Nuclear dynamics in a time-dependent approach

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"PAN-AMERICAN FEW-BODY PHYSICS BOOTCAMP: FOSTERING COLLABORATION"

ECT*, TRENTO, ITALY

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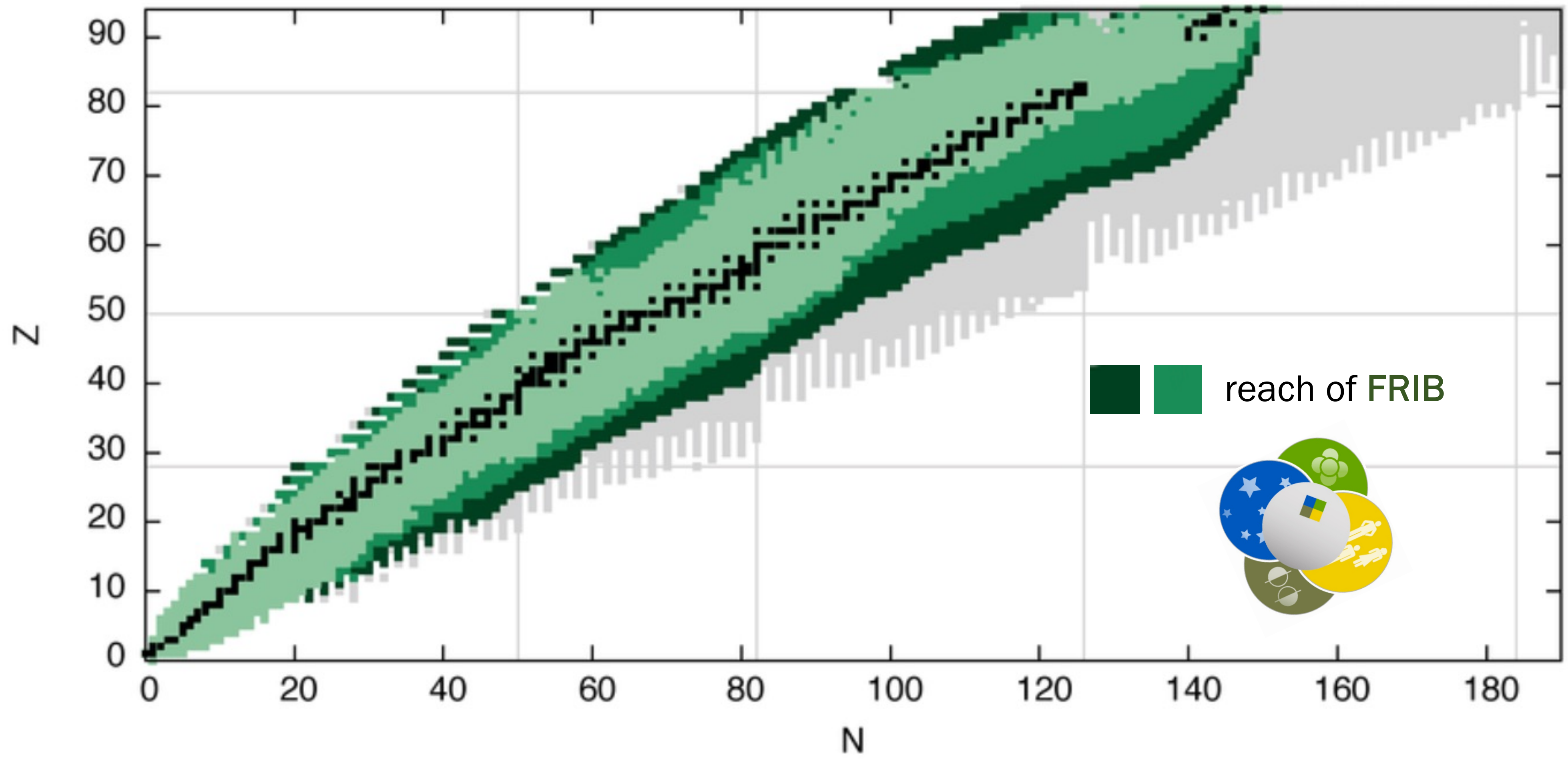
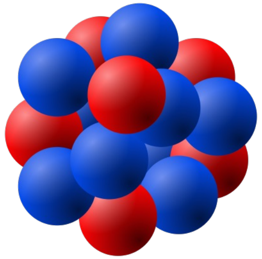
New discoveries on the horizon at the edge of stability!



R. Surman and M. Mumpower, EPJ Web of Conferences **178**, 04002 (2018).

Ab initio nuclear theory



"…we 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"

A. Ekström et al, Front. Phys. 11:1129094 (2023).

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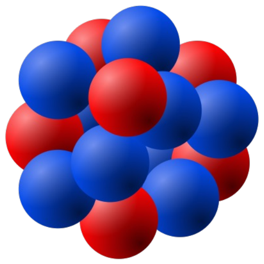

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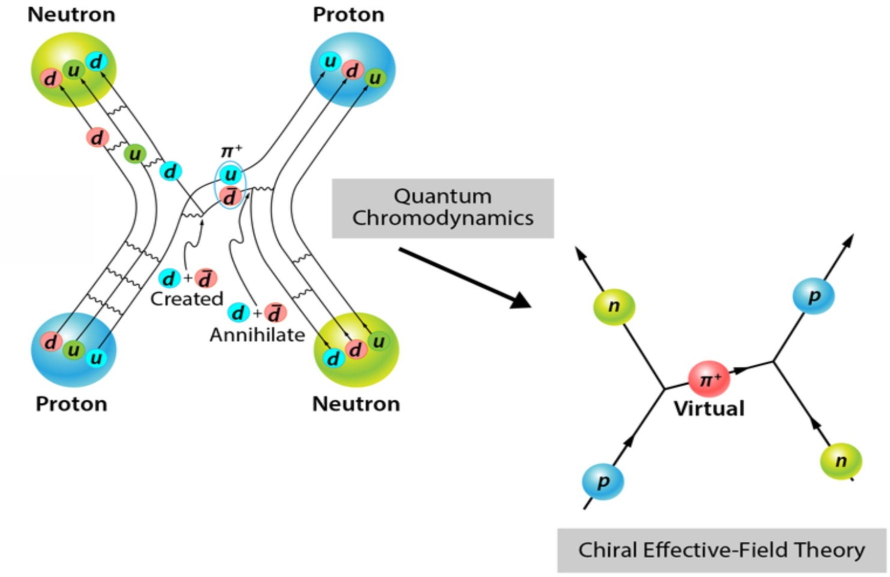
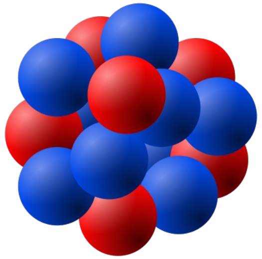


APS/Alan Stonebraker

- ❑ Building blocks: **protons and neutrons**.
- ❑ Nuclear forces from **chiral effective field theory.**

Ab initio nuclear theory



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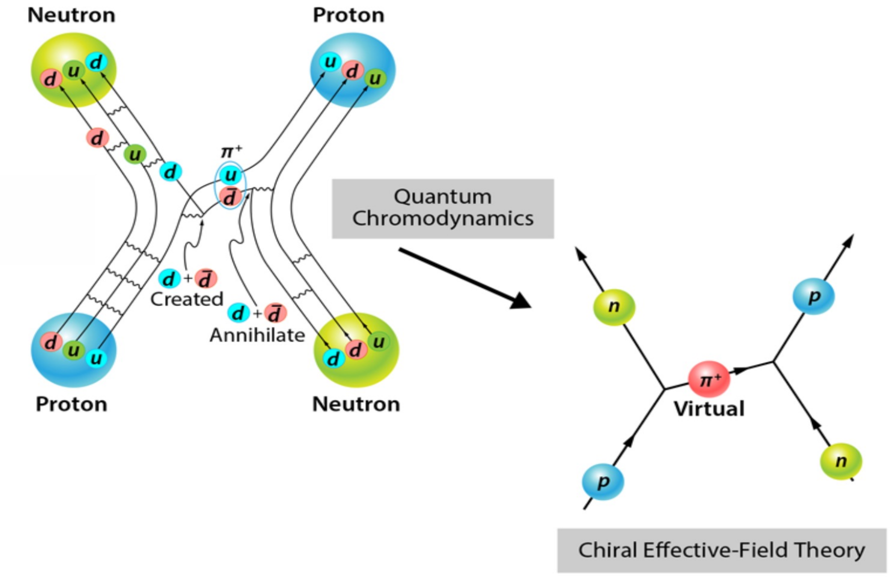

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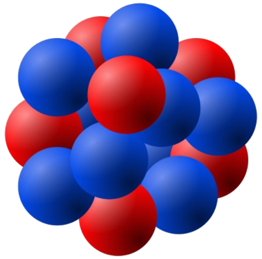
- ❑ Building blocks: protons and neutrons.
- ❑ Nuclear forces from chiral effective field theory.

