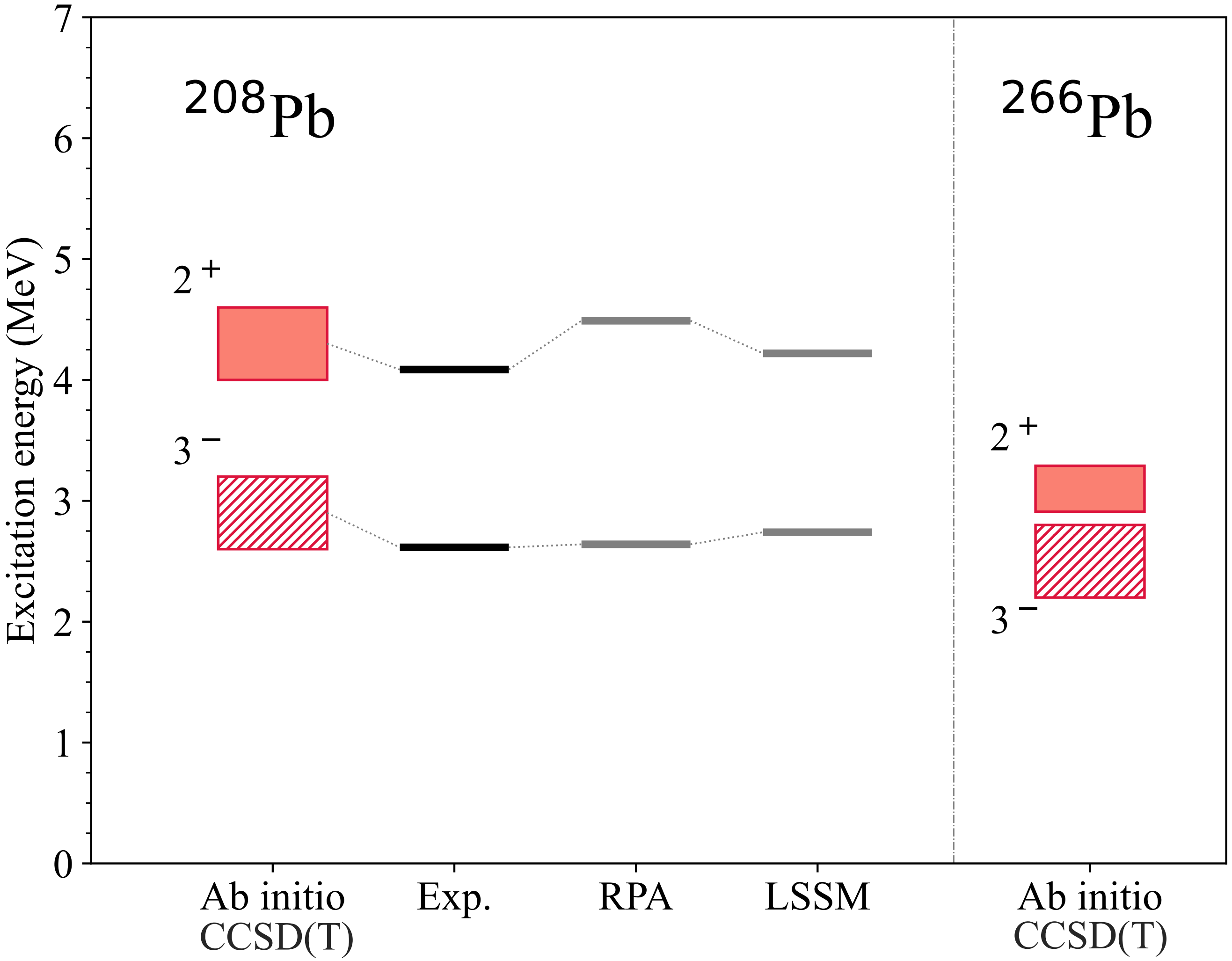
1.8/2.0 (EM) interaction



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

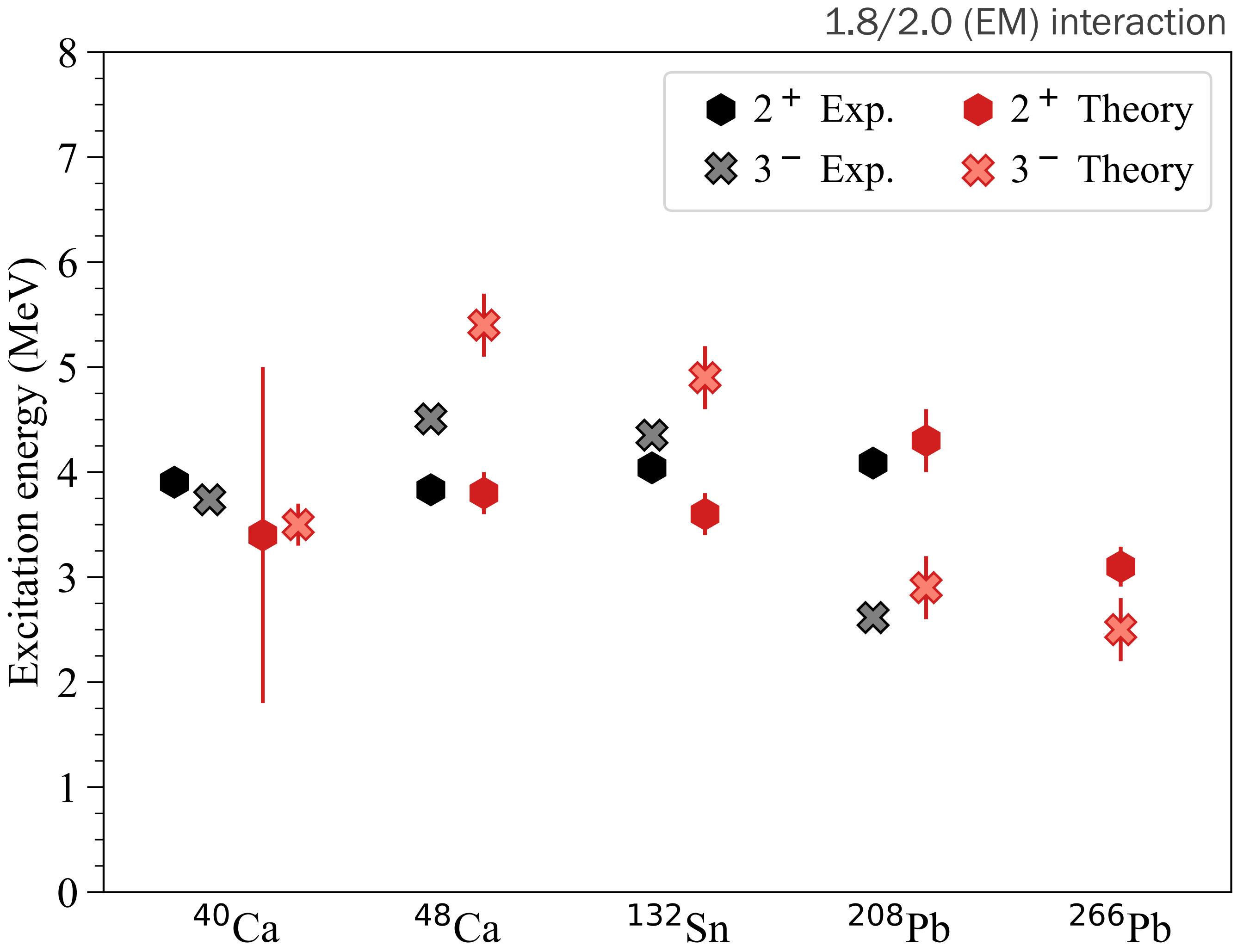
Structure of ^{208}Pb and ^{266}Pb

1.8/2.0 (EM) interaction



