



Facility for Rare Isotope Beams
at Michigan State University



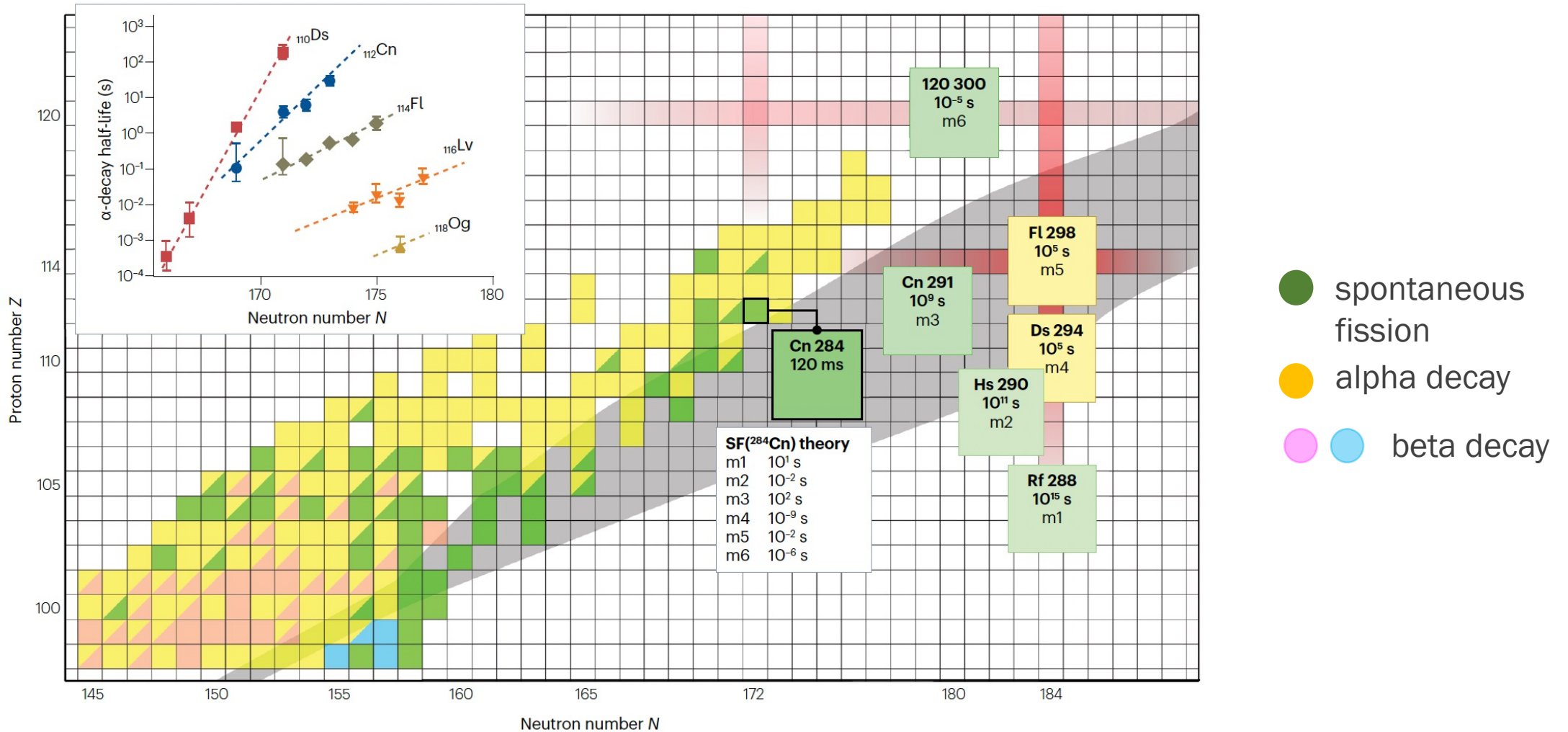
Coupled-cluster computations of superheavy nuclei

FRANCESCA BONAITI, FRIB&ORNL

PAINT 2026 WORKSHOP @ TRIUMF, VANCOUVER

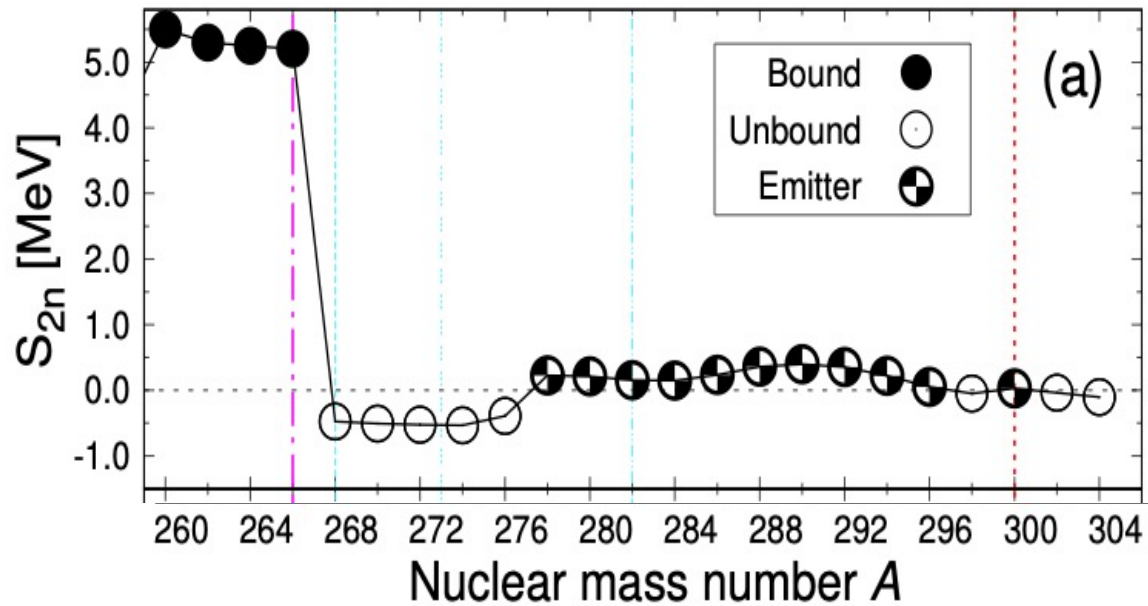
FEBRUARY 24, 2026

Searches for the “island of stability”

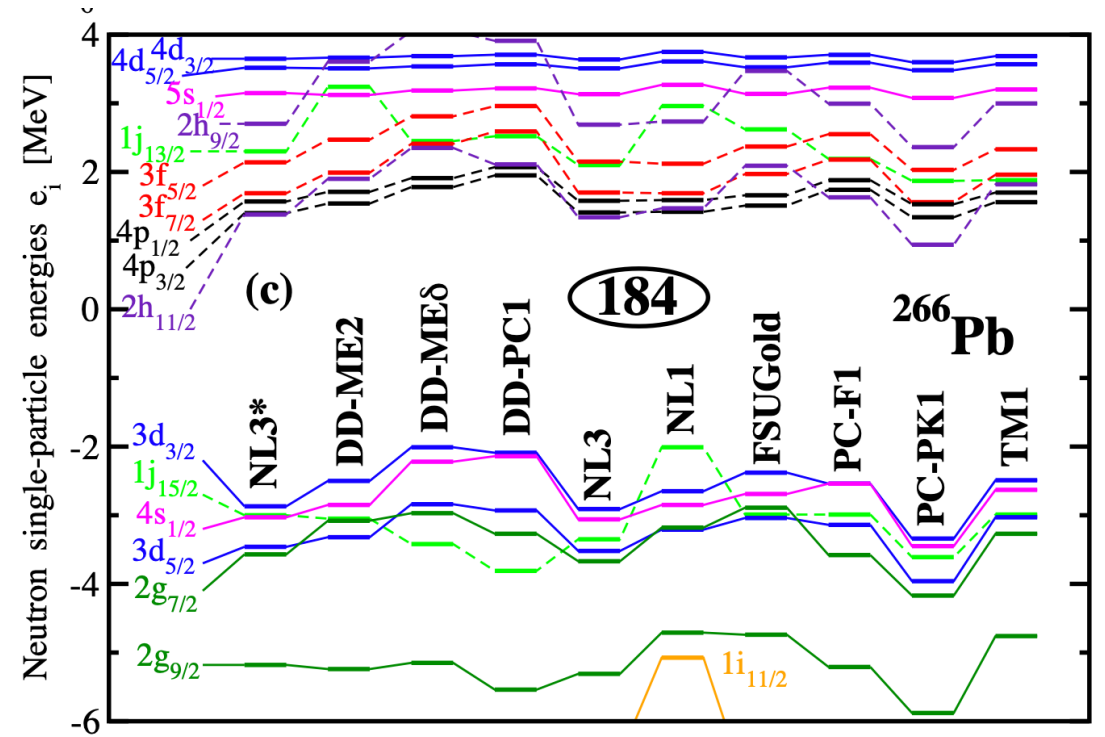


What is the next shell closure
we find beyond ^{208}Pb ?

A possible candidate: ^{266}Pb



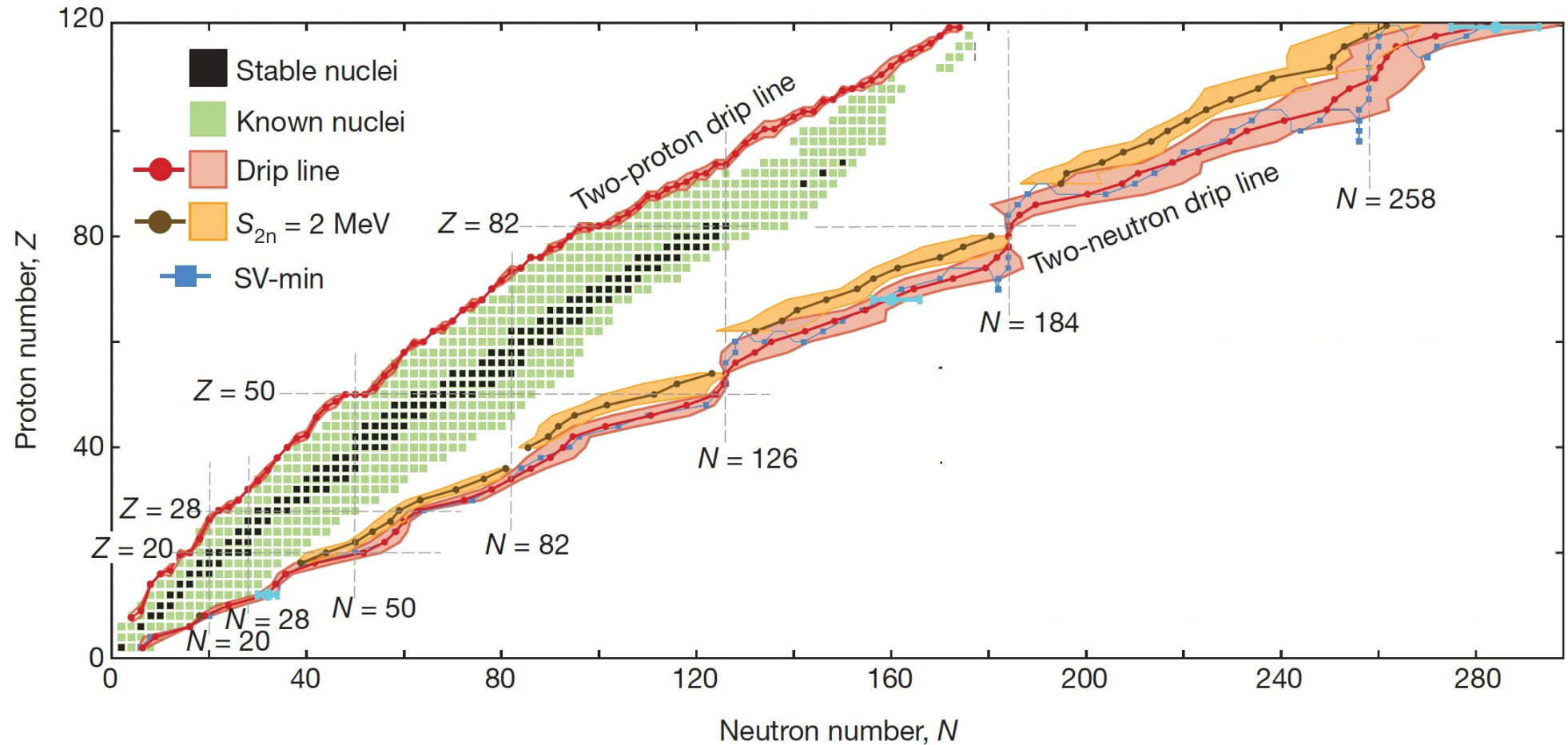
S. Kim et al, PRC 105, 034340 (2022).