Key facts on chiral EFT:

- ❑ Low-energy approximation of QCD.
- ❑ Separation of scales allows for systematic order-by-order expansion in powers of momenta.

Ab initio nuclear theory



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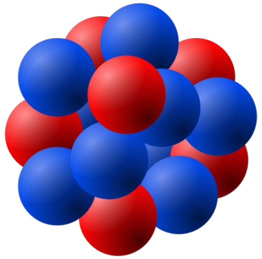
$$H = T + V_{NN} + V_{3N}$$

We solve the quantum many-body problem with controlled approximations.

Ab initio nuclear theory



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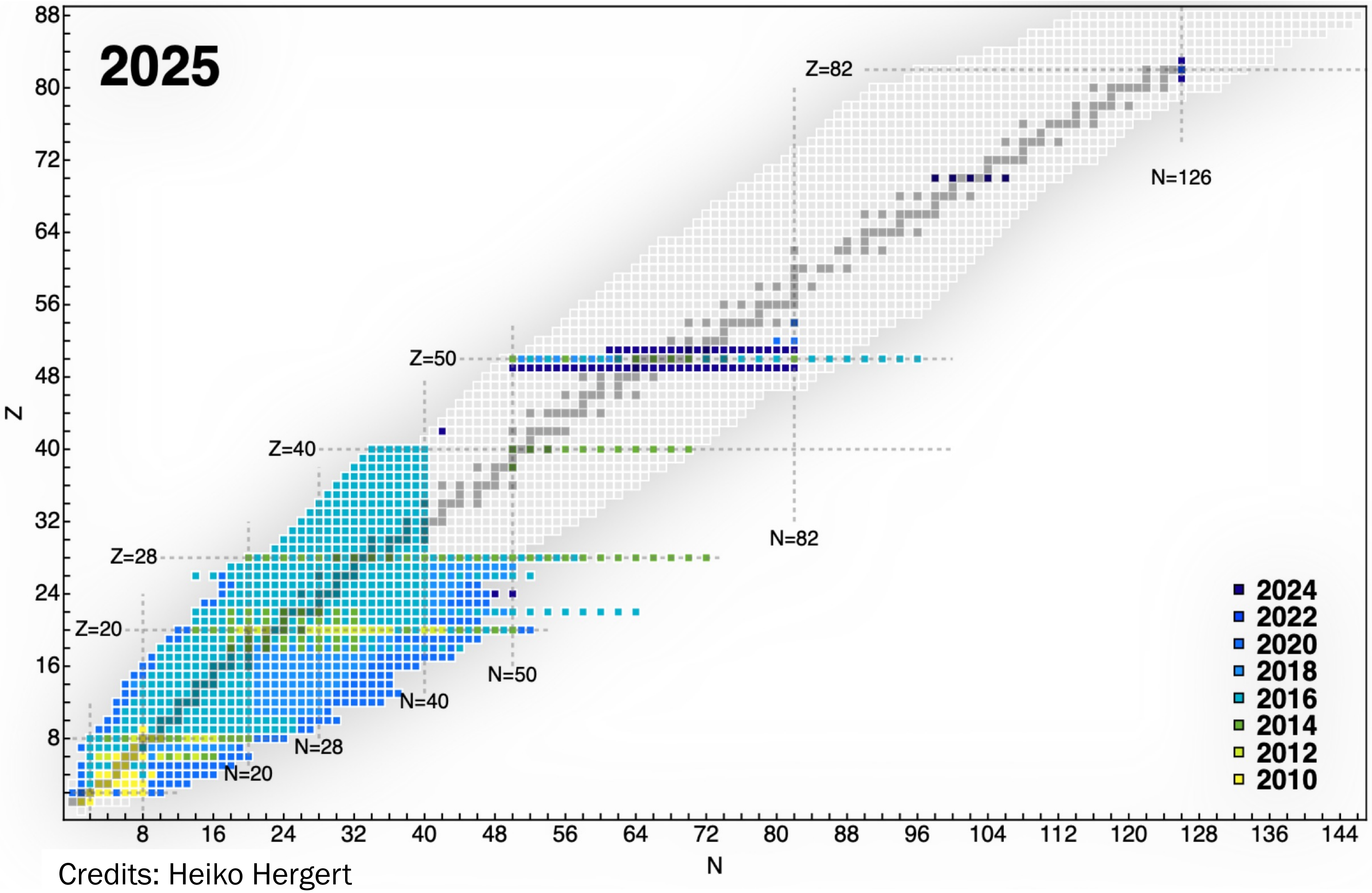
Many methods on the market:
coupled-cluster, in medium similarity renormalization group, no-core shell model, Quantum Monte Carlo …