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

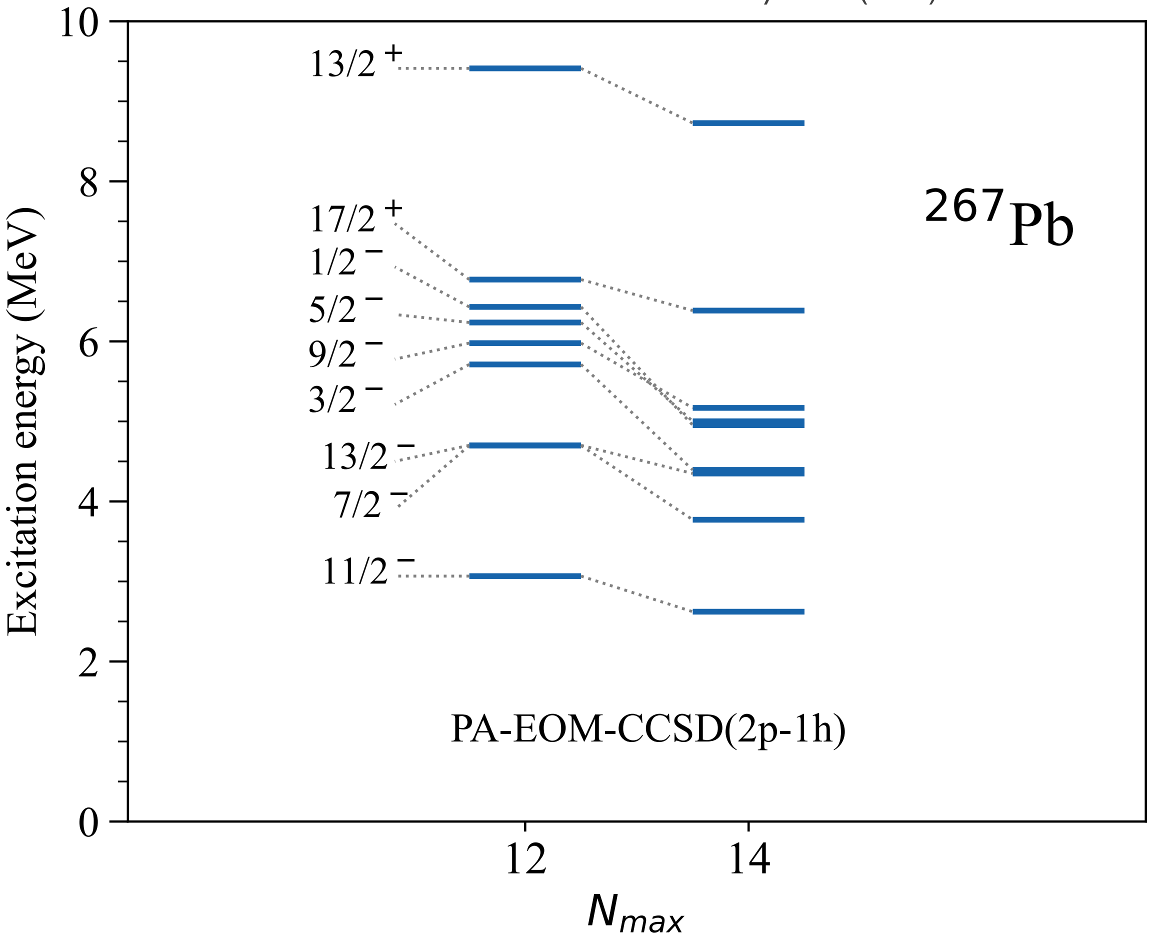
From light to heavy doubly magic nuclei



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

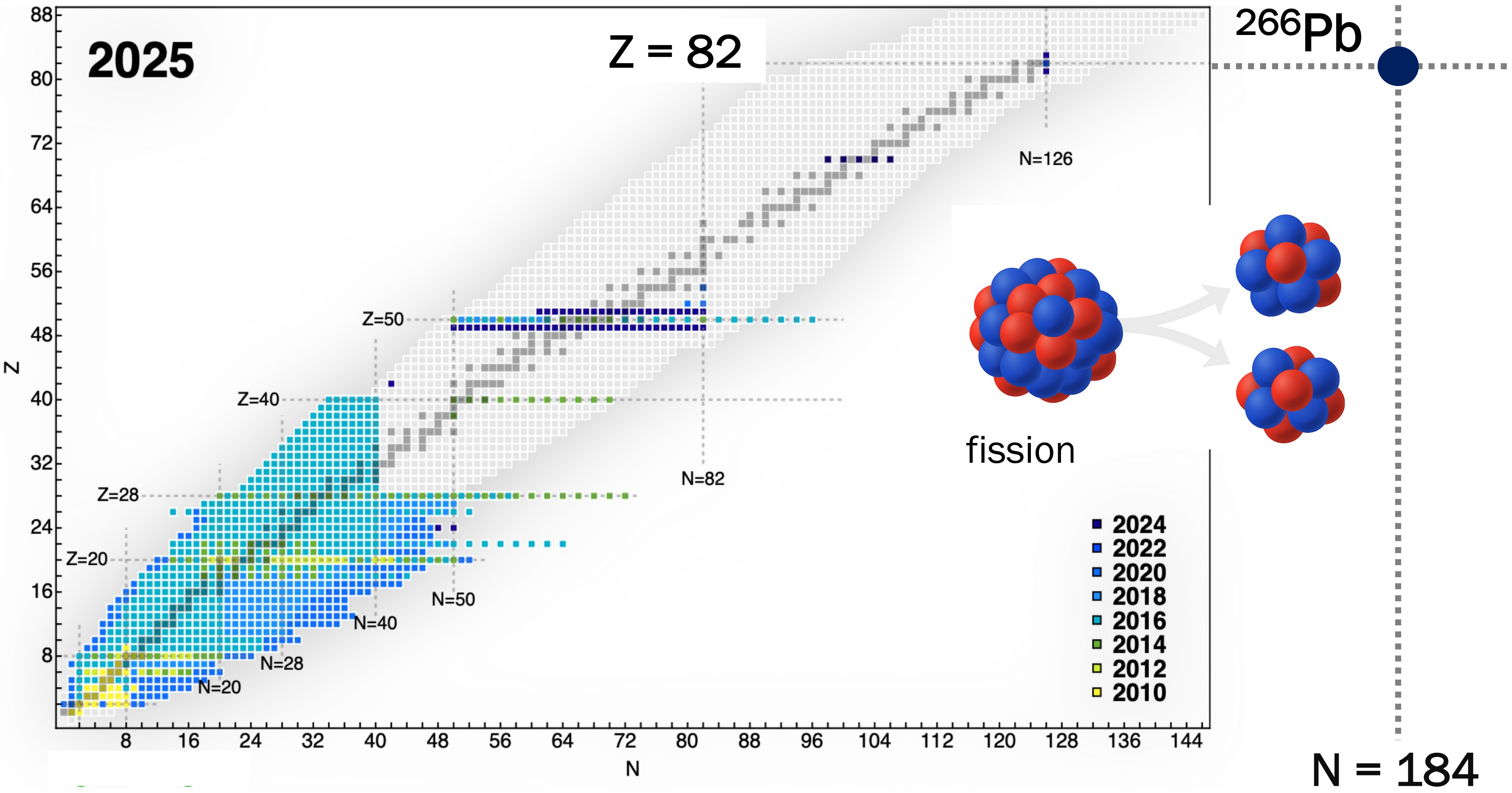
Is ^{266}Pb the last bound lead isotope?