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

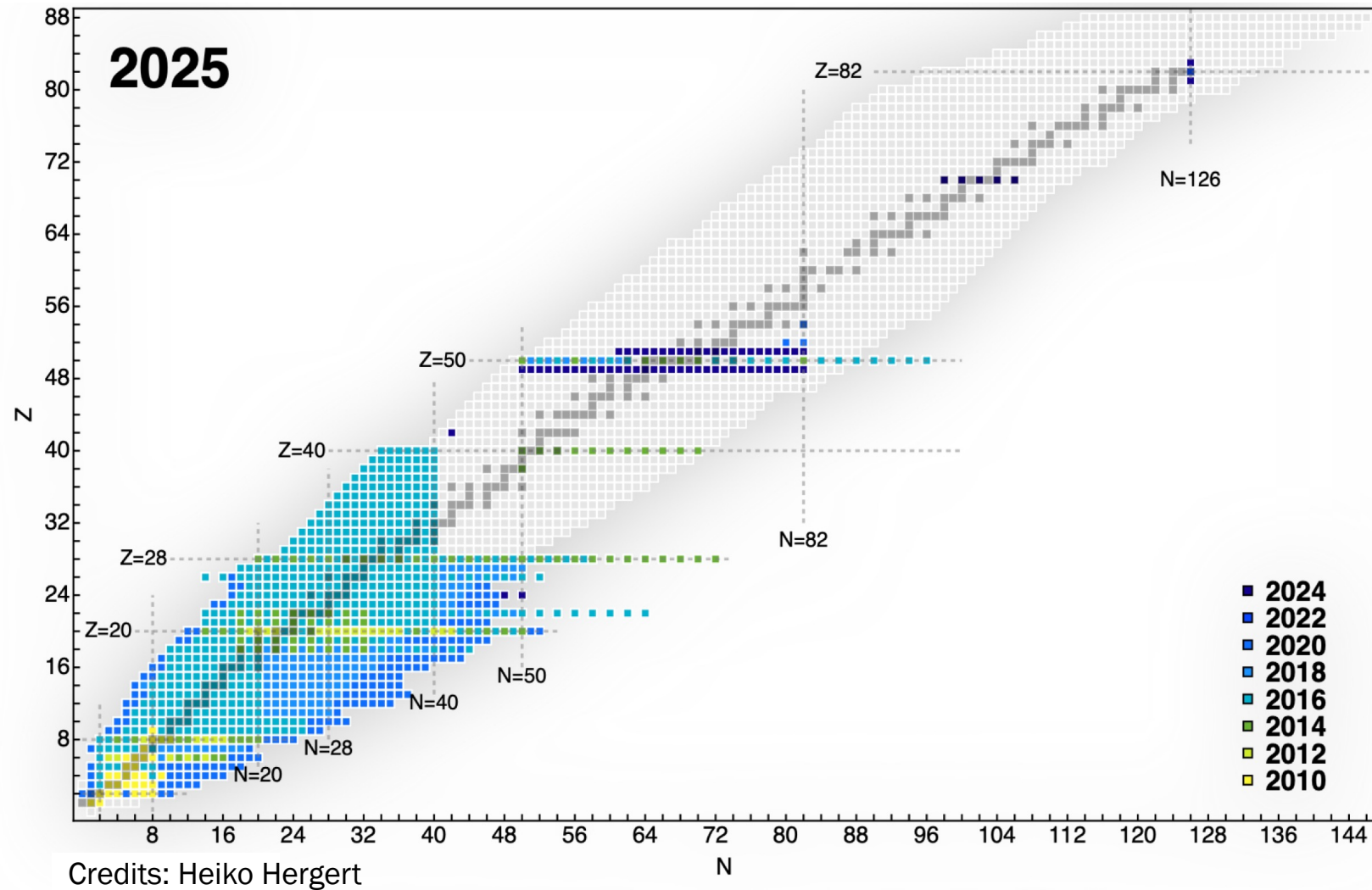
Separation energies and single-particle energies results from mean-field calculations indicate possible doubly-magic nature of ^{266}Pb .

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



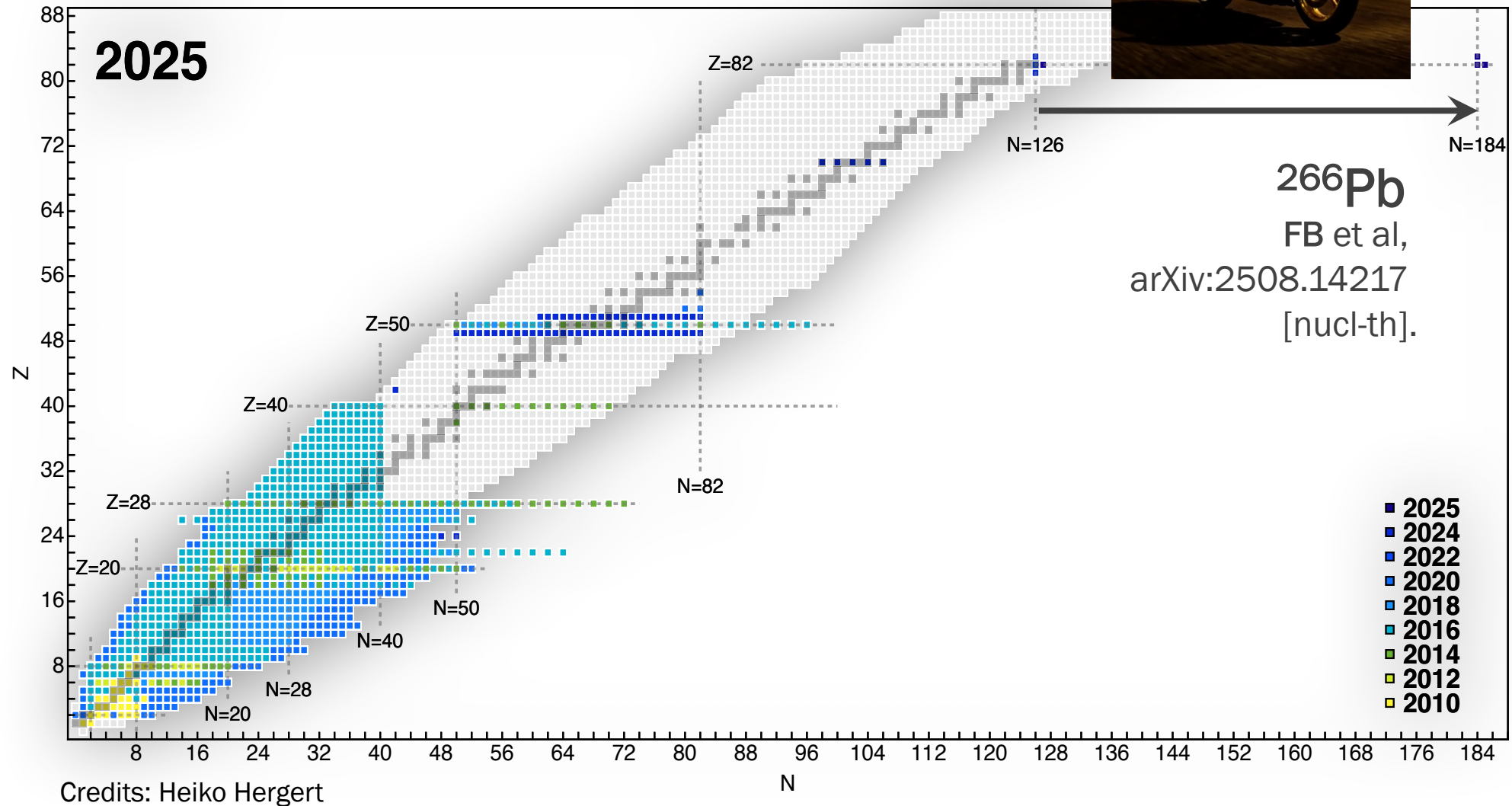
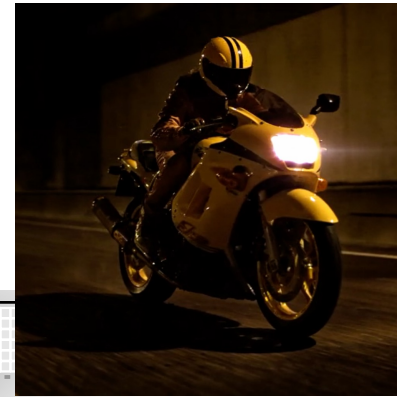
We can now tackle these
questions from an *ab initio*
perspective!

Until July 2025...



Credits: Heiko Hergert

... and now!



Coupled-cluster theory

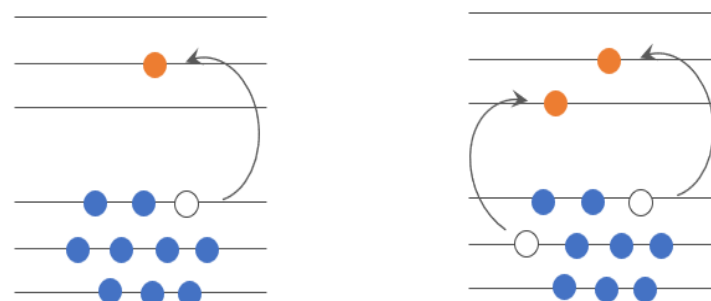
- Starting point: **Hartree-Fock** reference state $|\Phi_0\rangle$
- Add correlations via:

$$|\Psi_0\rangle = e^T |\Phi_0\rangle$$

with

$$T = \sum t_i^a a_a^\dagger a_i + \sum t_{ij}^{ab} a_a^\dagger a_b^\dagger a_j a_i + \dots$$

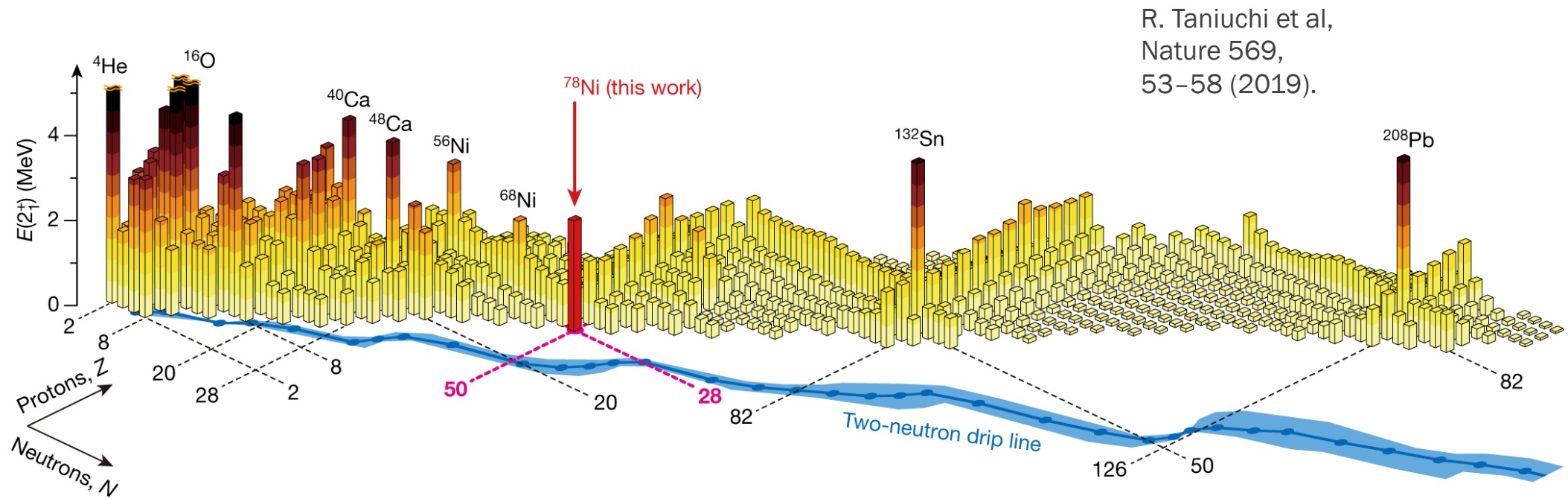
singles and
doubles
(CCSD)