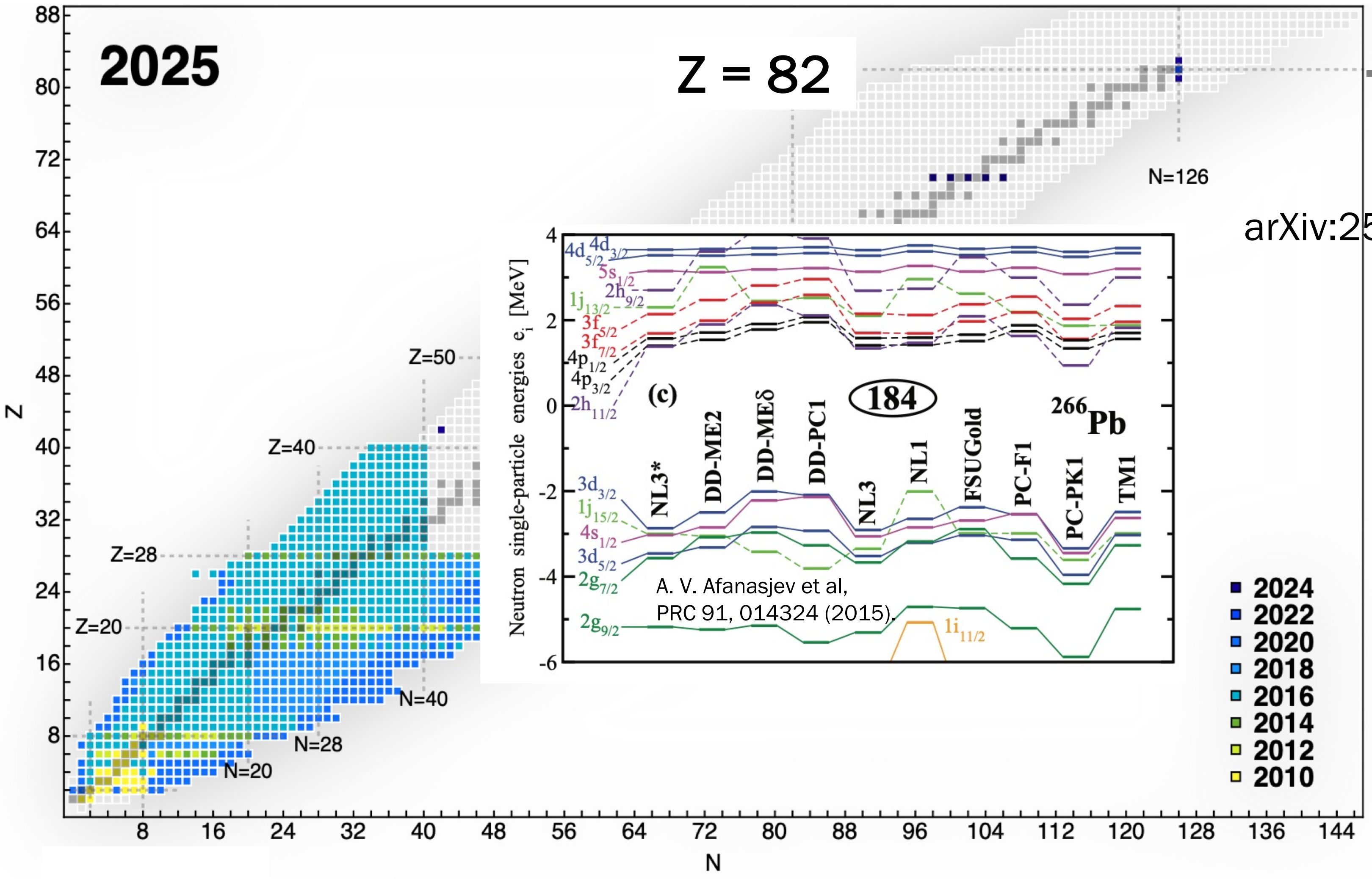
Huge progress in the last ~10 years…

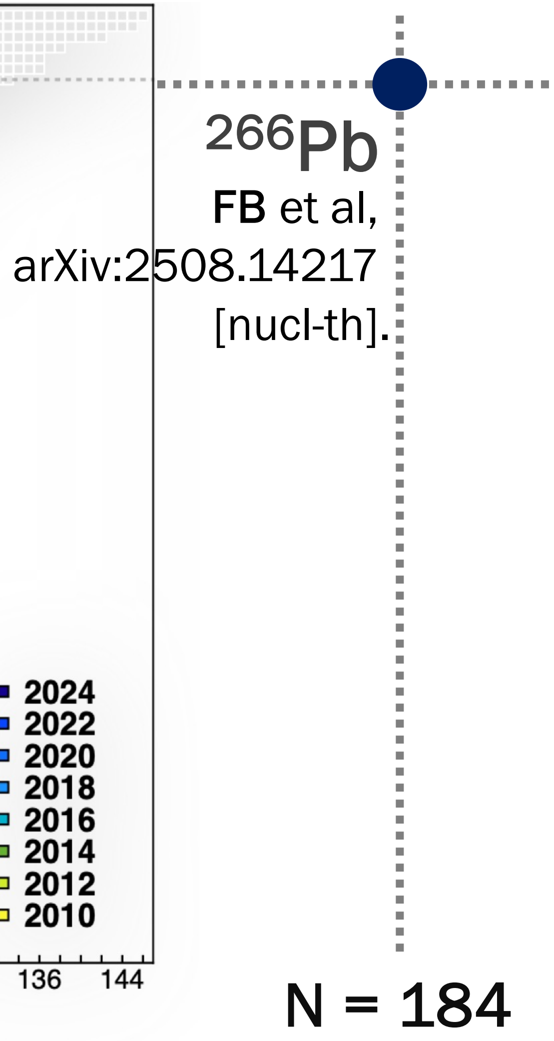
HPC advances + many-body methods scaling polynomially with A



Credits: Heiko Hergert

… but there is more to come!

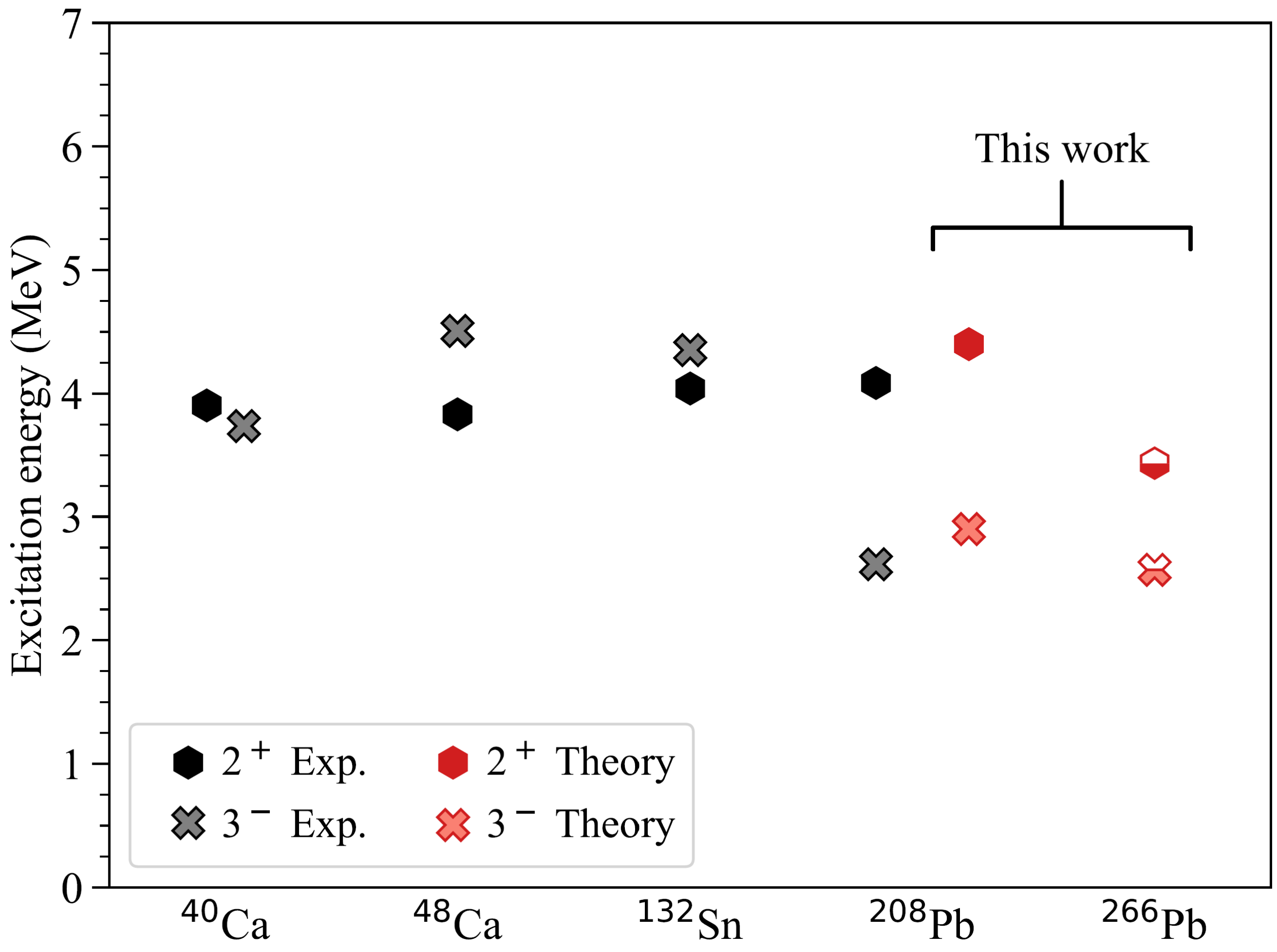




Now we can confirm this from an ab initio perspective!

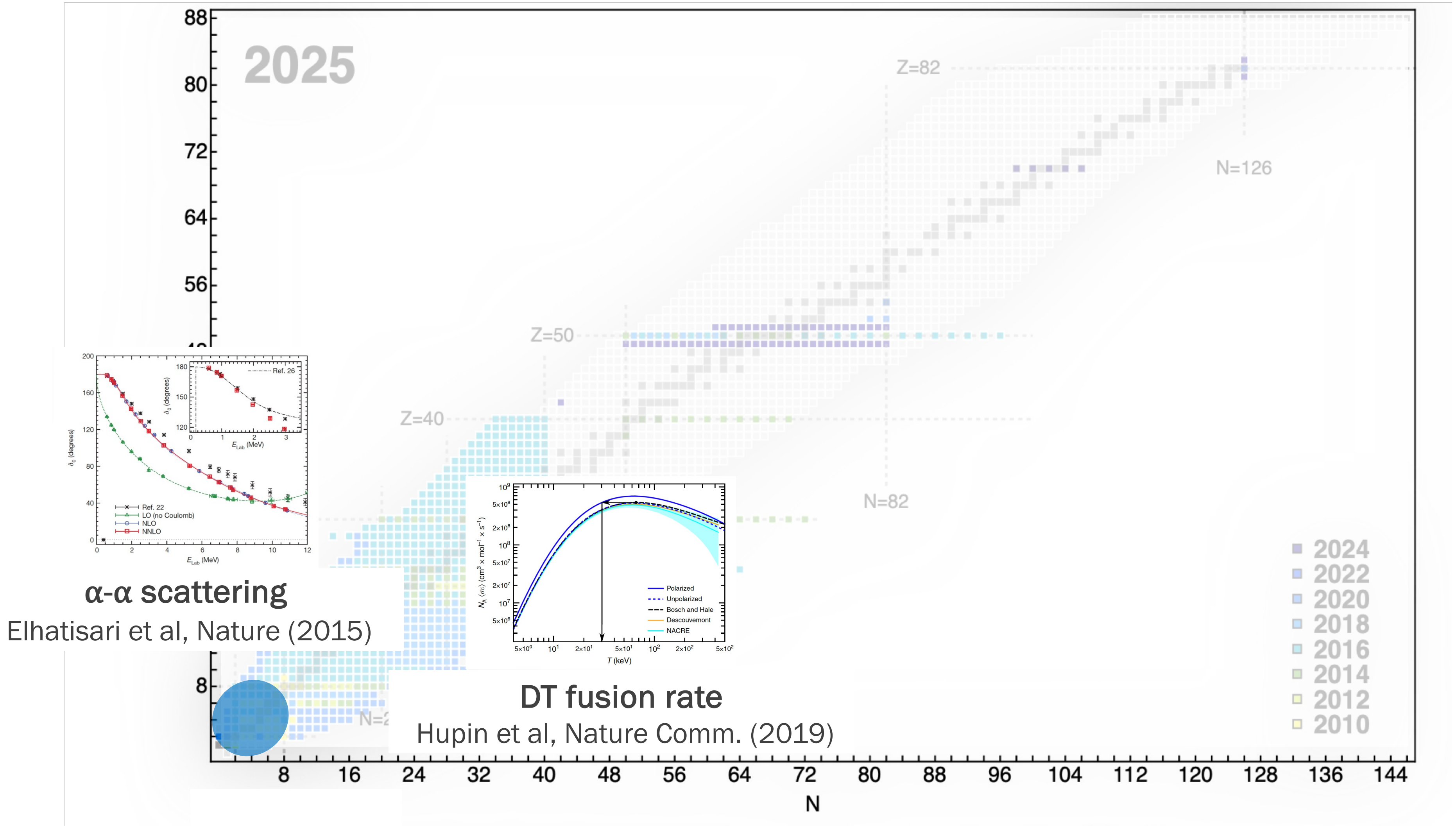
The doubly-magic nuclei ^{208}Pb and ^{266}Pb