1.8/2.0 (EM) interaction



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

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

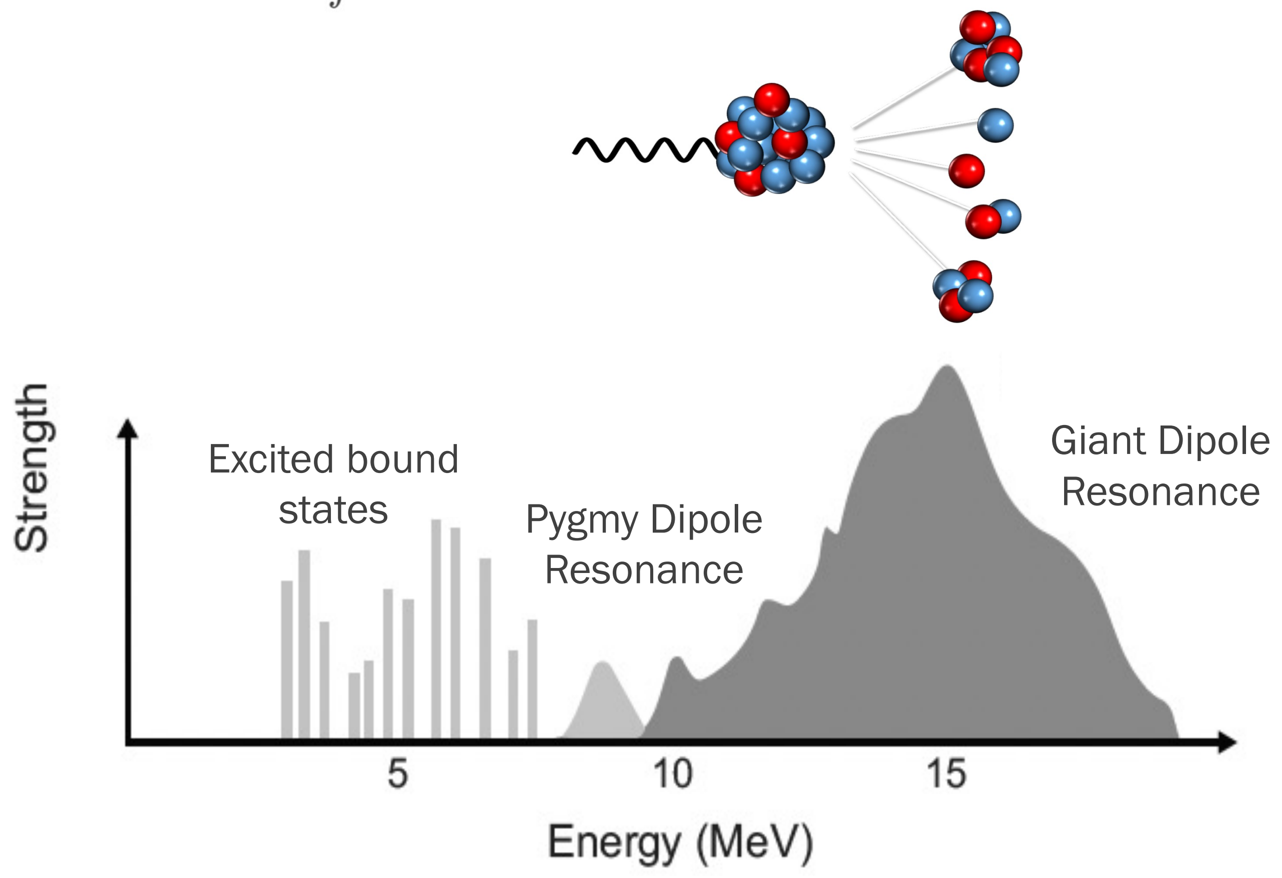


How to solve the time-dependent Schrödinger equation from a first-principles perspective?

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

Nuclear response functions

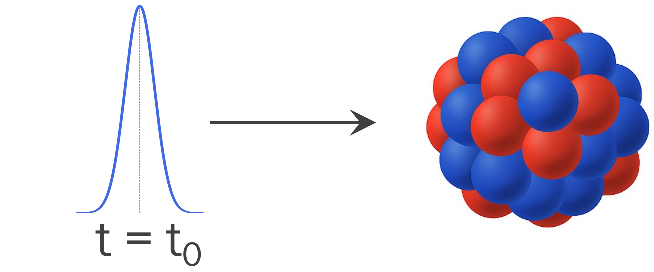
$$R(\omega) = \sum\!\!\!\!\!\!\!\int_f \left| \langle \Psi_f | \Theta | \Psi_0 \rangle \right|^2 \delta(E_f - E_0 - \omega)$$



Responses in a time-dependent approach

Goal: solving

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



with

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

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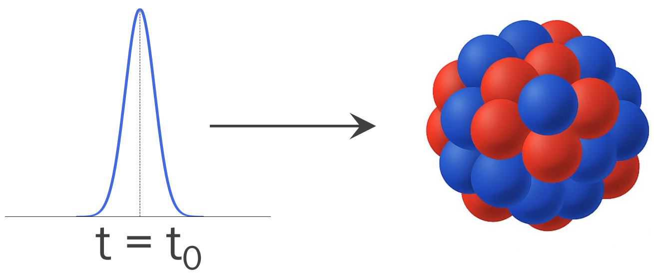

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For small ε, first-order time-dependent perturbation theory yields:

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

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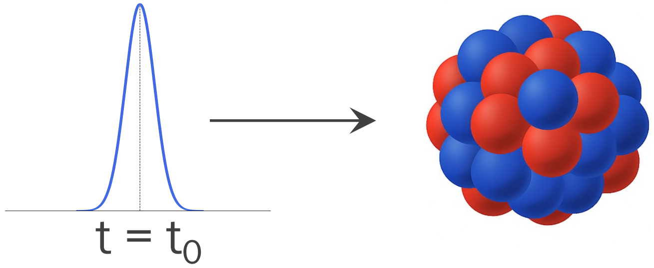

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Fourier transform

Responses in a time-dependent approach

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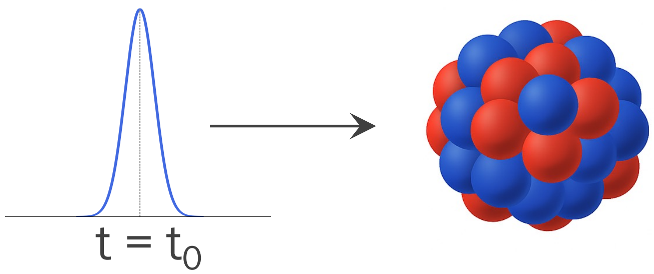
$$i\hbar \frac{d}{dt}|\Psi(t)\rangle = \hat{H}(t)\,|\Psi(t)\rangle$$



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

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

Fourier transform

Time-dependent coupled-cluster theory

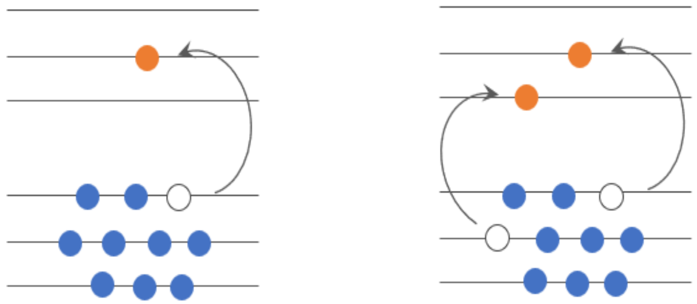
- Starting point: Hartree-Fock reference state $|\Phi_0\rangle$
- Add correlations via:

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

with

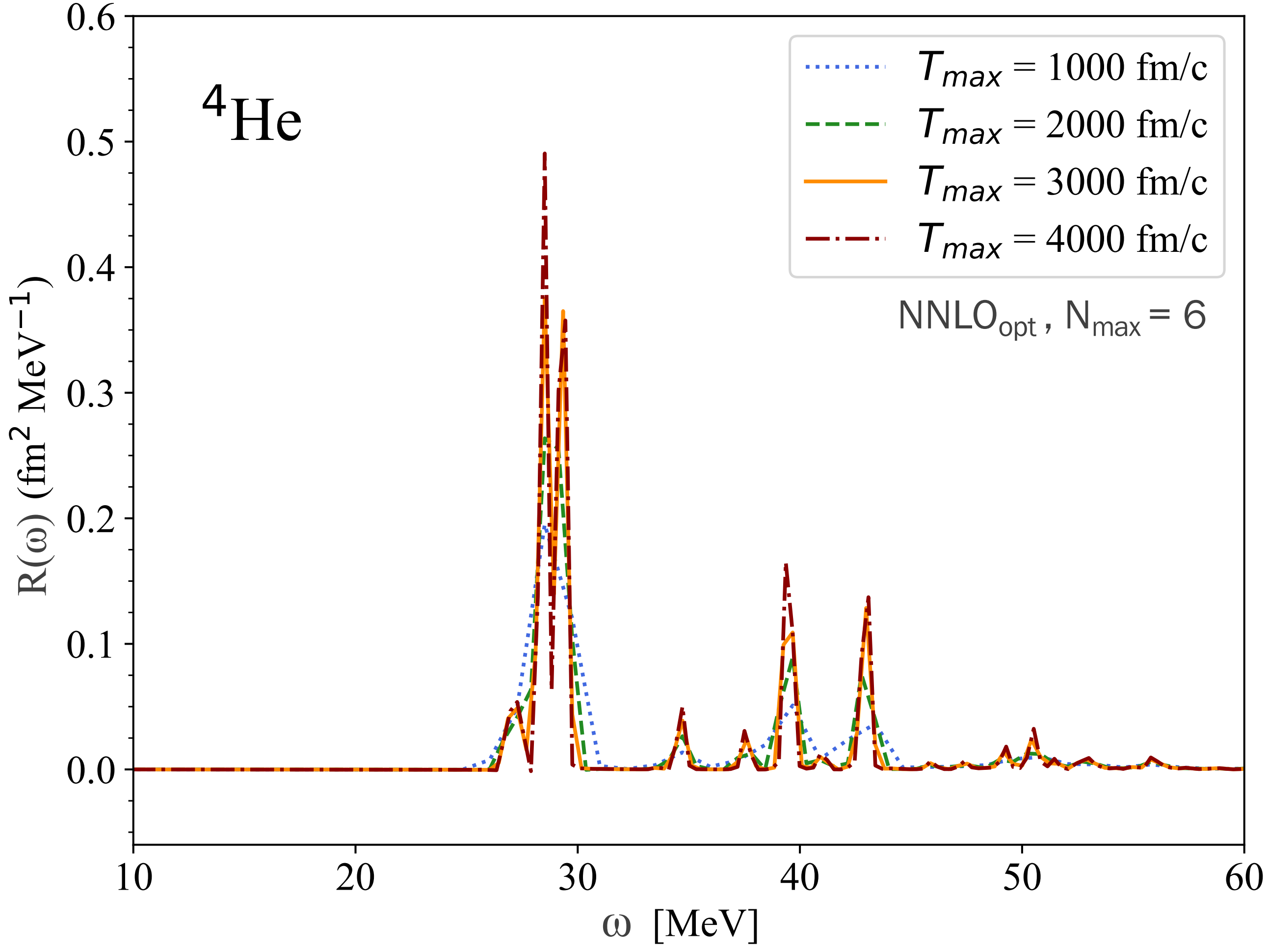
$$T(t) = t_0(t) + \sum_{ia} t_i^a(t) a_a^\dagger a_i + \sum_{ijab} t_{ij}^{ab}(t) a_a^\dagger a_b^\dagger a_j a_i + \dots$$

singles and
doubles
(CCSD)



G. Hagen, T. Papenbrock, M. Hjorth-Jensen, D. J. Dean, RPP 77, 096302 (2014).

Simulation time and resolution



Resolution

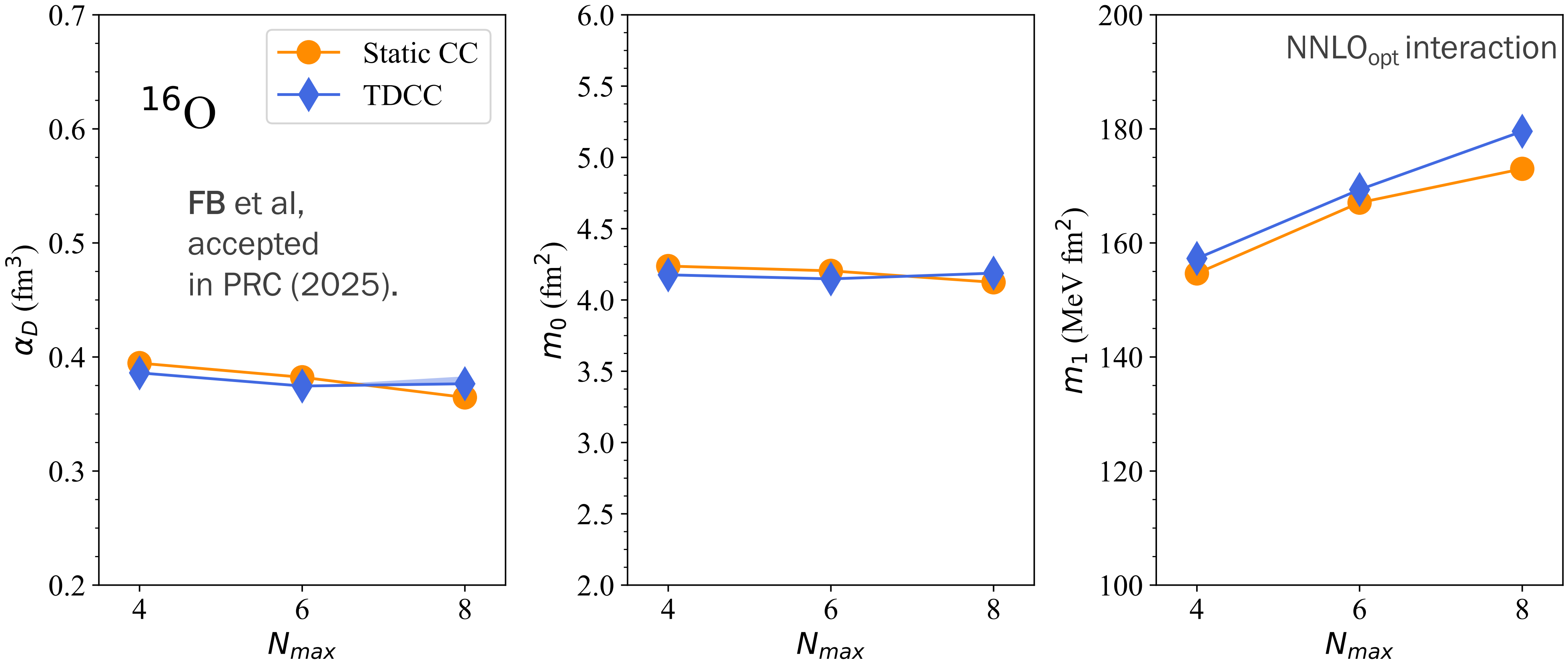
$$\boxed{\Delta\omega} = \frac{2\pi\hbar c}{\boxed{t_{max}}}$$

Maximum simulation time

FB et al, accepted in PRC (2025).