triples excitations
with the **CCSD(T)**
framework

→ coefficients
from **coupled-
cluster equations**

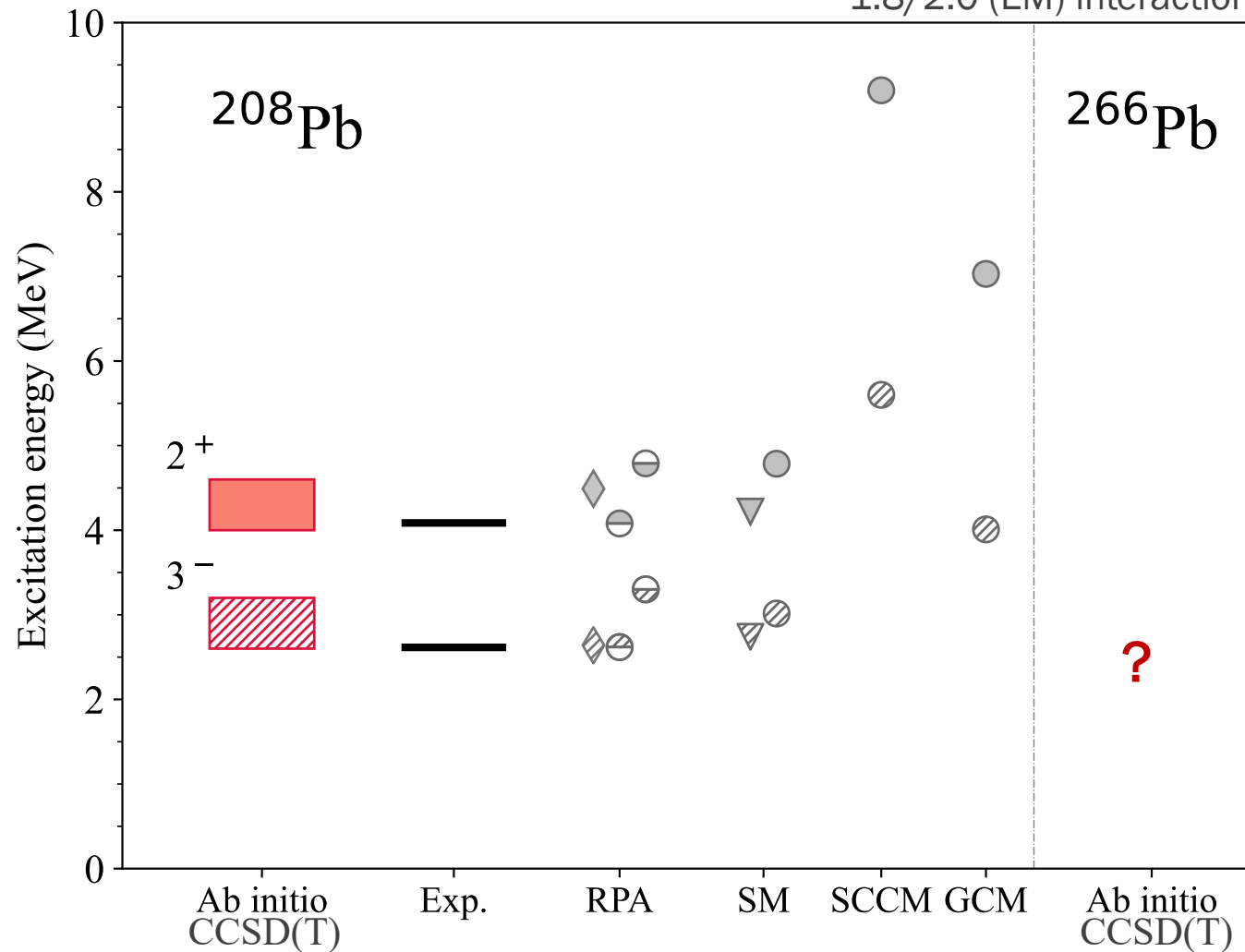
“Doubly magic” signatures: the first 2^+ state



Goal: predicting the excited spectrum of ^{266}Pb from first principles.

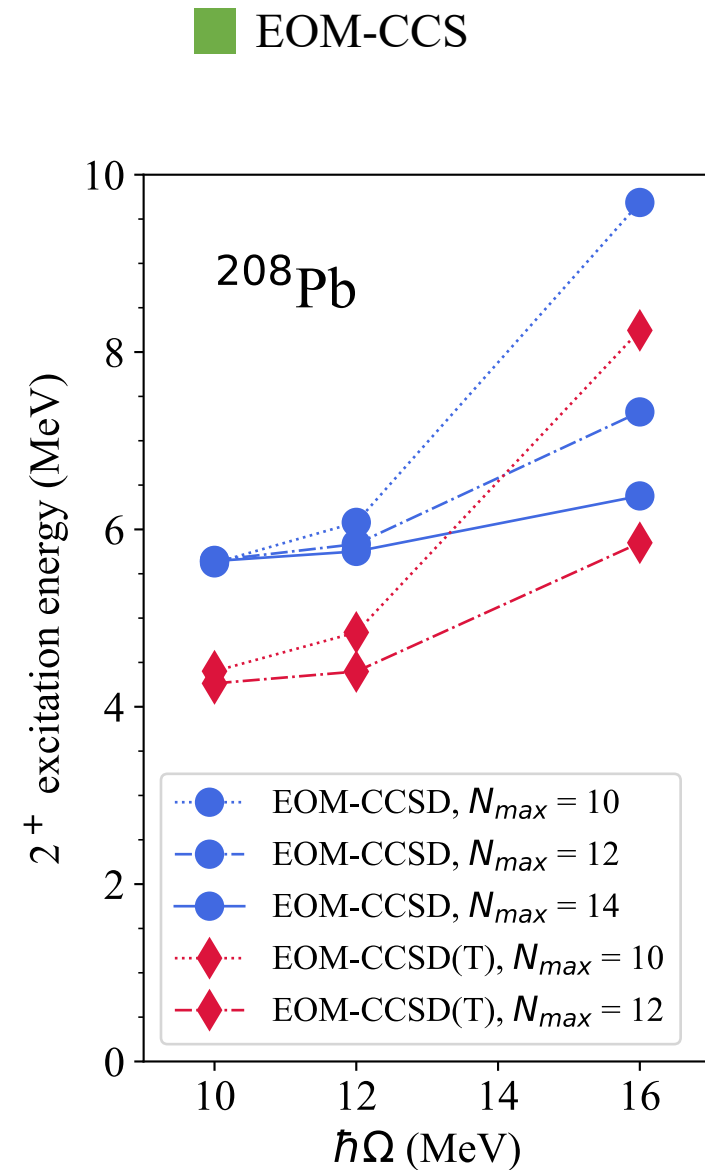
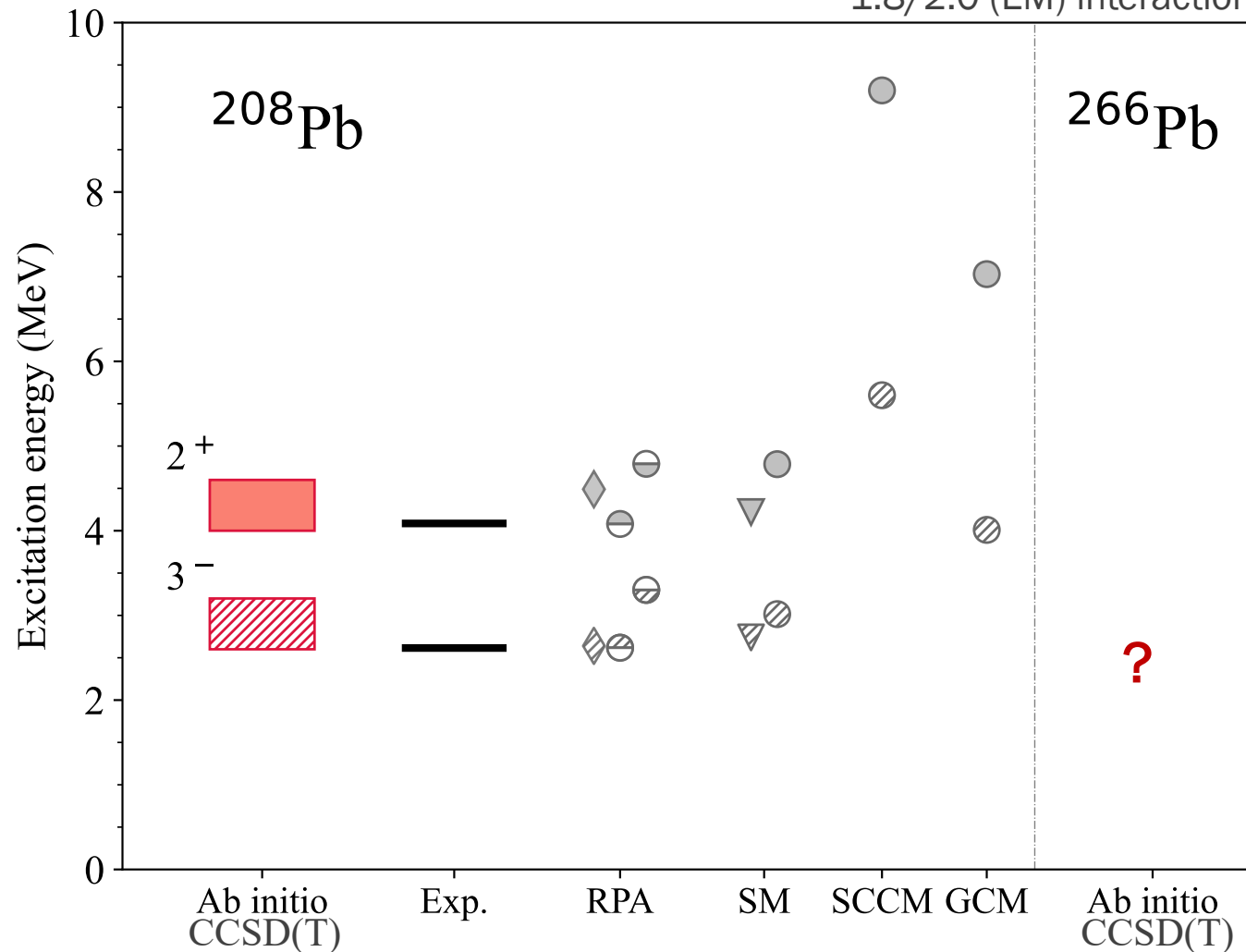
Excited states in ^{208}Pb