1.8/2.0 (EM) “magic” interaction



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

Some milestones have been reached, but still a long way to go to understand nuclear dynamics!



α-α scattering
Elhatisari et al, Nature (2015)

DT fusion rate
Hupin et al, Nature Comm. (2019)

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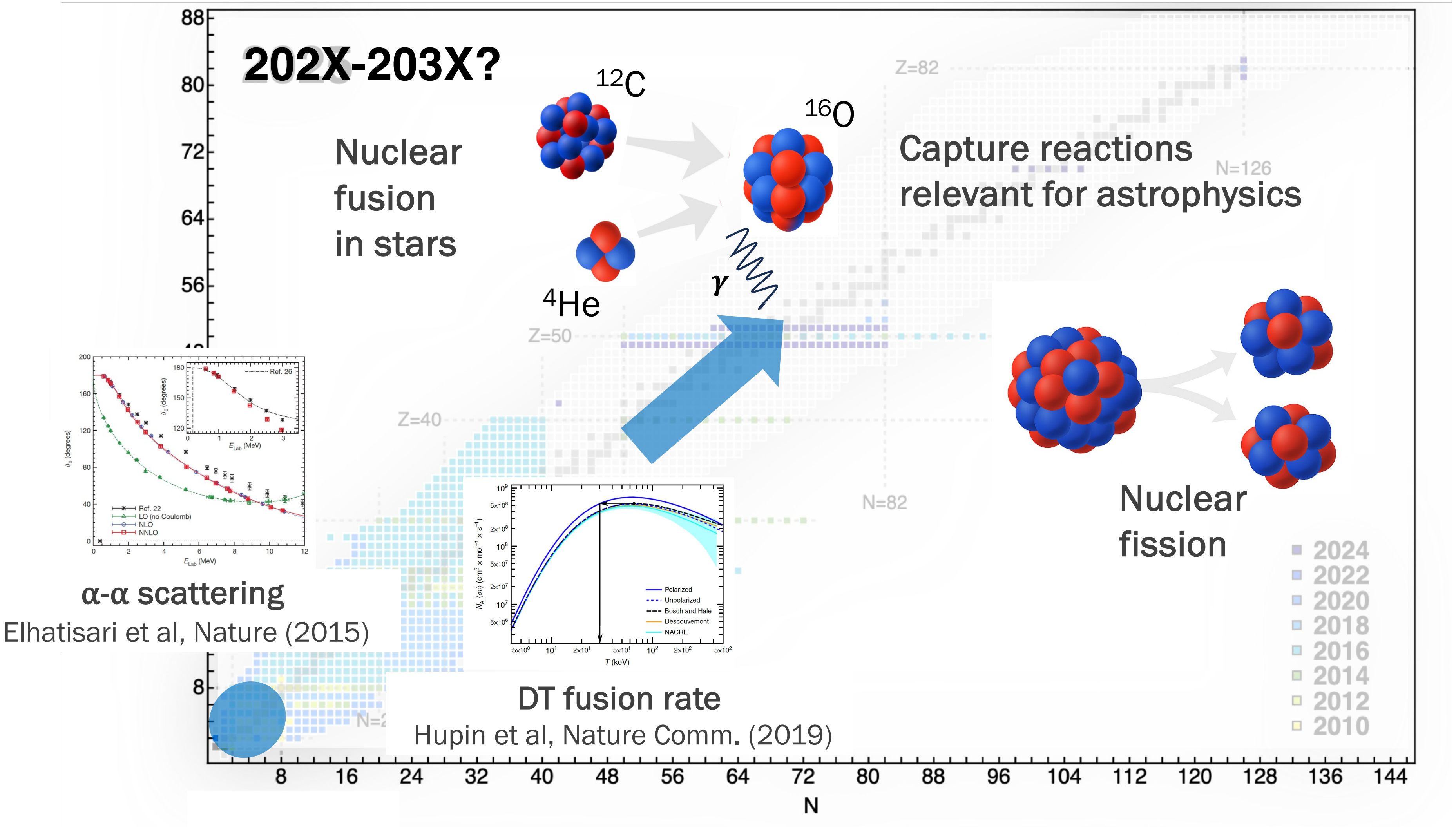


How to solve the time-dependent Schrödinger equation from a first-principles perspective?

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

Coupled-cluster theory

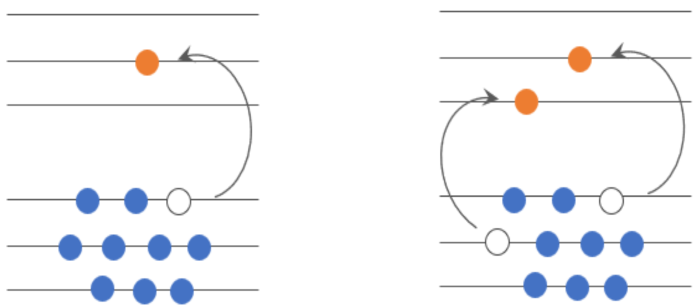
- ❑ Starting point: Hartree-Fock reference state $|\Phi_0\rangle$
- ❑ Add correlations via:

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

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)



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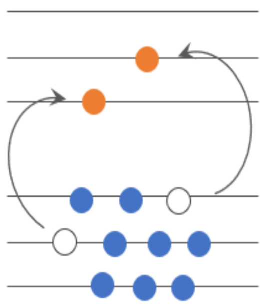
An even cheaper scheme:
doubles (CCD)



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Time-dependent coupled-cluster equations

Time-dependent coupled-cluster (TDCC) ansatz:

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

We obtain:

$$i\hbar \boxed{e^{-T(t)}\partial_t e^{T(t)}}|\Phi_0\rangle = \boxed{e^{-T(t)}\hat{H}(t)e^{T(t)}}|\Phi_0\rangle$$

similarity-transformed Hamiltonian

$$e^{-T(t)}\partial_t e^{T(t)} = \partial_t + \dot{T}(t)$$

$$\longrightarrow$$

$$i\hbar\dot{t}_0(t) = \langle\Phi_0|\overline{H}|\Phi_0\rangle$$
$$i\hbar\dot{t}_i^a(t) = \langle\Phi_i^a|\overline{H}|\Phi_0\rangle$$
$$i\hbar\dot{t}_{ij}^{ab}(t) = \langle\Phi_{ij}^{ab}|\overline{H}|\Phi_0\rangle$$

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

Time evolution from the mean-field

- Fission is typically modeled within **mean-field approaches** (time-dependent Hartree-Fock).

- Do we need to **add correlations** and go beyond this description?

- We can evaluate this is to **introduce correlation dynamically** and look at **time evolution of the system** starting from the **Hartree-Fock reference**.