Static CC vs time-dependent CC: ^{16}O

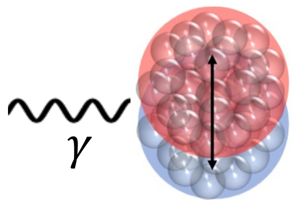
$$\alpha_D = 2\alpha \int d\omega\, \omega^{-1} R(\omega) \qquad m_0 = \int d\omega R(\omega) \qquad m_1 = \int d\omega\, \omega R(\omega)$$

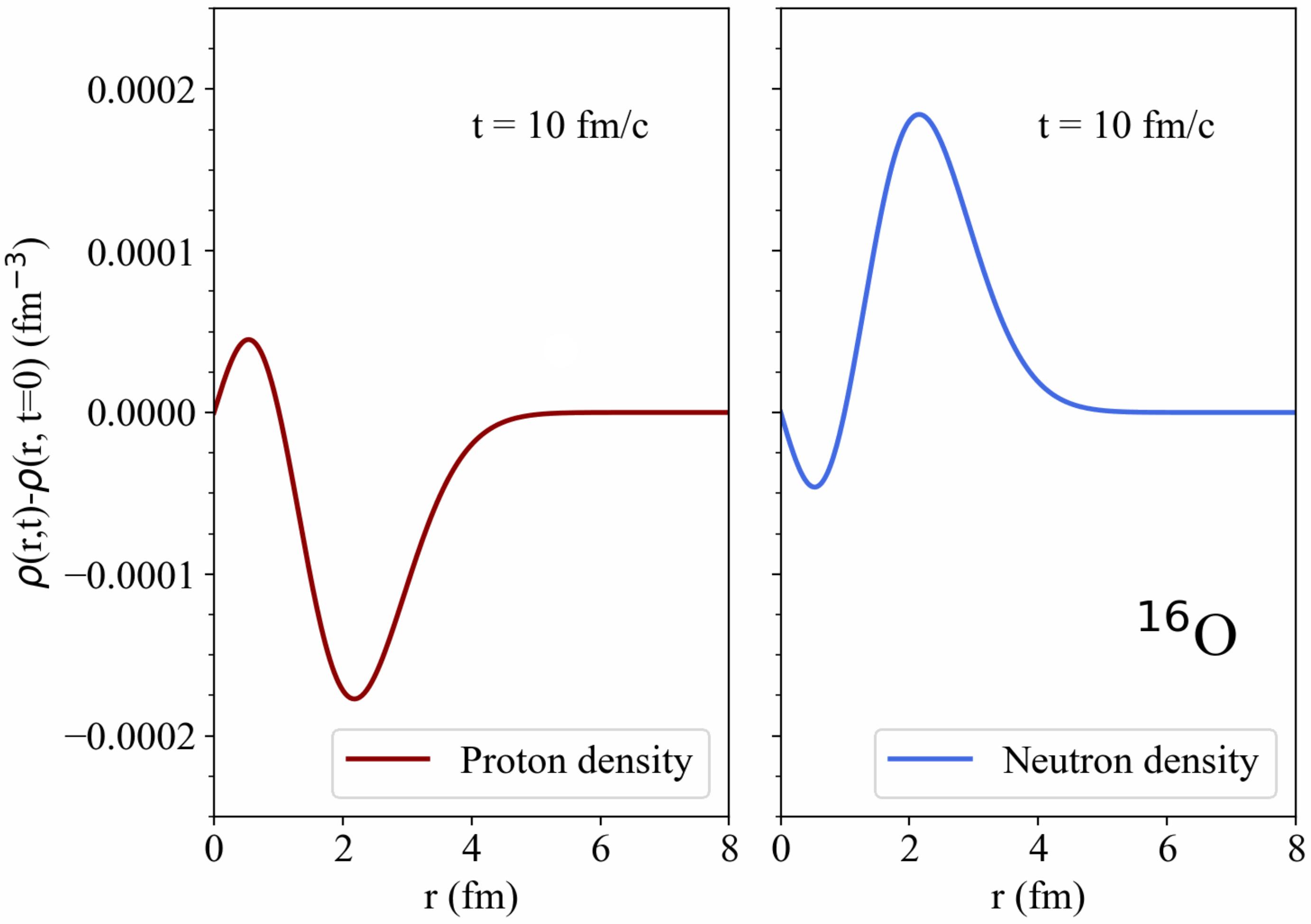


Very small deviations between the two completely independent approaches!

Collective oscillations in real time

^{16}O



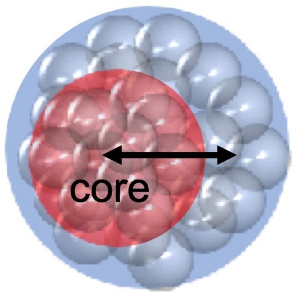


$NNLO_{opt}$,
$N_{max} = 6$

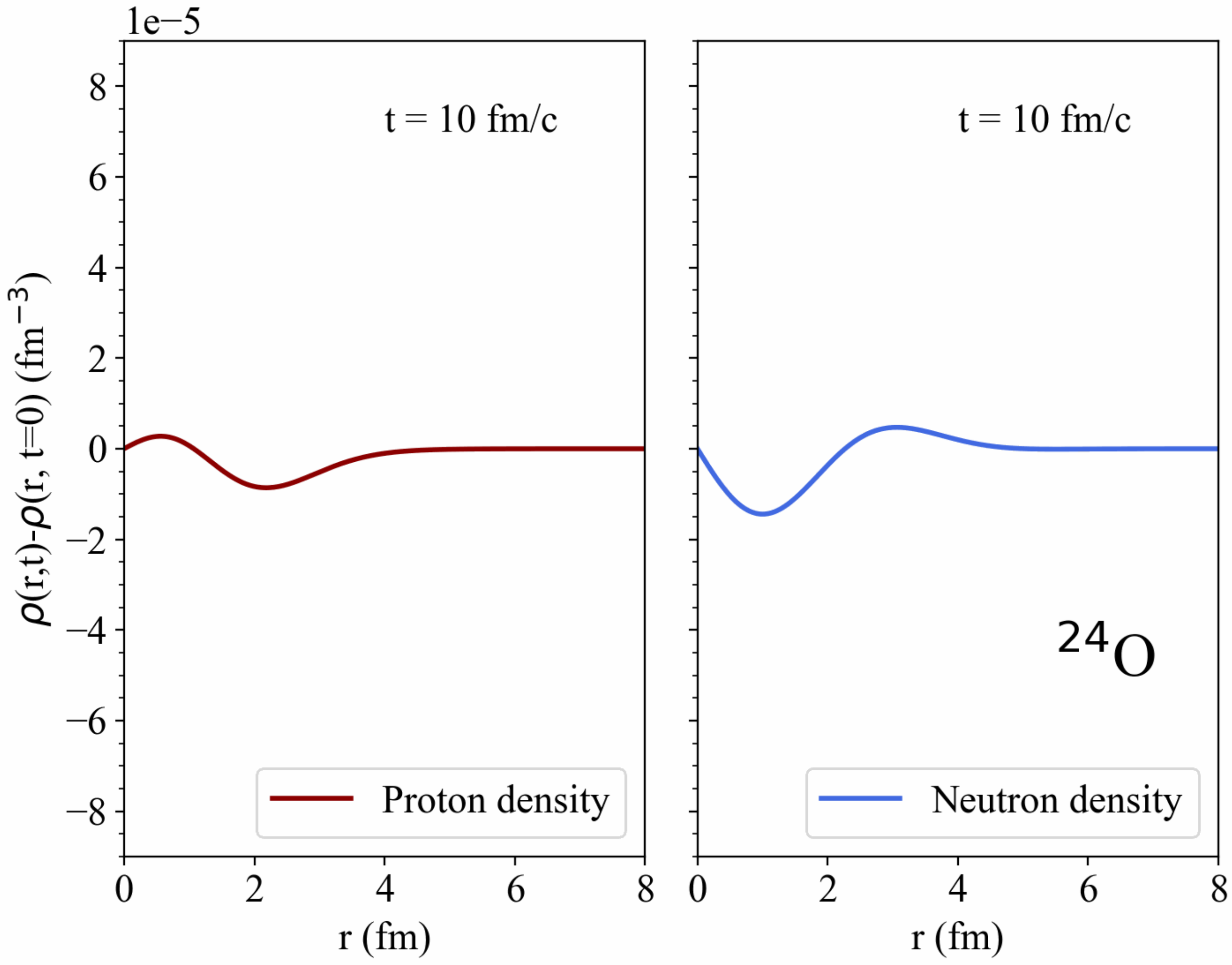
FB et al, accepted in PRC (2025).