1.8/2.0 (EM) interaction



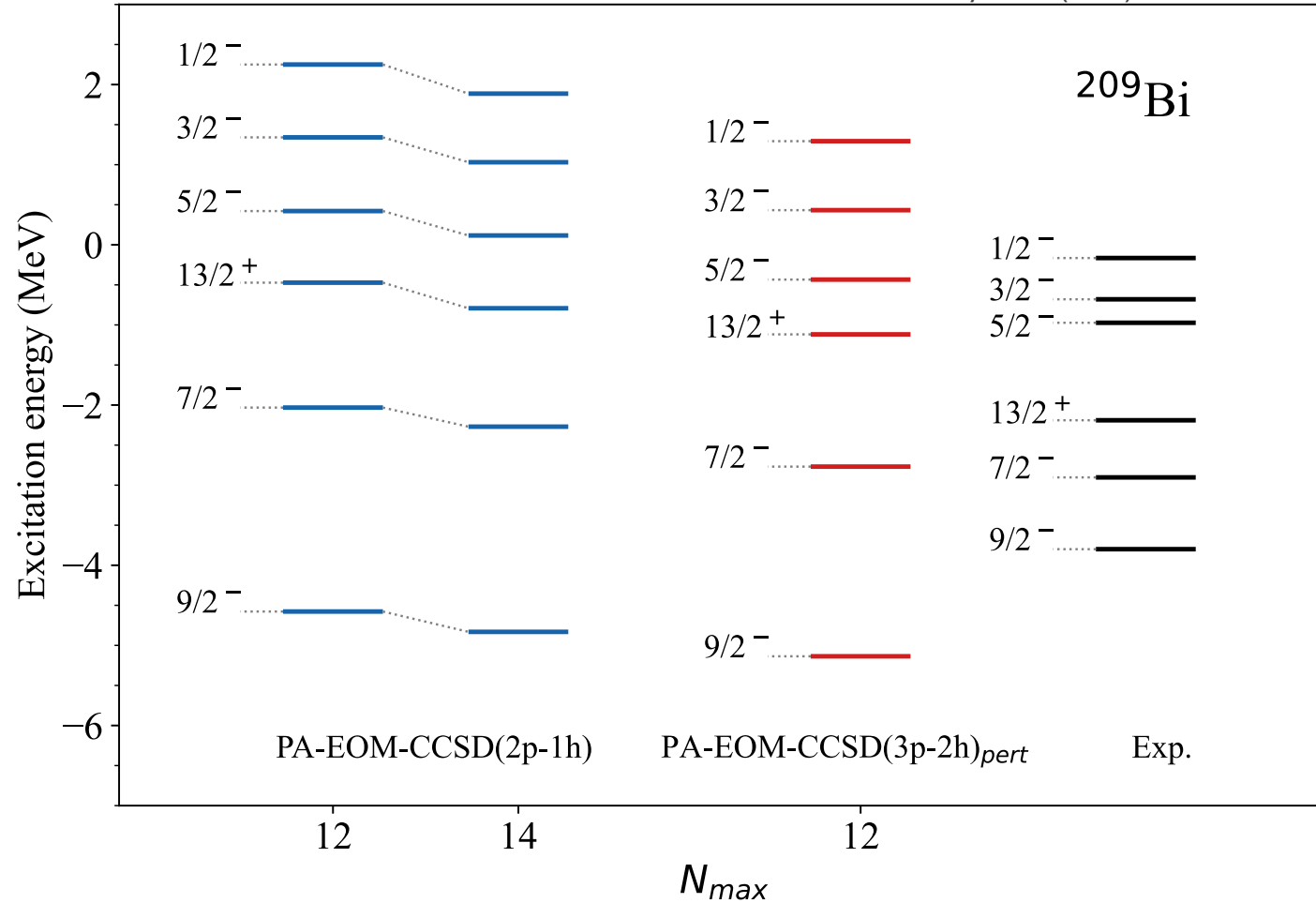
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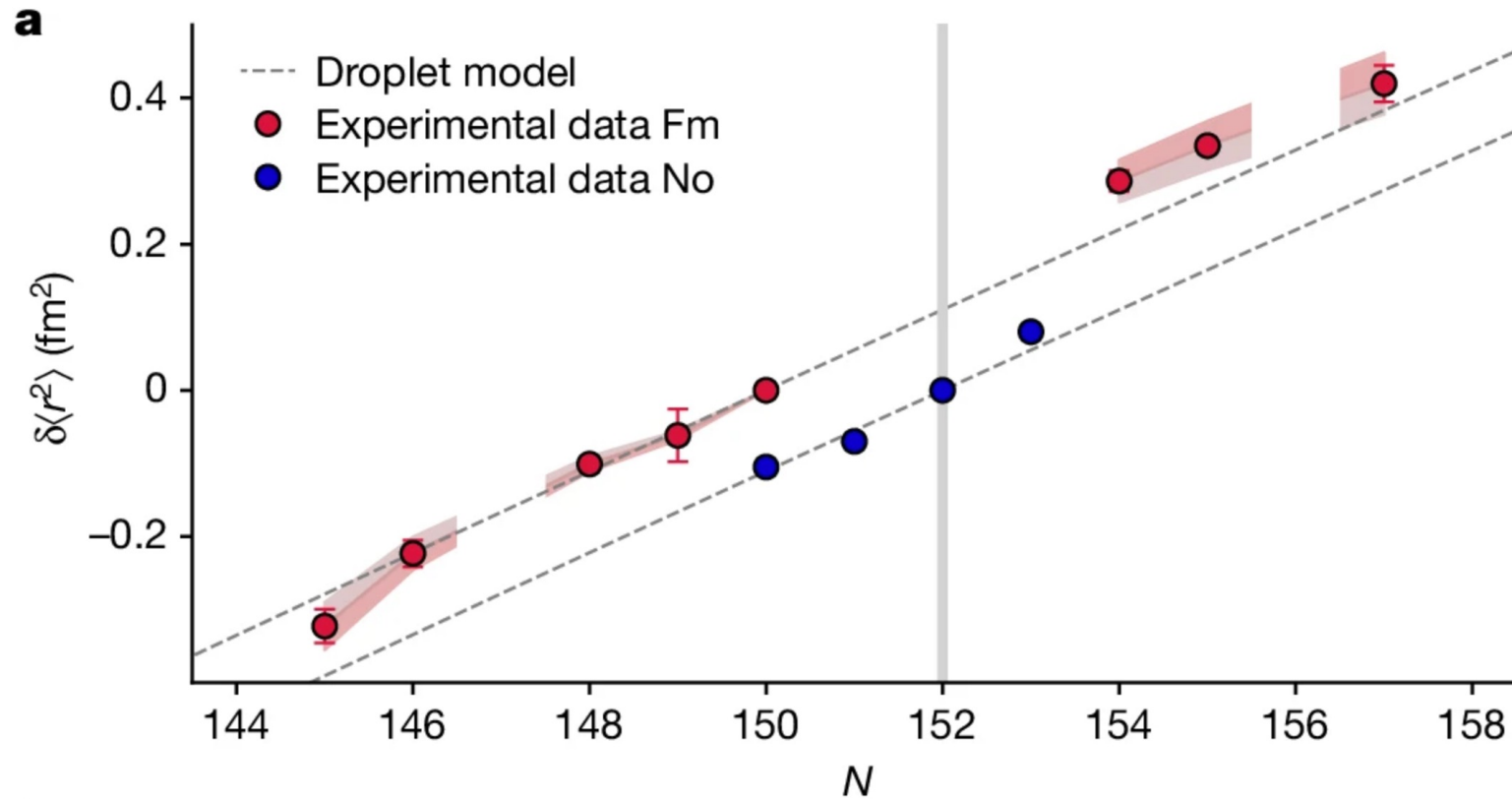
Excited states of ^{209}Bi

1.8/2.0 (EM) interaction



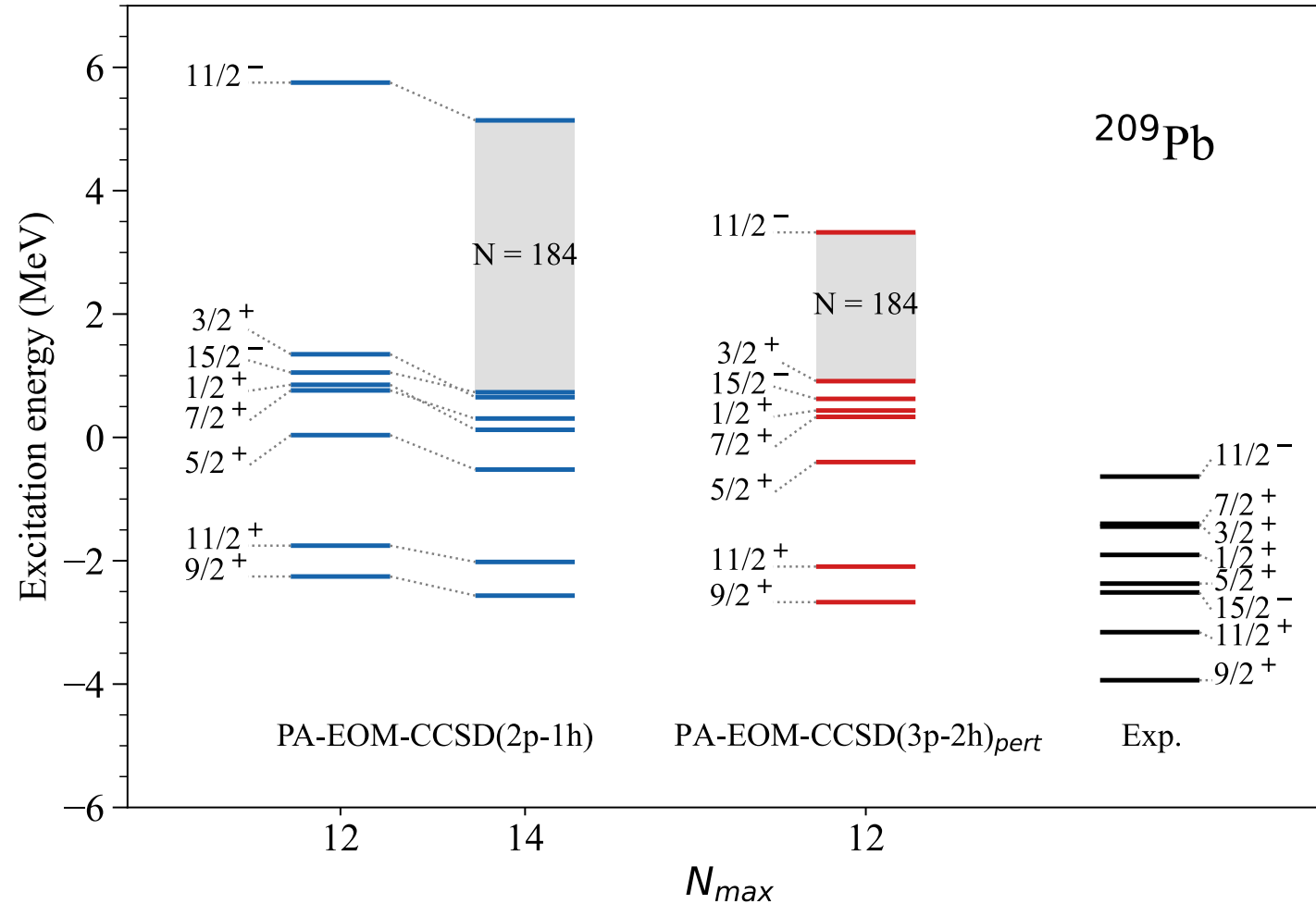
- To identify the **next shell gaps**, we look at **excited spectra of neighbouring nuclei** as an estimate of **single-particle energies**.
- Gap at Z=92? Double magicity of ^{216}U ruled out due to presence of high-spin isomer.