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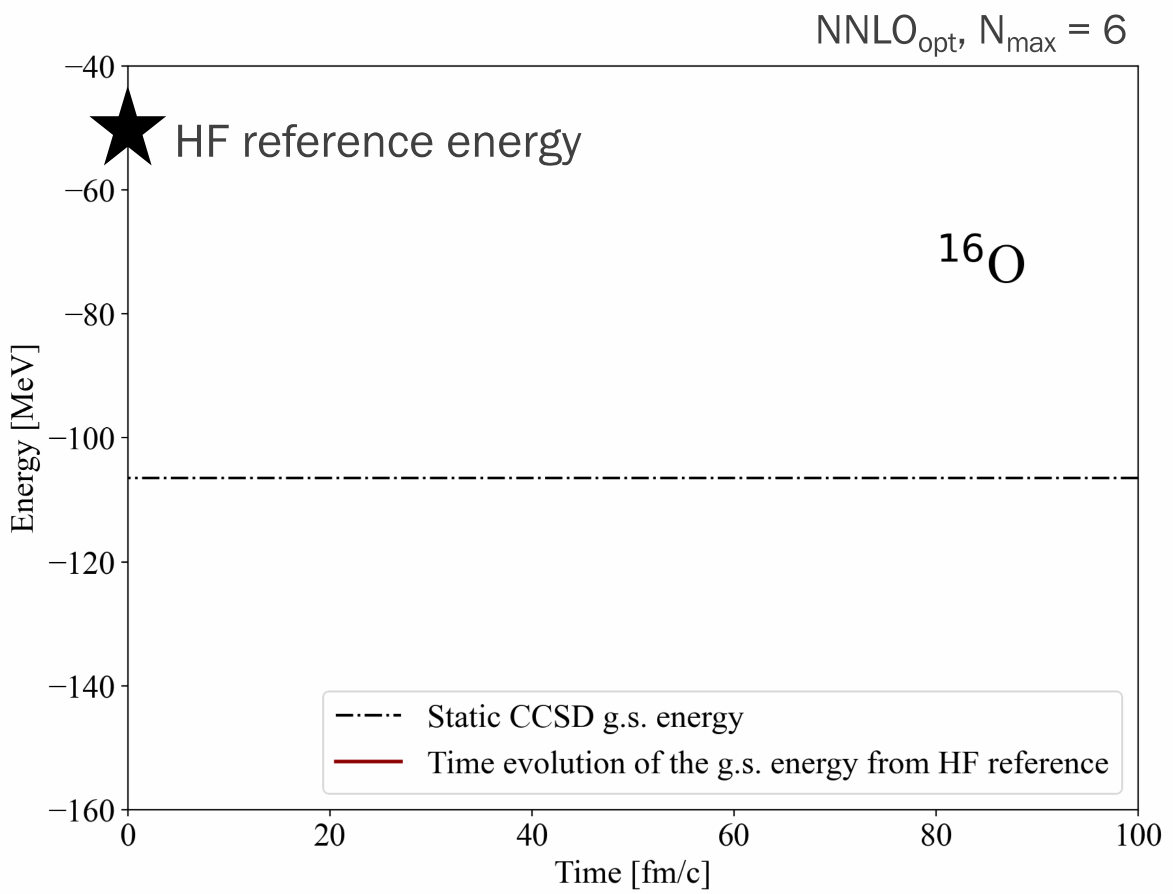

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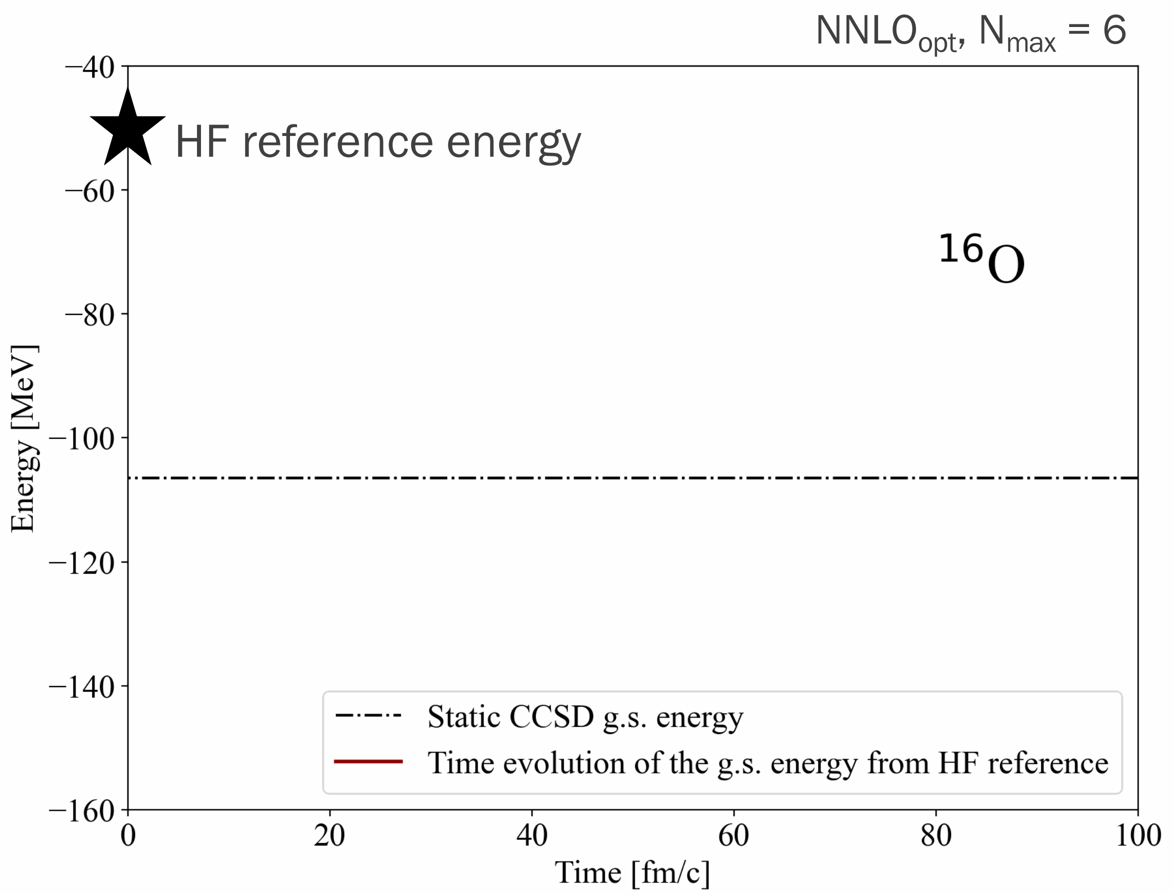

We can look at the **typical time scales and amplitudes** of **nuclear density fluctuations**.

Nuclear density fluctuations: ^{48}Ca

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

- ❑ We calculate the density fluctuation with respect to its average over time.

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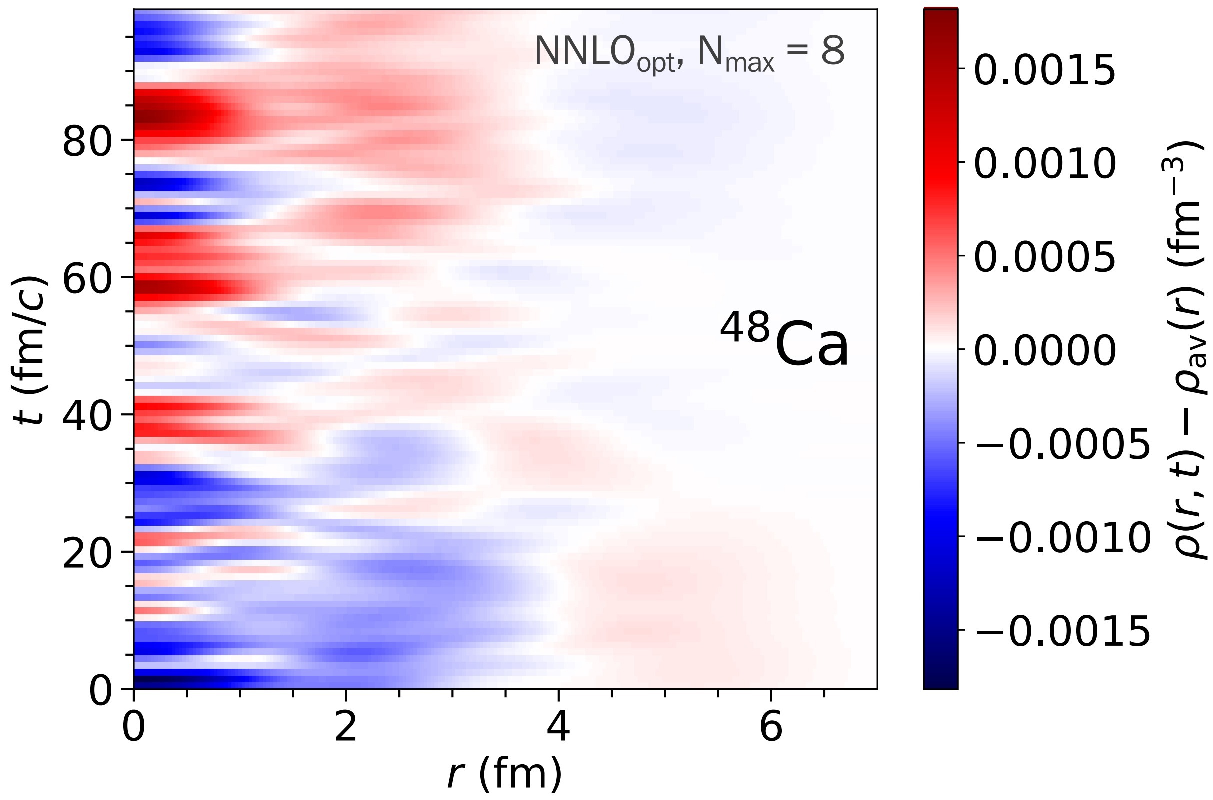