Collective oscillations in real time

^{24}O



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



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

FB et al, accepted in PRC (2025).

What happens when we increase ε?

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

- Up to now, ε = 0.1 MeV/fm, where we are still in the linear regime.
- Non-linearities emerge when the perturbation becomes comparable to typical scale of H_0.
- For ^{16}O, $B(E1)^{1/2}$ ~ 0.01 e fm [TUNL database], so we need ε = 100 MeV/fm to get a perturbation ~ MeV.

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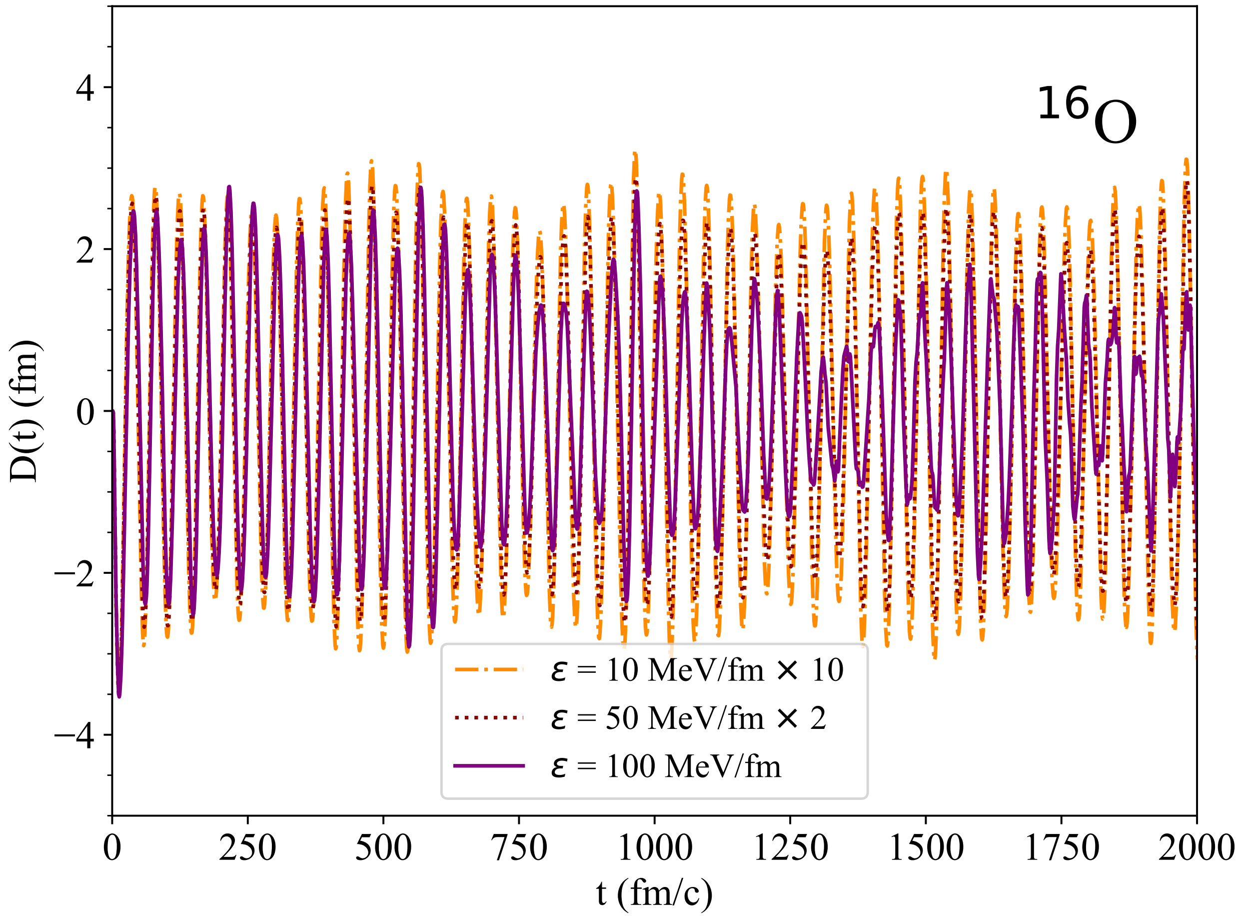
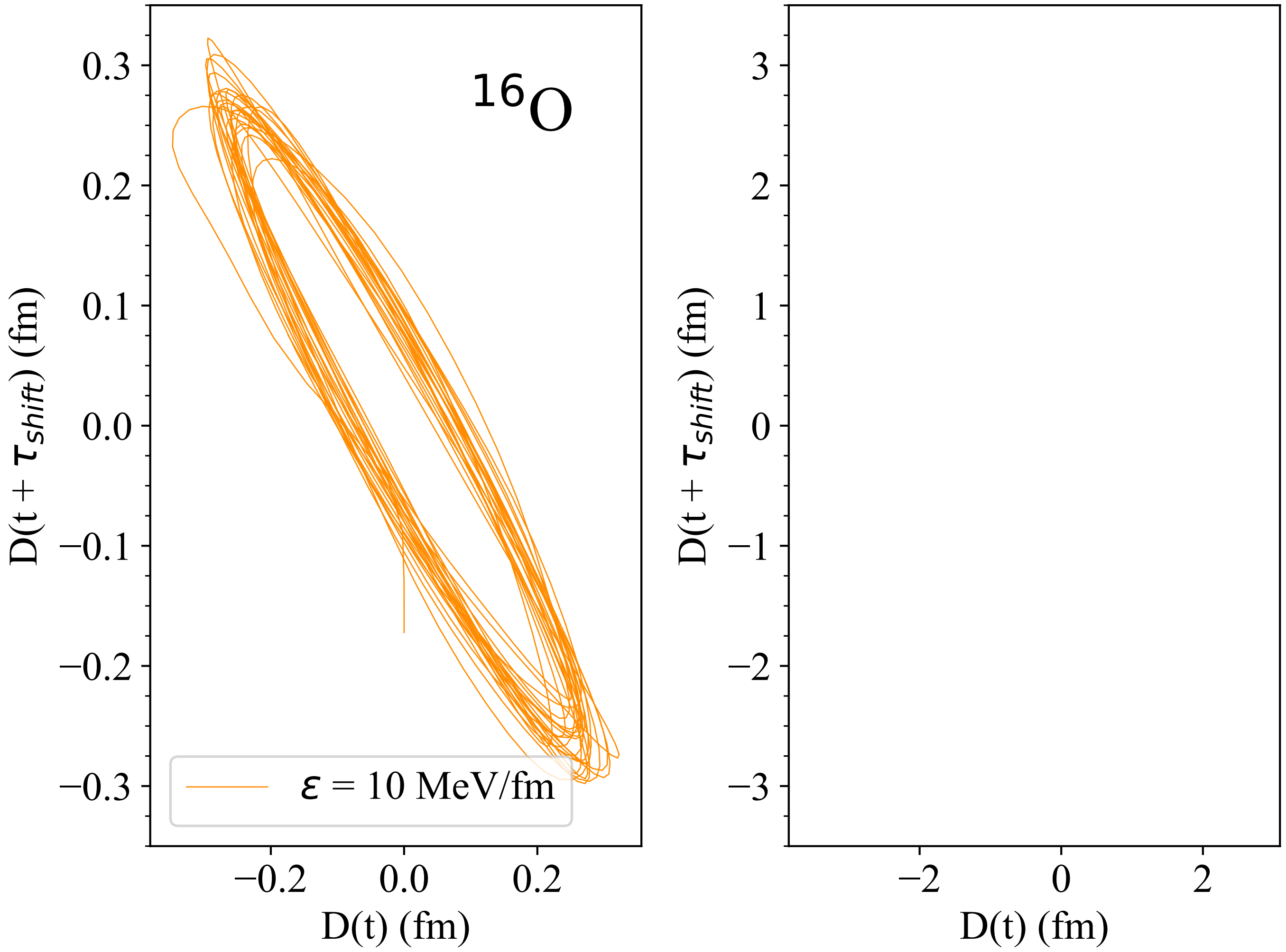