“Shell diffusion effects” in superheavies

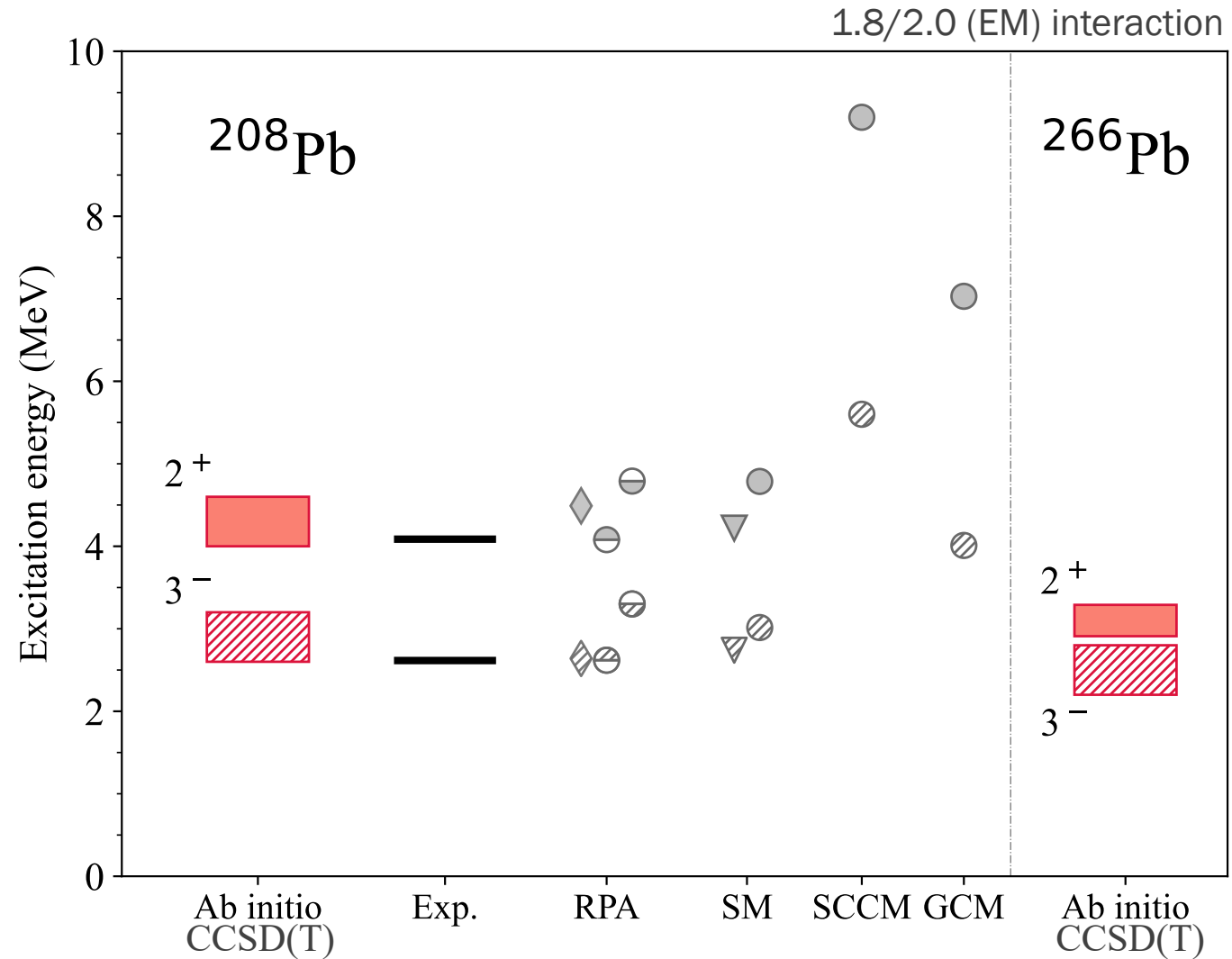


Excited states of ^{209}Pb

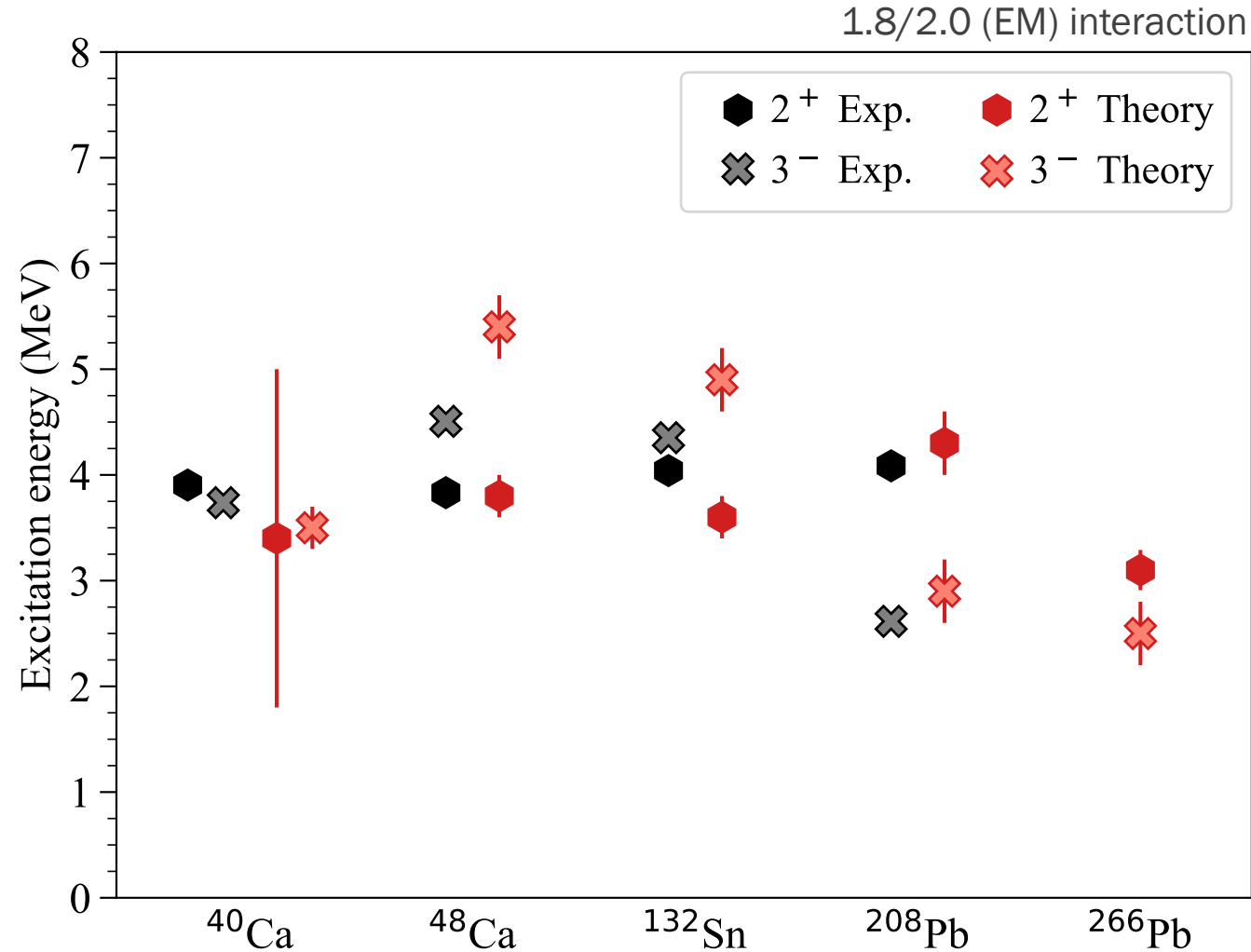
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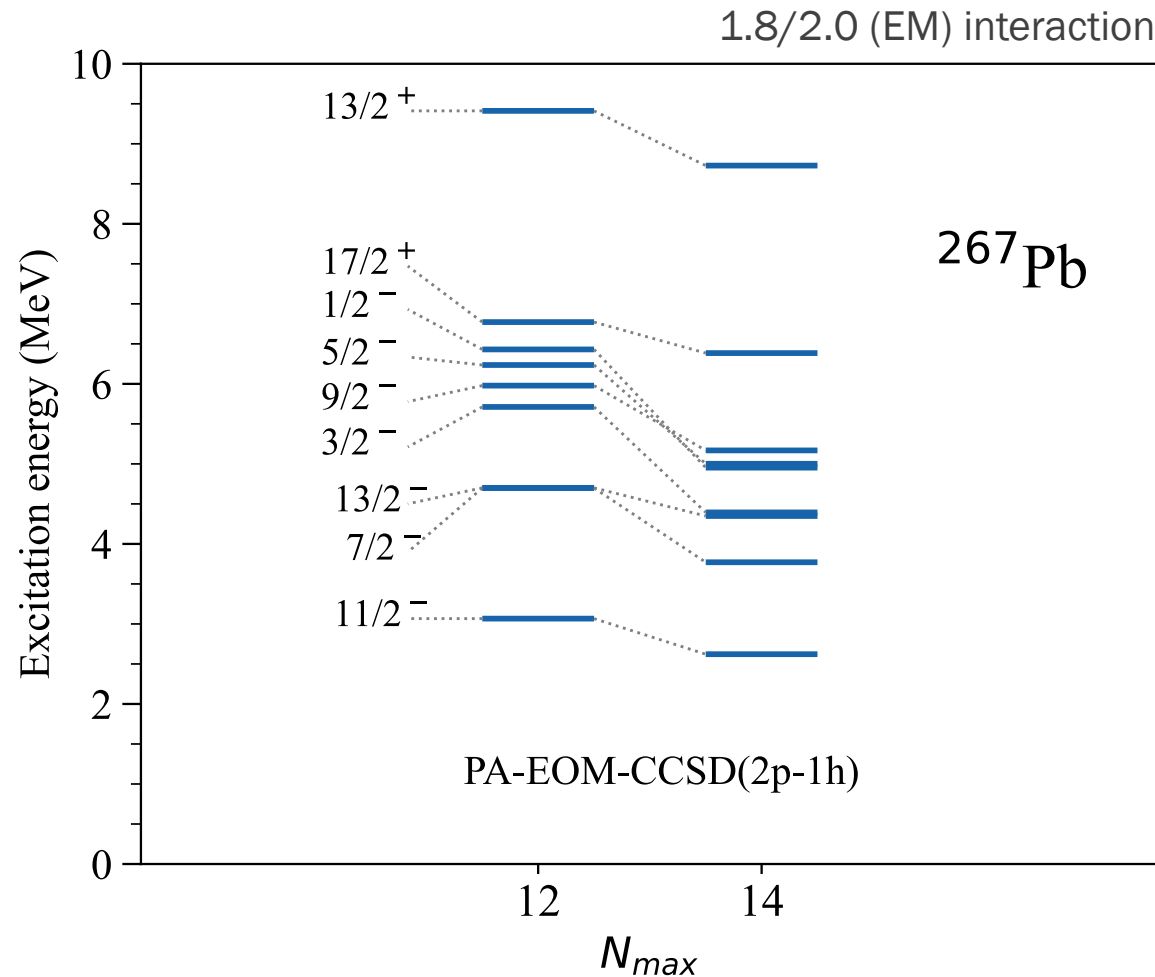
^{266}Pb is doubly magic



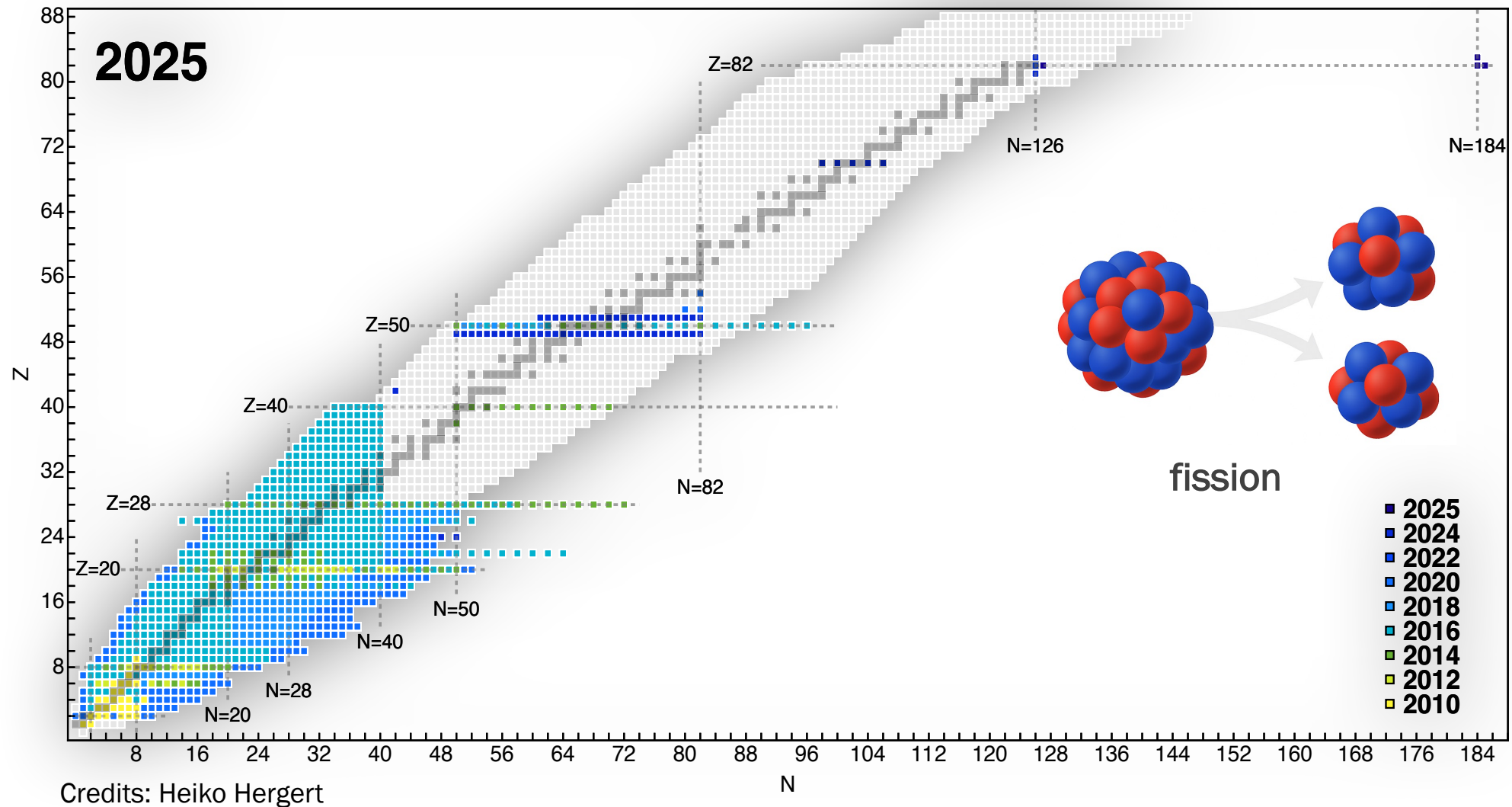
From light to heavy doubly magic nuclei



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



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?