FB et al, in preparation.

Nuclear density fluctuations: ^{48}Ca

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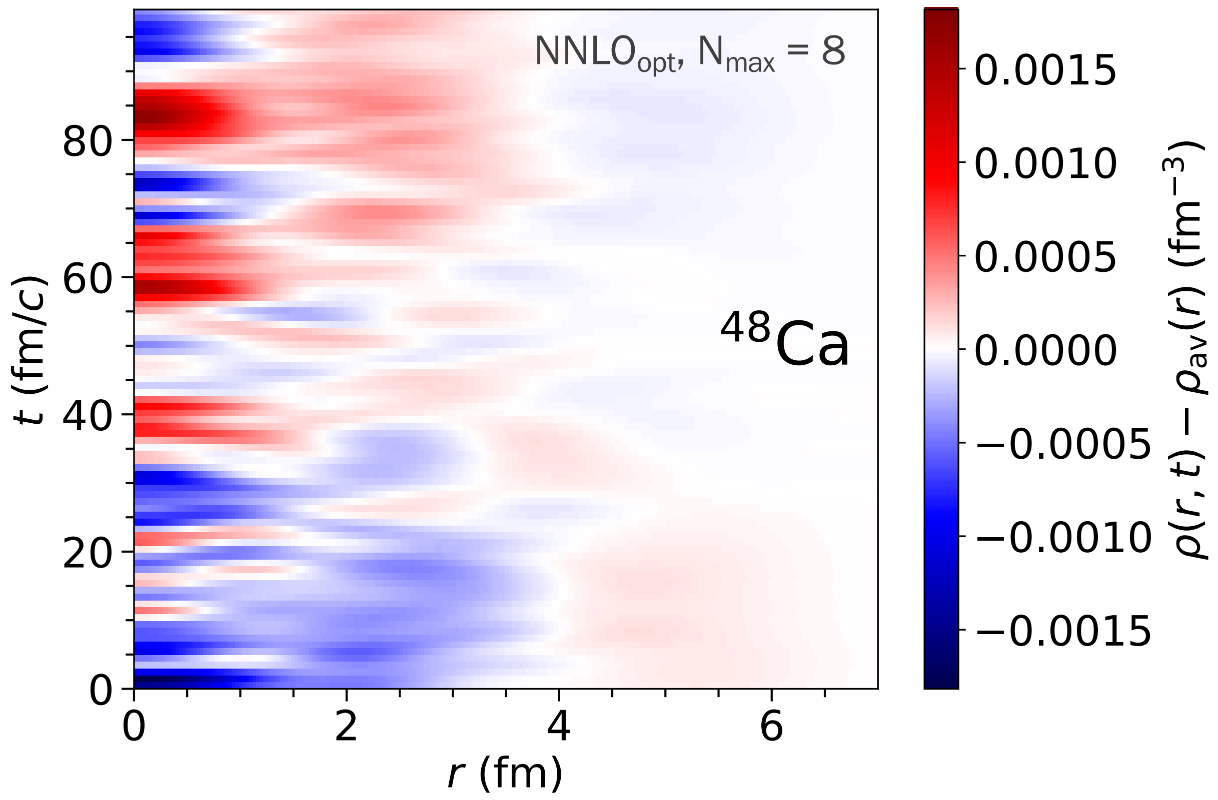
- ❑ We calculate the **density fluctuation** with respect to its **average over time.**



Short-range oscillations, with period of ~5 fm/c → **one order of magnitude** less than **typical equilibration times in nuclear reactions**.

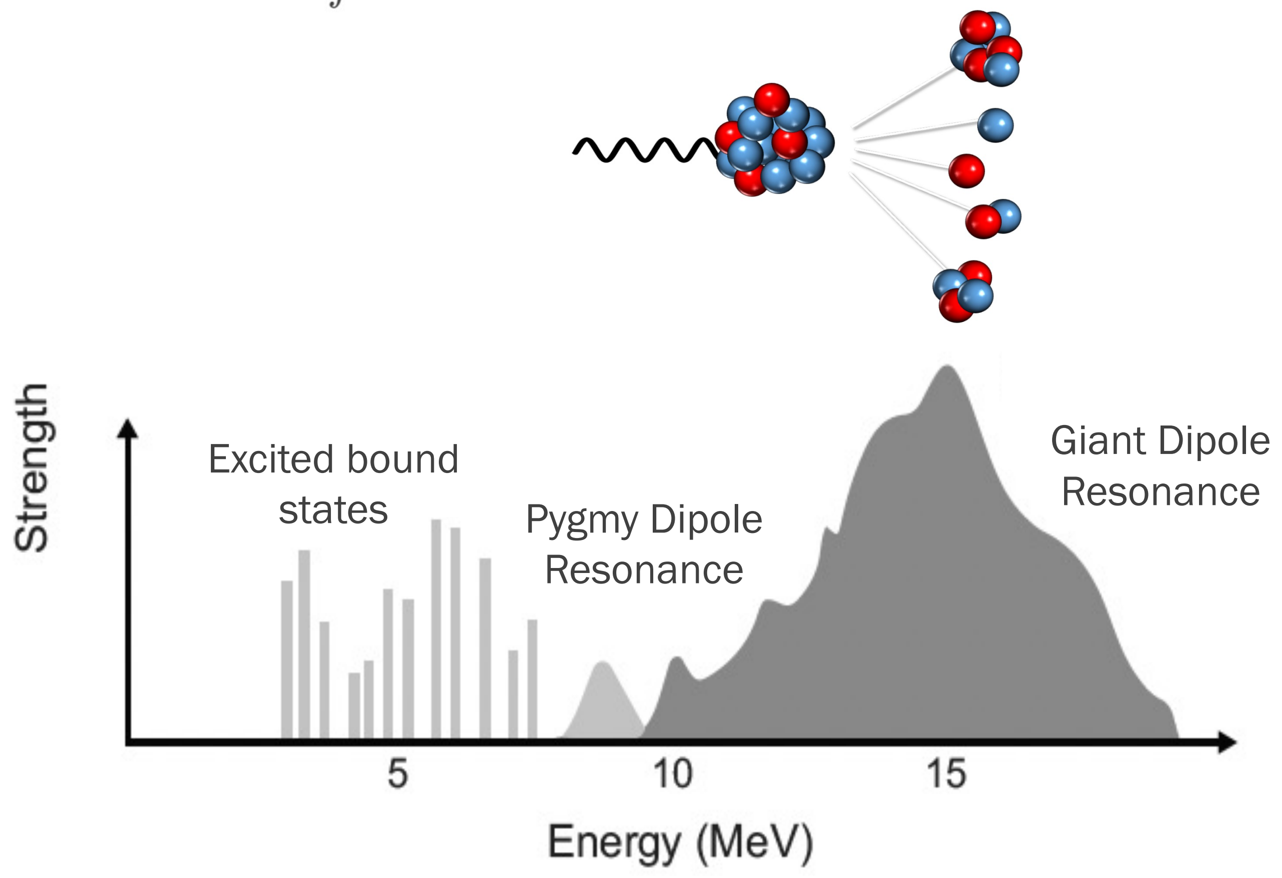
Jedele et al, PRL 118, 062501 (2017).