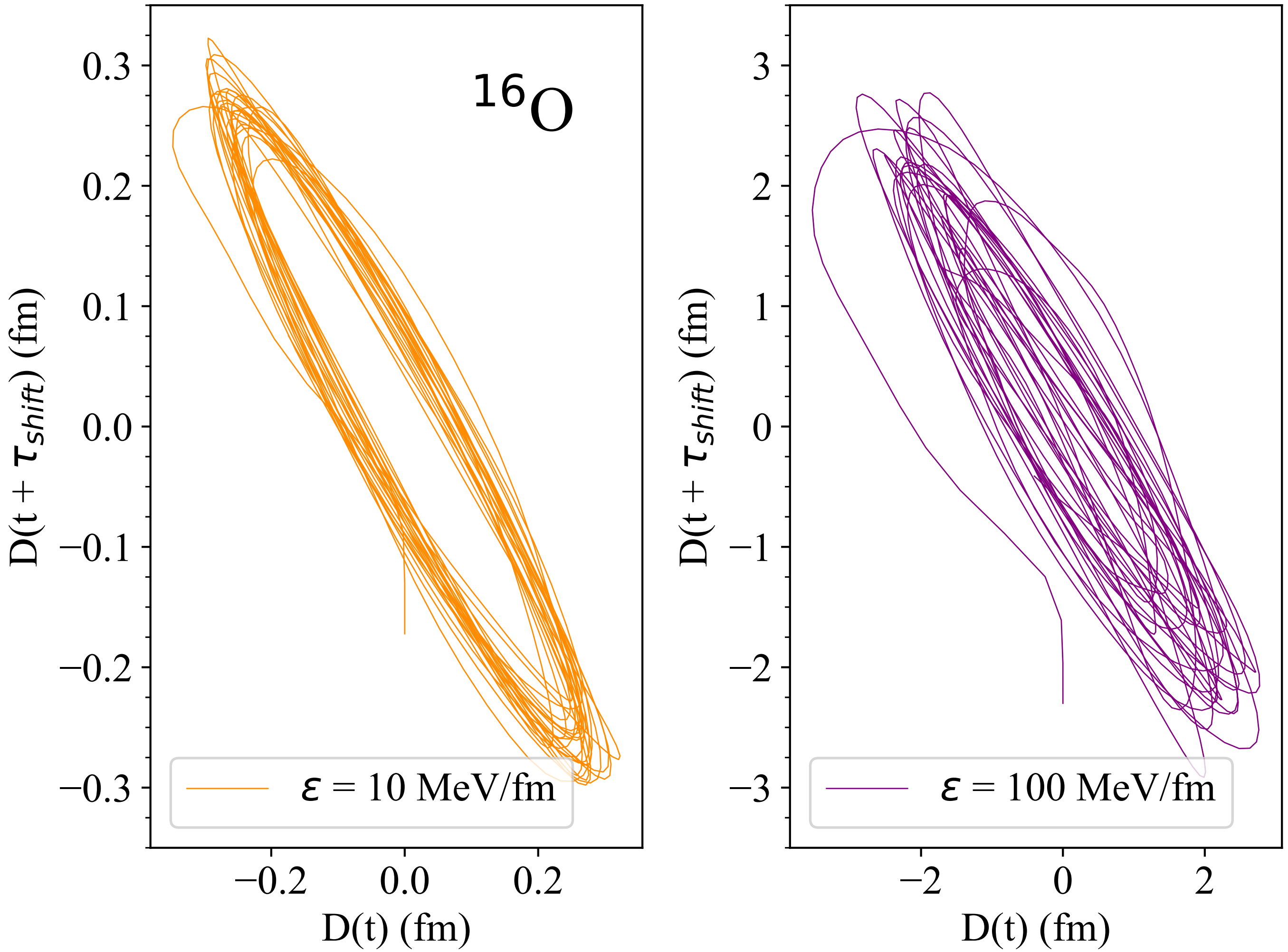
FB et al, arXiv:2510.19940 [nucl-th].

From order…



FB et al, arXiv:2510.19940 [nucl-th].

From order to chaos



FB et al, arXiv:2510.19940 [nucl-th].

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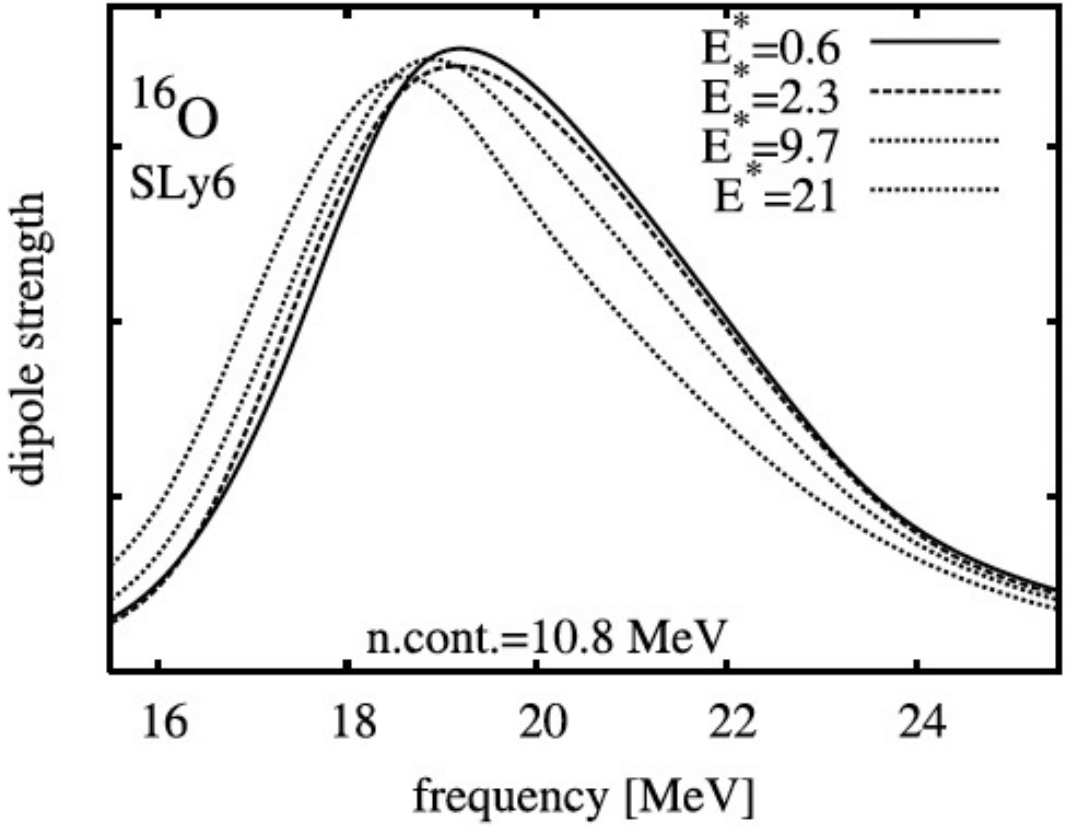

P.-G. Reinhard et al, Eur. Phys. J. A 32, 19–23 (2007).