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

Coupled-cluster theory

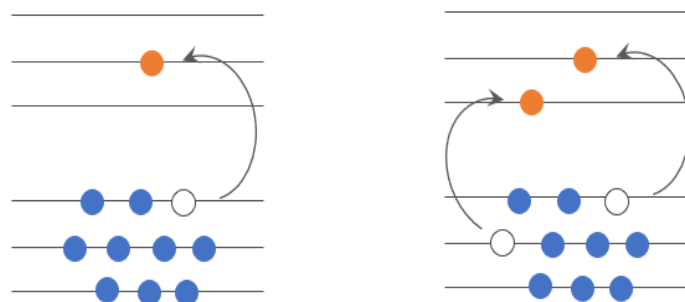
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singles and
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→ **CC equations**
become **ordinary**
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Coupled-cluster theory

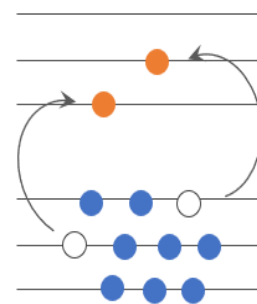
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One can also only isolate
doubles (CCD)



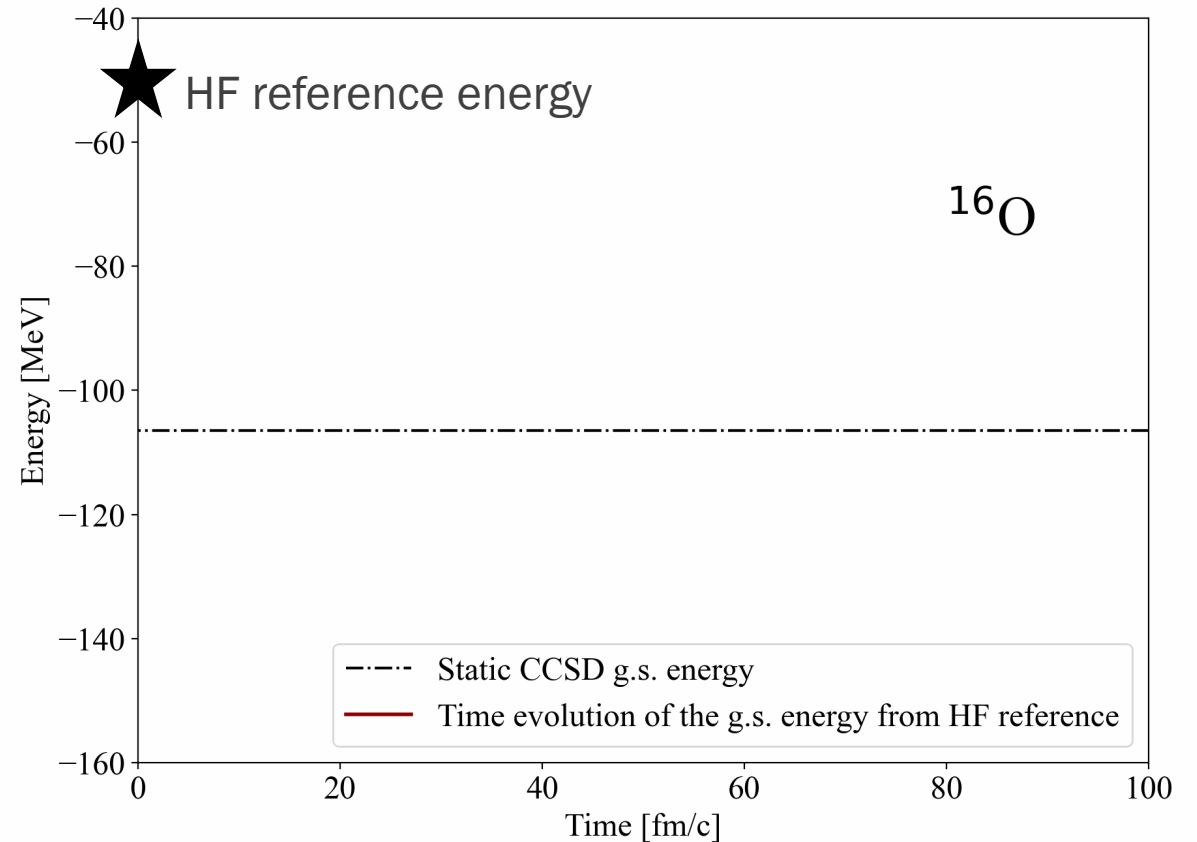
→ **CC equations**
become **ordinary differential eqs** for
the **time-dependent amplitudes**

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**.

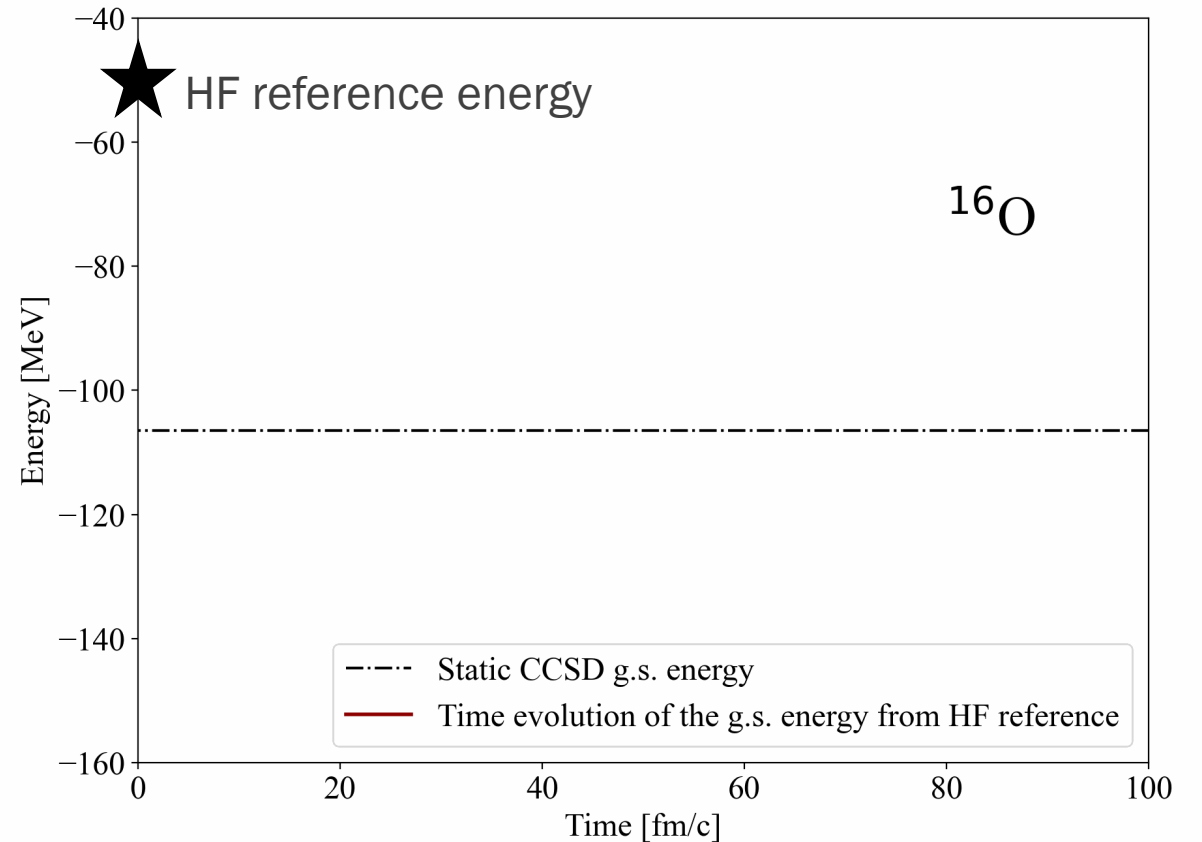
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We can look at the **typical time scales and amplitudes** of **nuclear density fluctuations**.

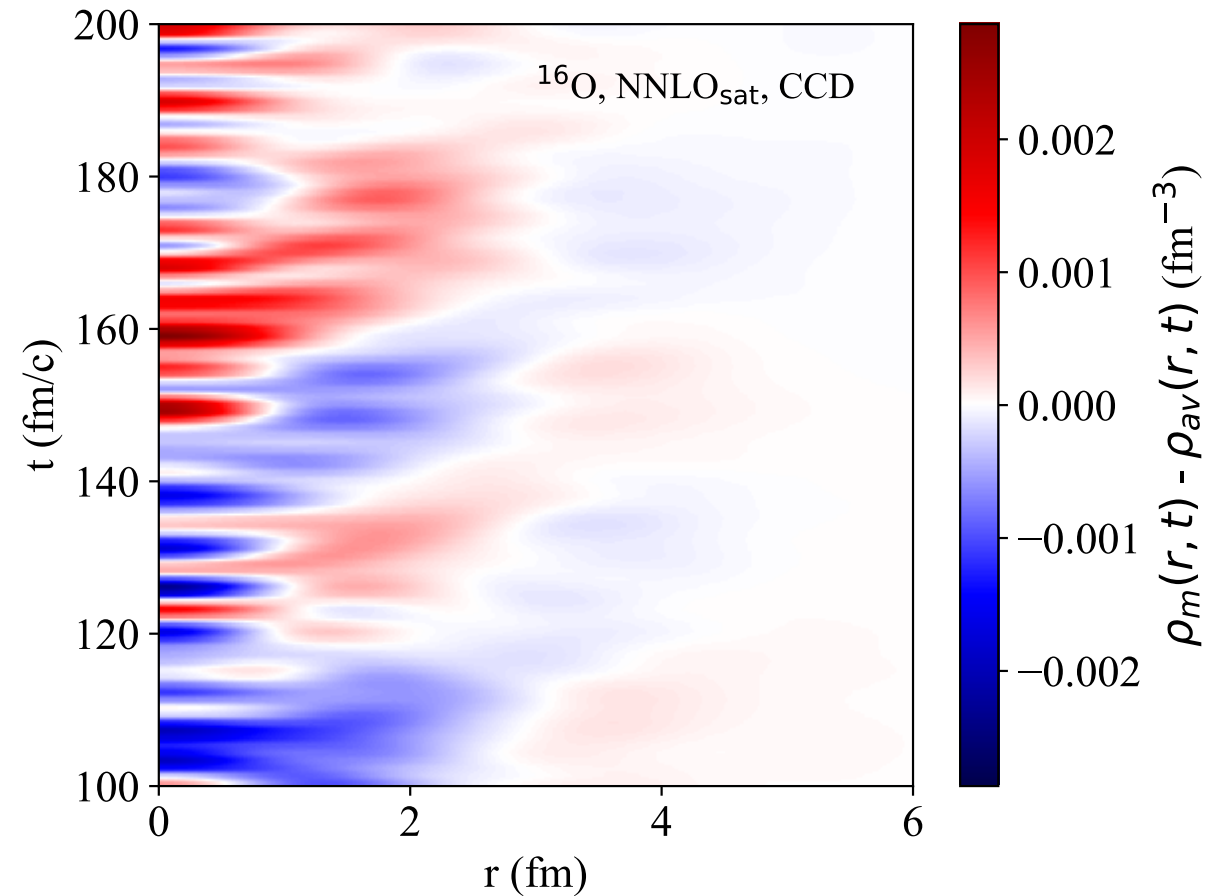
Nuclear density fluctuations: ^{16}O

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

Nuclear density fluctuations: ^{16}O

FB et al, in preparation.