FB et al, in preparation.

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

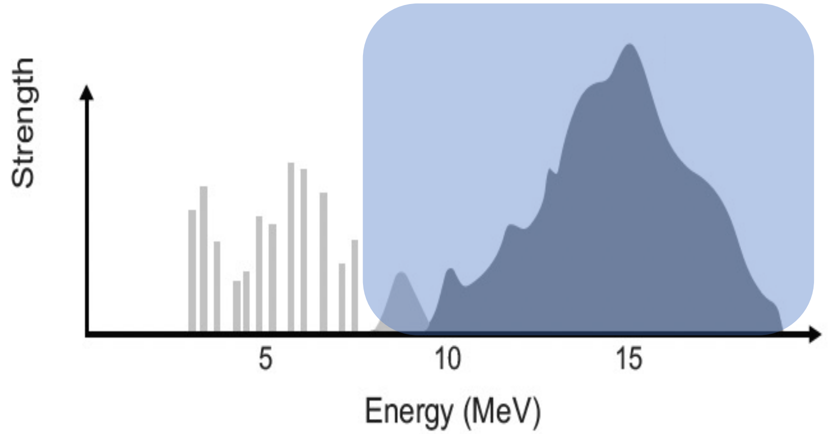
Nuclear response functions

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

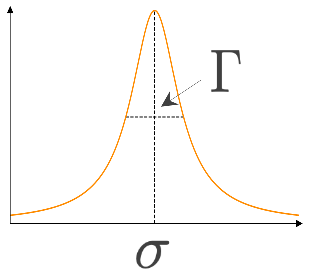


The static approach: LIT-CC

$$R(\omega)$$



Continuum problem



Lorentz Integral Transform (LIT)

$$L(\sigma,\Gamma) = \frac{\Gamma}{\pi}\int d\omega \, \frac{R(\omega)}{(\omega-\sigma)^2+\Gamma^2}$$

$$L(\sigma,\Gamma) = \frac{\Gamma}{\pi}\langle\Psi_L|\Psi_R\rangle$$

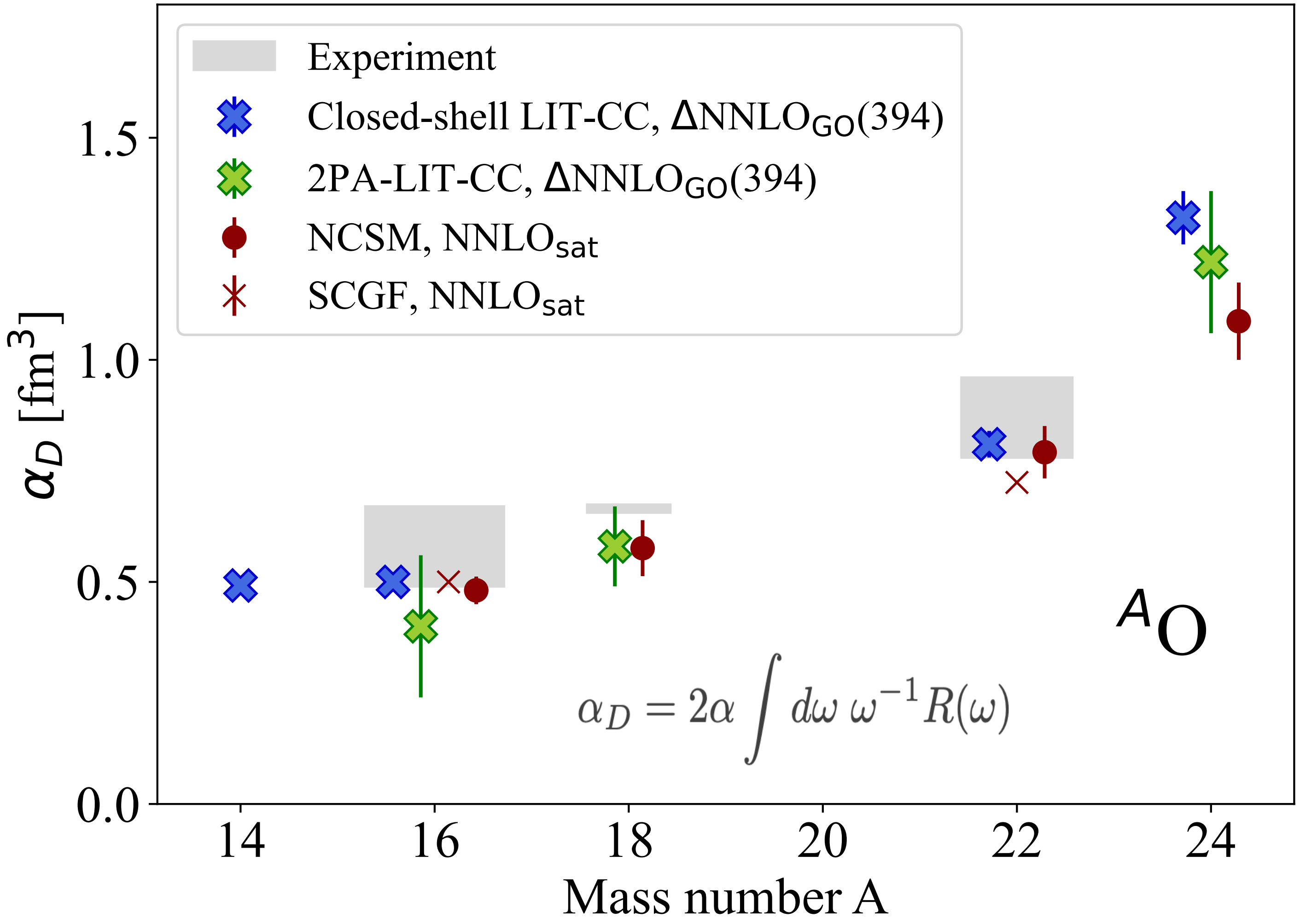
where

$$\left(\overline{H} - E_0 - \sigma - i\Gamma\right)|\Psi_R\rangle = \overline{\Theta}\,|\Phi_0\rangle$$

Bound-state like problem

S. Bacca, N. Barnea, G. Hagen, G. Orlandini, T. Papenbrock, PRL **111**, 122502 (2013).

α_D along the oxygen chain

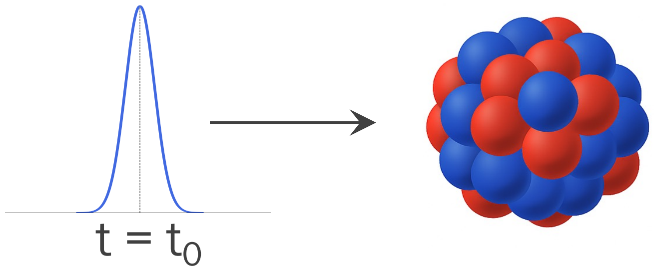


FB et al., PRC 110, 044306 (2024).

Responses in a time-dependent approach

Goal: solving

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



with

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

Responses in a time-dependent approach

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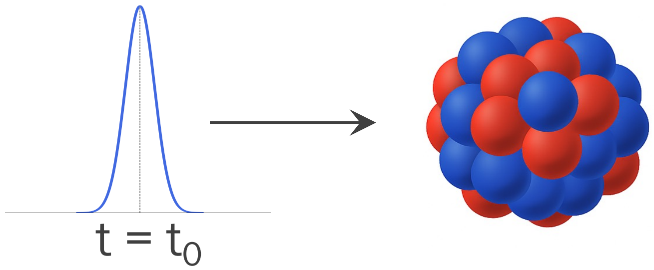

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For small ε, first-order time-dependent perturbation theory yields:

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

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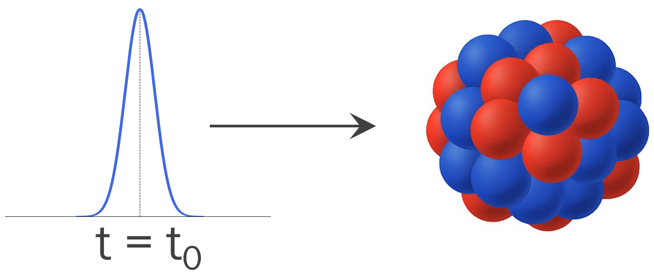

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$$D(t) = \langle\Psi(t)|\hat{D}|\Psi(t)\rangle \xrightarrow{\quad\quad} \tilde{D}(\omega)$$