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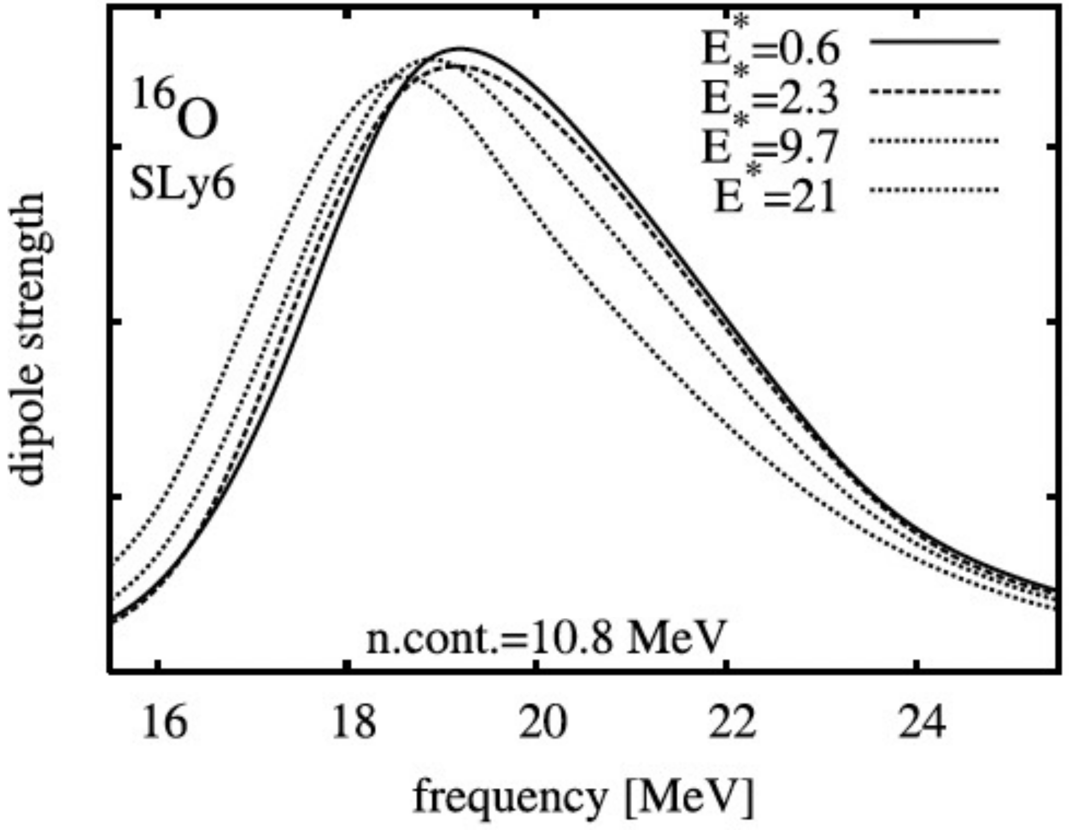

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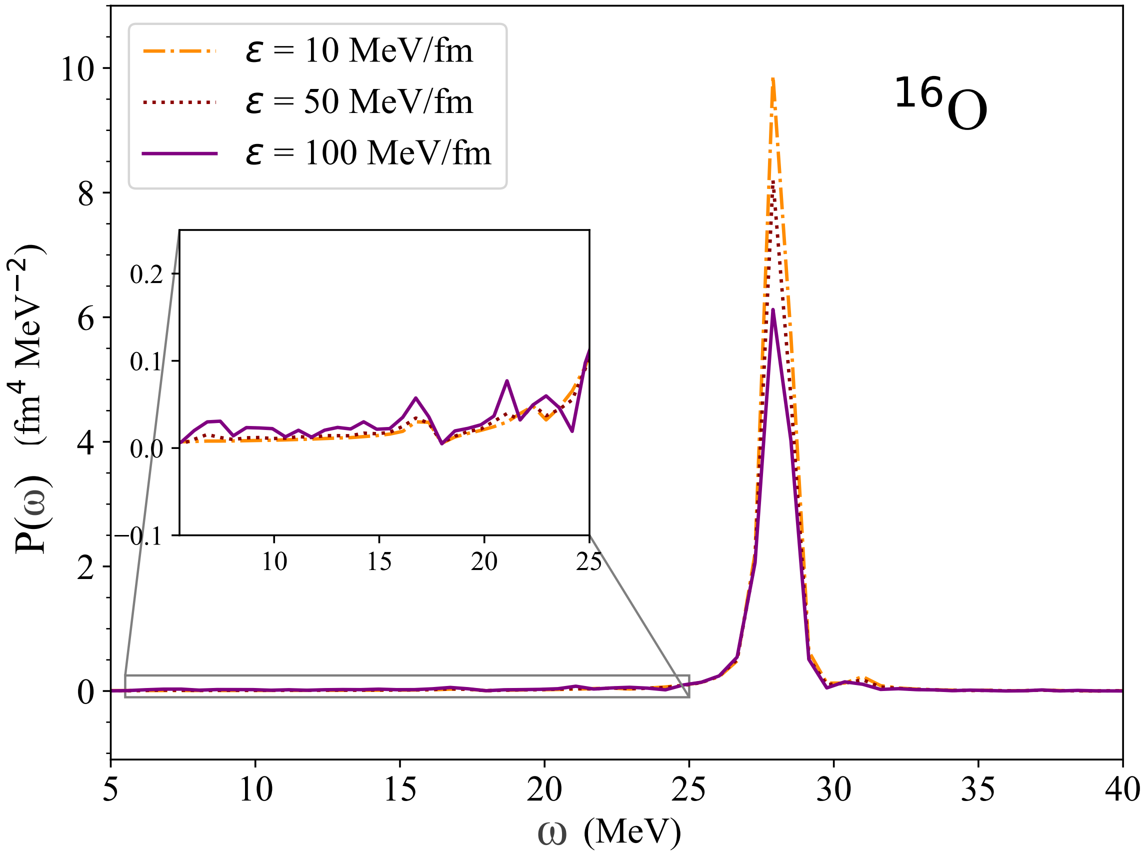

FB et al, arXiv:2510.19940 [nucl-th].

Conclusions

- We showed the doubly-magic nature of ^{266}Pb from first principles.
- We are able to visualize collective oscillations as pygmy and giant dipole resonances and explore the strong-field limit by incorporating time dependence in our many-body framework.
- We aim to couple this with calculations on the lattice (see Matthias Heinz's talk), a natural framework where to achieve a microscopic description of nuclear dynamics.

Stay tuned!

Thanks to my collaborators:

@ORNL/UTK: Gaute Hagen, Matthias Heinz, Gustav R. Jansen, Ben Johnson-Toth, Thomas Papenbrock, Maxwell Rothman
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@JGU Mainz: Sonia Bacca, Tim Egert, Weiguang Jiang, Francesco Marino
@LLNL: Cody Balos, Carol Woodward
@TU Darmstadt: Andrea Porro, Alex Tichai, Achim Schwenk

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FRIB Theory Alliance

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