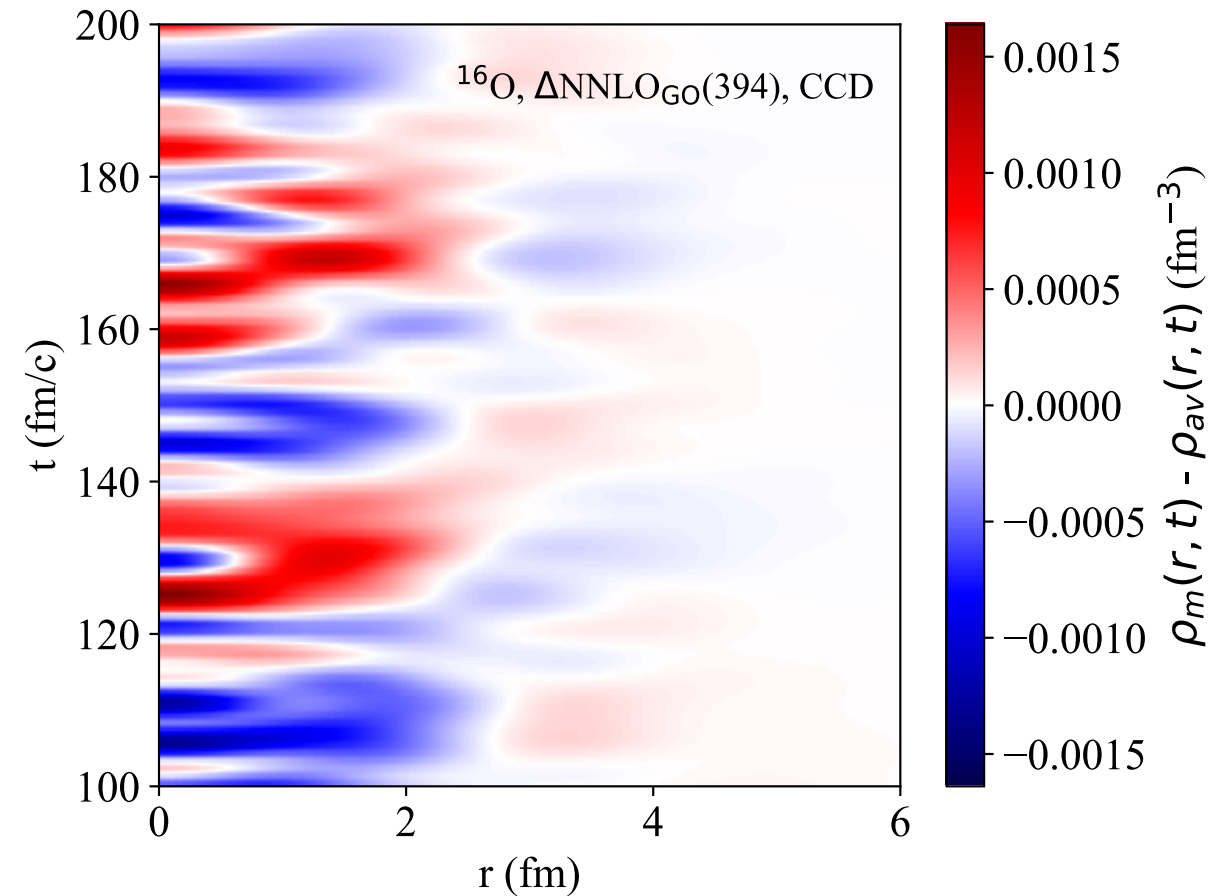
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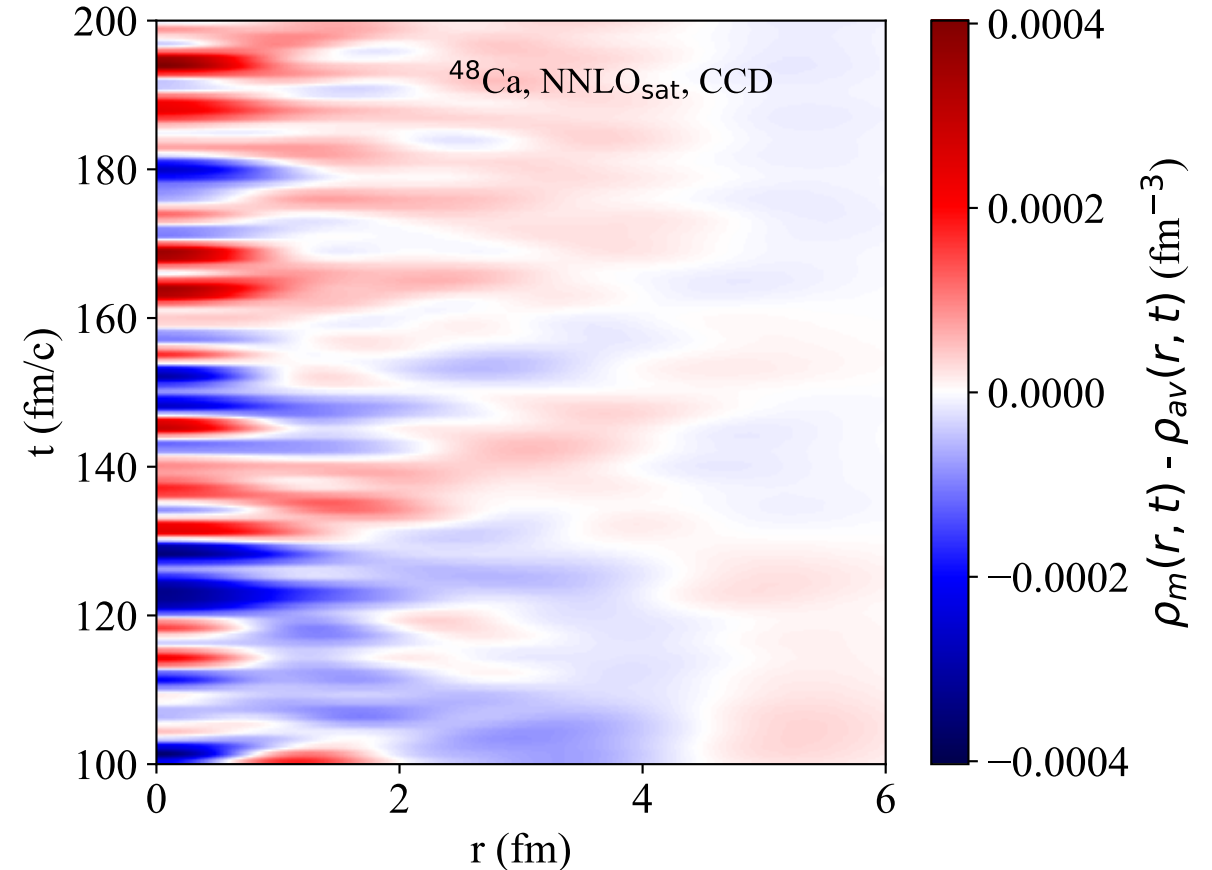
- We isolate effect of **2p-2h correlations** by considering a **CCD calculation**.
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Nuclear density fluctuations: ^{48}Ca

FB et al, in preparation.

- We isolate effect of **2p-2h correlations** by considering a **CCD calculation**.
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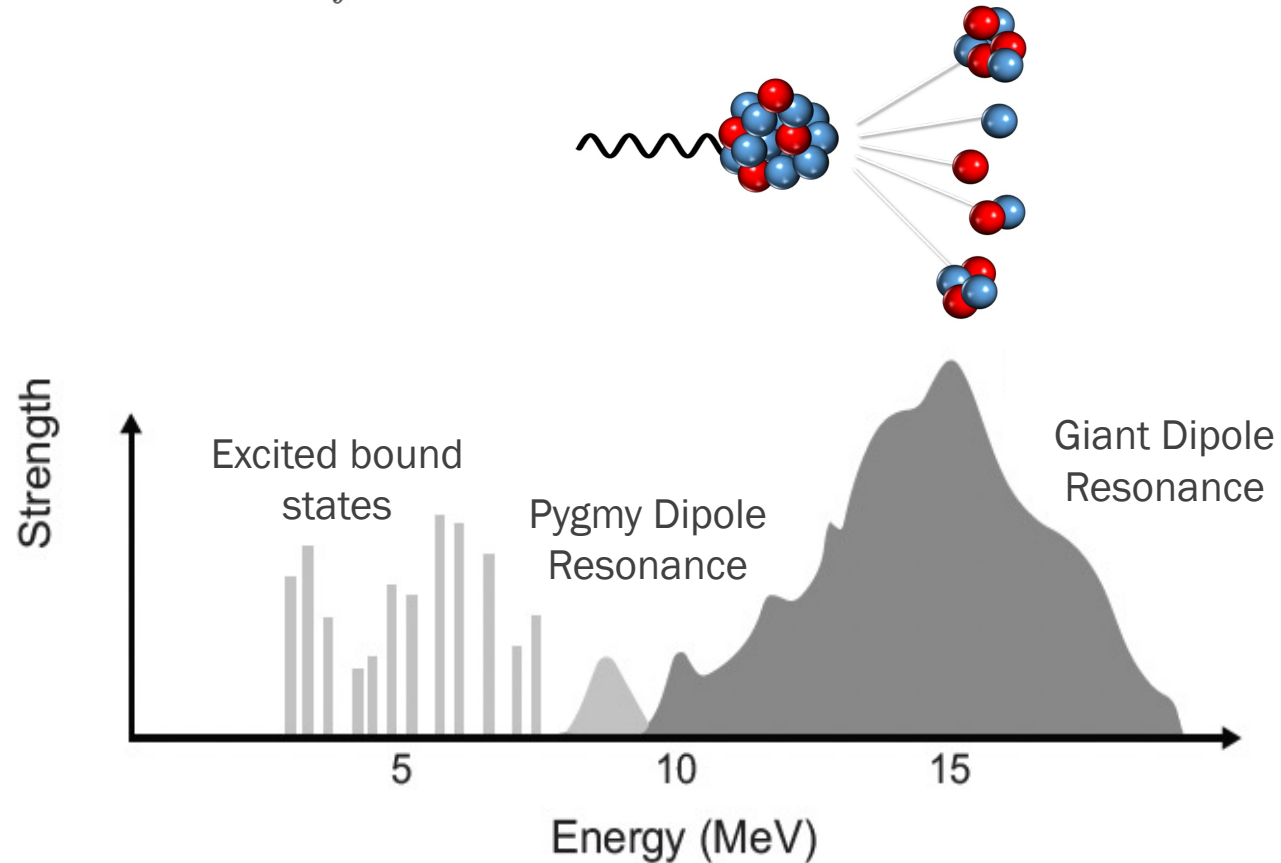


Short-range oscillations, with periods of up to 3-5 $\text{fm}/c \rightarrow$
one order of magnitude less than typical equilibration times in nuclear reactions.

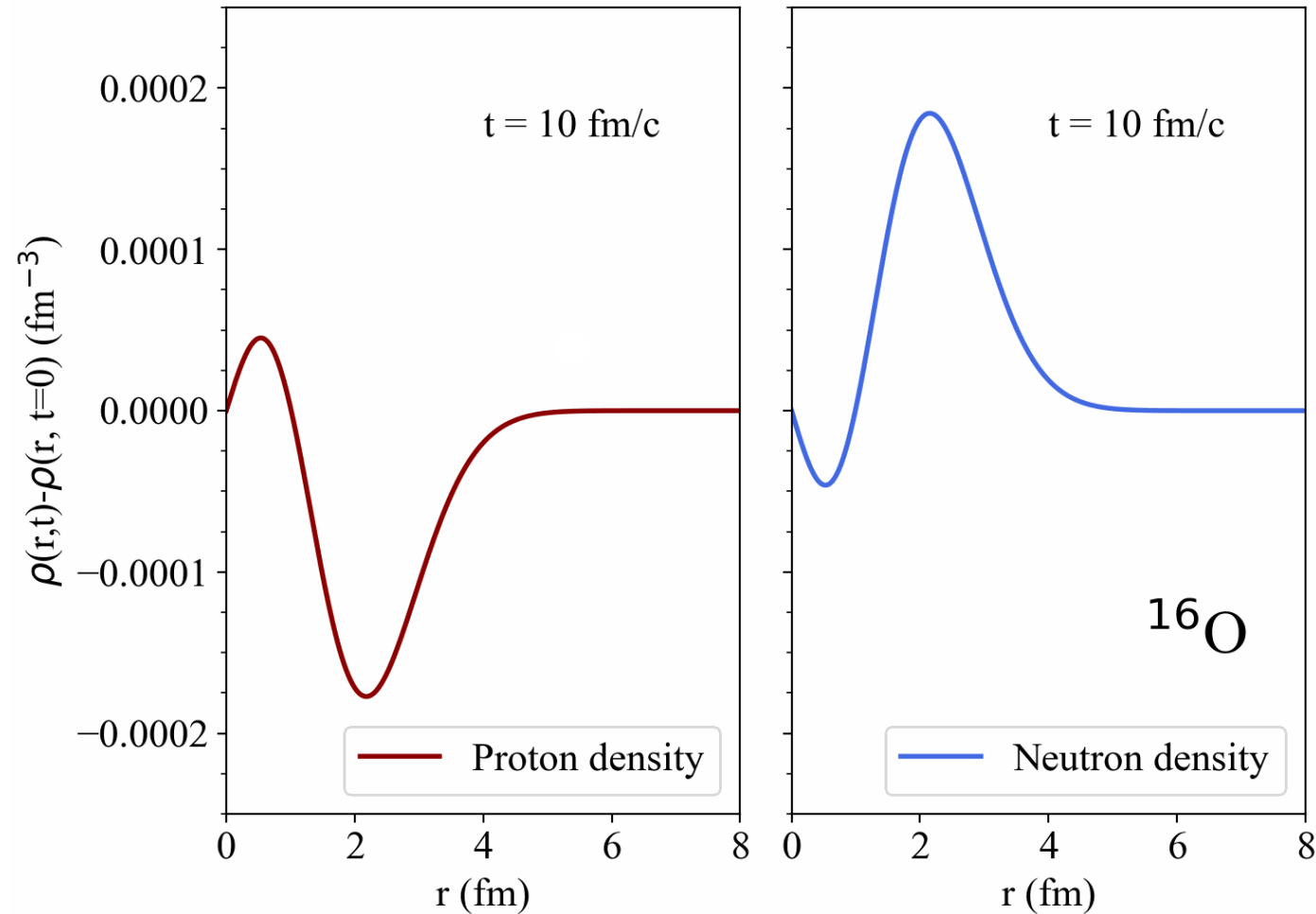
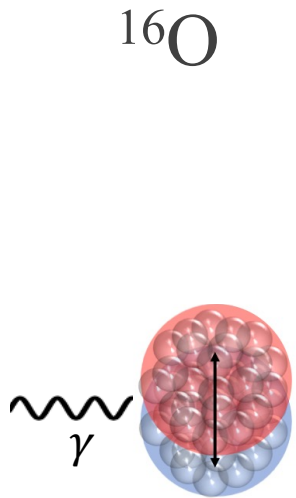
A simple physics case:
nuclear response functions from
a time-dependent perspective

Nuclear response functions

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



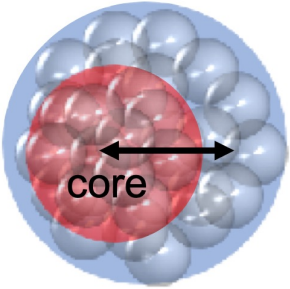
Collective oscillations in real time



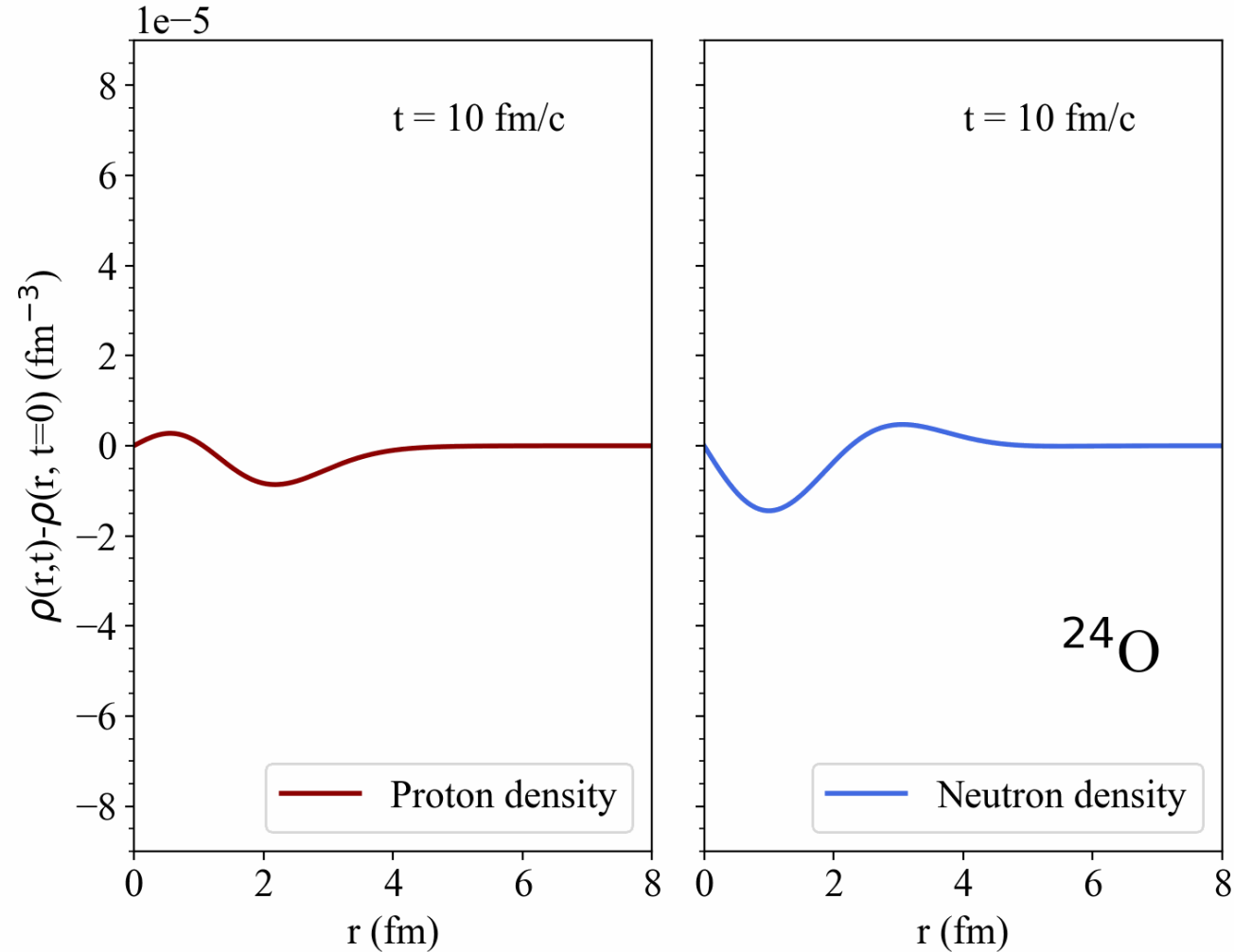
NNLO_{opt},
 $N_{\text{max}} = 6$

Collective oscillations in real time

^{24}O



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

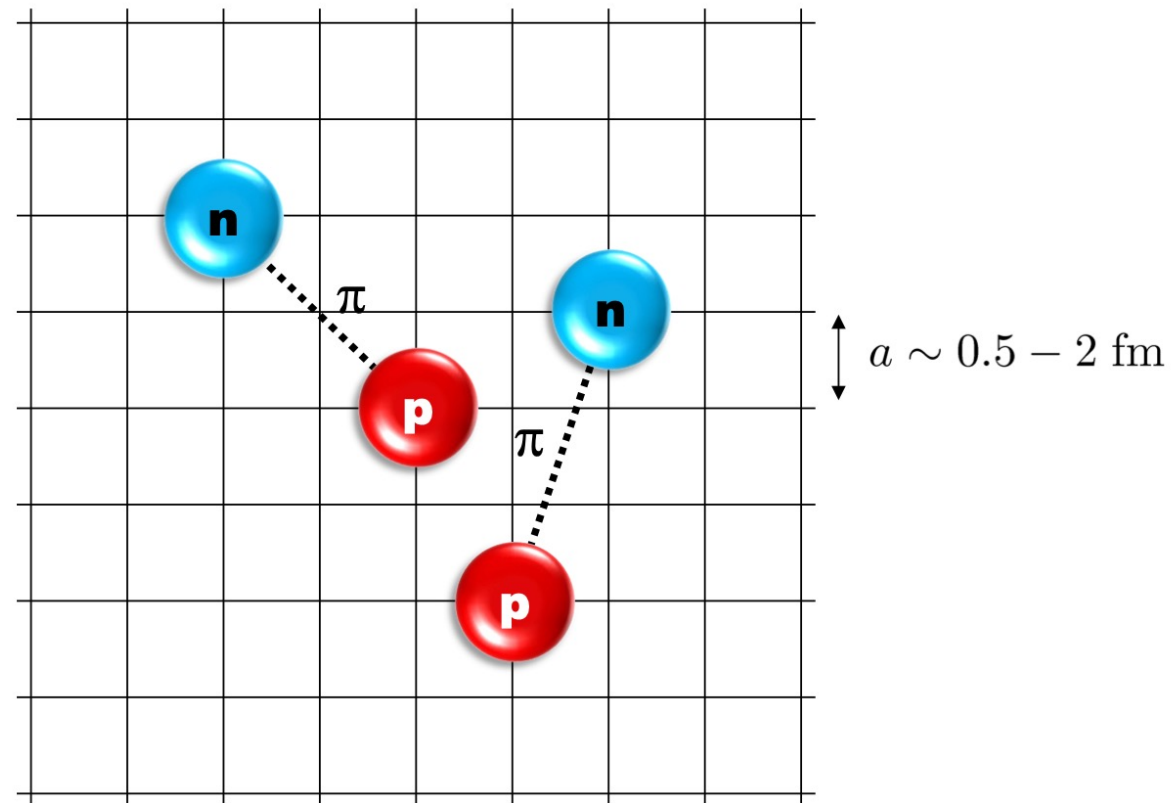


NNLO_{opt},
 $N_{\text{max}} = 6$

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

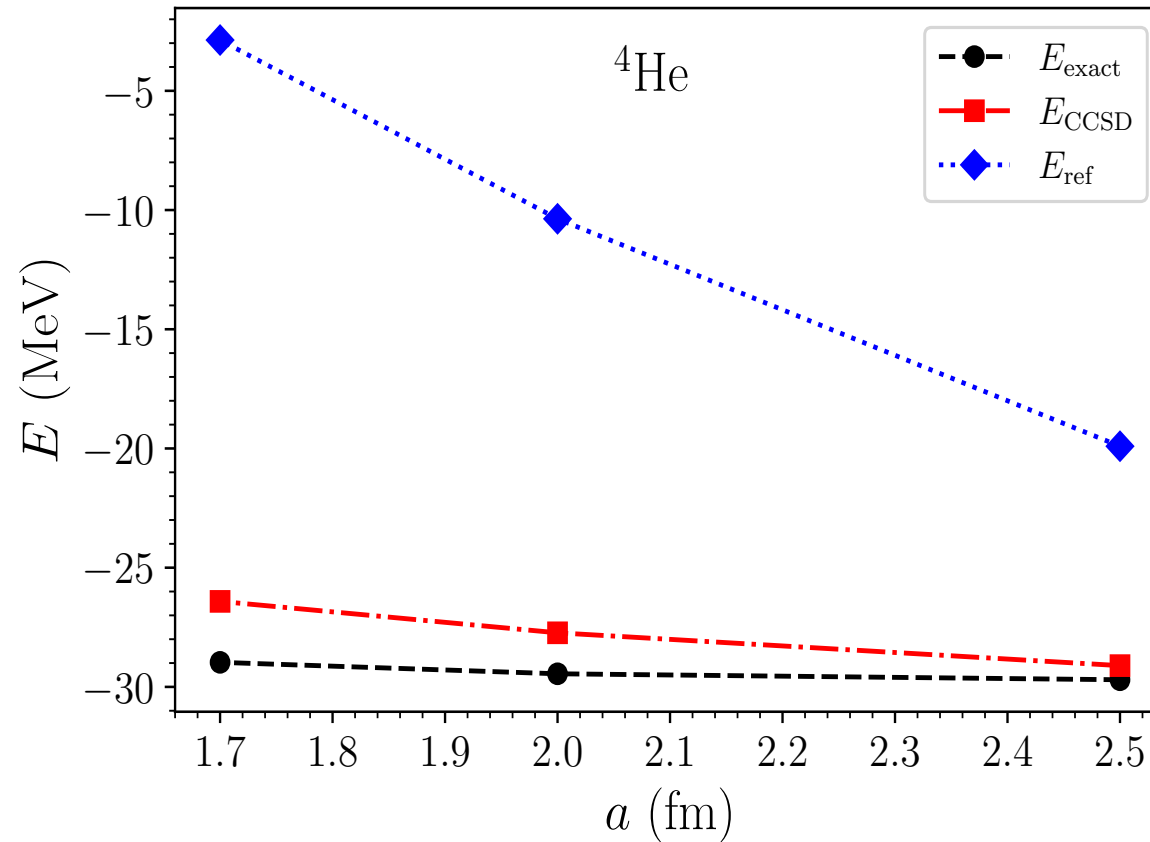
A natural framework: nuclei on the lattice

- ❑ We can exploit the **short-range nature** of the **nuclear force**! Correlations are only between **neighbours**.
- ❑ Computational cost scales with **volume** → problem becomes **sparse** and we can do calculations on a **laptop**!
- ❑ 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: ${}^4\text{He}$



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

Conclusions

- ❑ We showed the **doubly-magic nature of ^{266}Pb** from **first principles**.
- ❑ We found that many-body correlations beyond the mean-field generate **short-range density fluctuations** one order of magnitude faster than typical equilibration times in nuclear reactions.
- ❑ We aim to couple time-dependent calculations with a **lattice** formulation, a natural framework where to achieve a microscopic description of **nuclear dynamics**.

Stay tuned!

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

@ORNL/UTK: Gaute Hagen, Matthias Heinz, Gustav R. Jansen,
Ben Johnson-Toth, Thomas Papenbrock, Maxwell Rothman

@FRIB/MSU: Kyle Godbey

@LLNL: Cody Balos, Carol Woodward

and to you for your attention!

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U.S. DEPARTMENT OF
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Theory
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NUCLEI
Nuclear Computational Low-Energy Initiative