Fourier transform

Responses in a time-dependent approach

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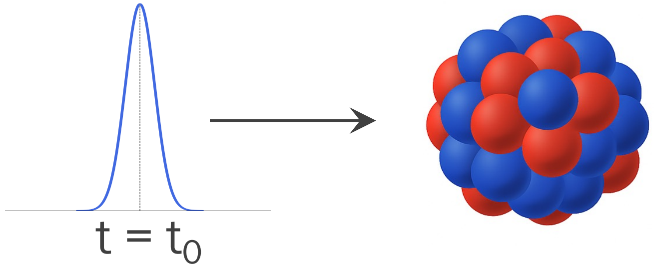

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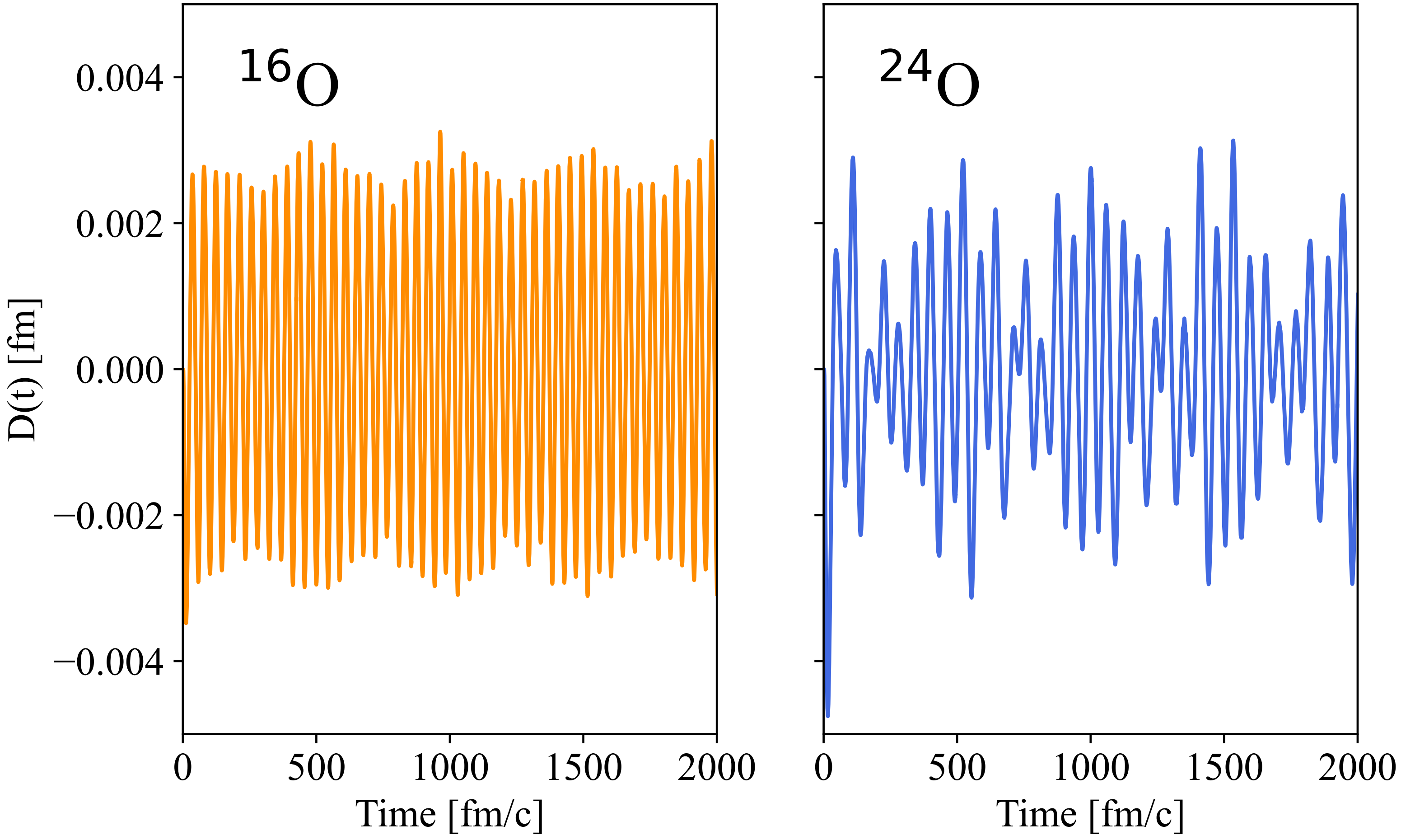
For small ε, first-order time-dependent perturbation theory yields:

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

Fourier transform

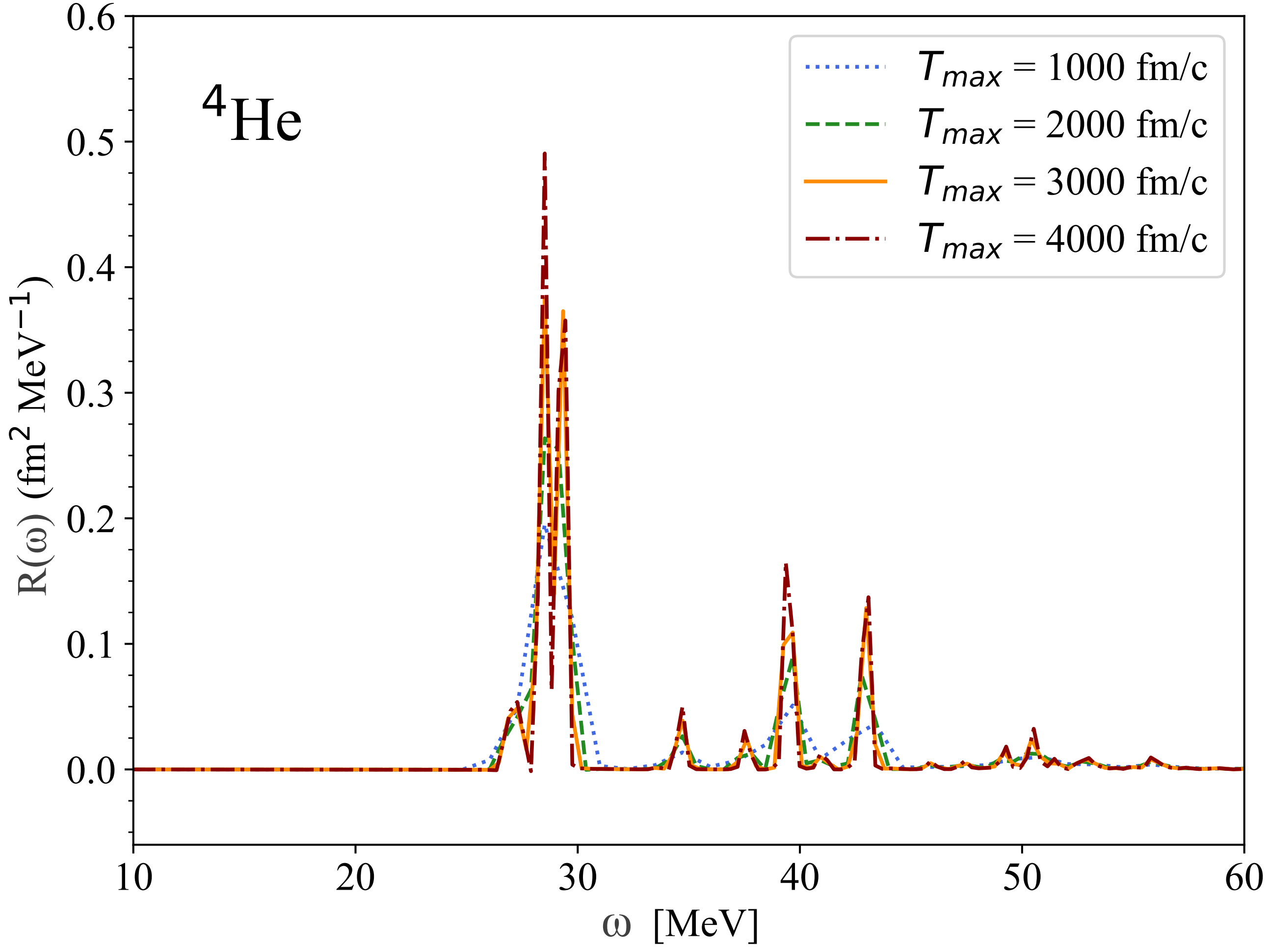
Time-dependent dipole moment

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



FB et al, in preparation.

Simulation time and resolution



Resolution

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

Maximum simulation time

FB et al, in preparation.

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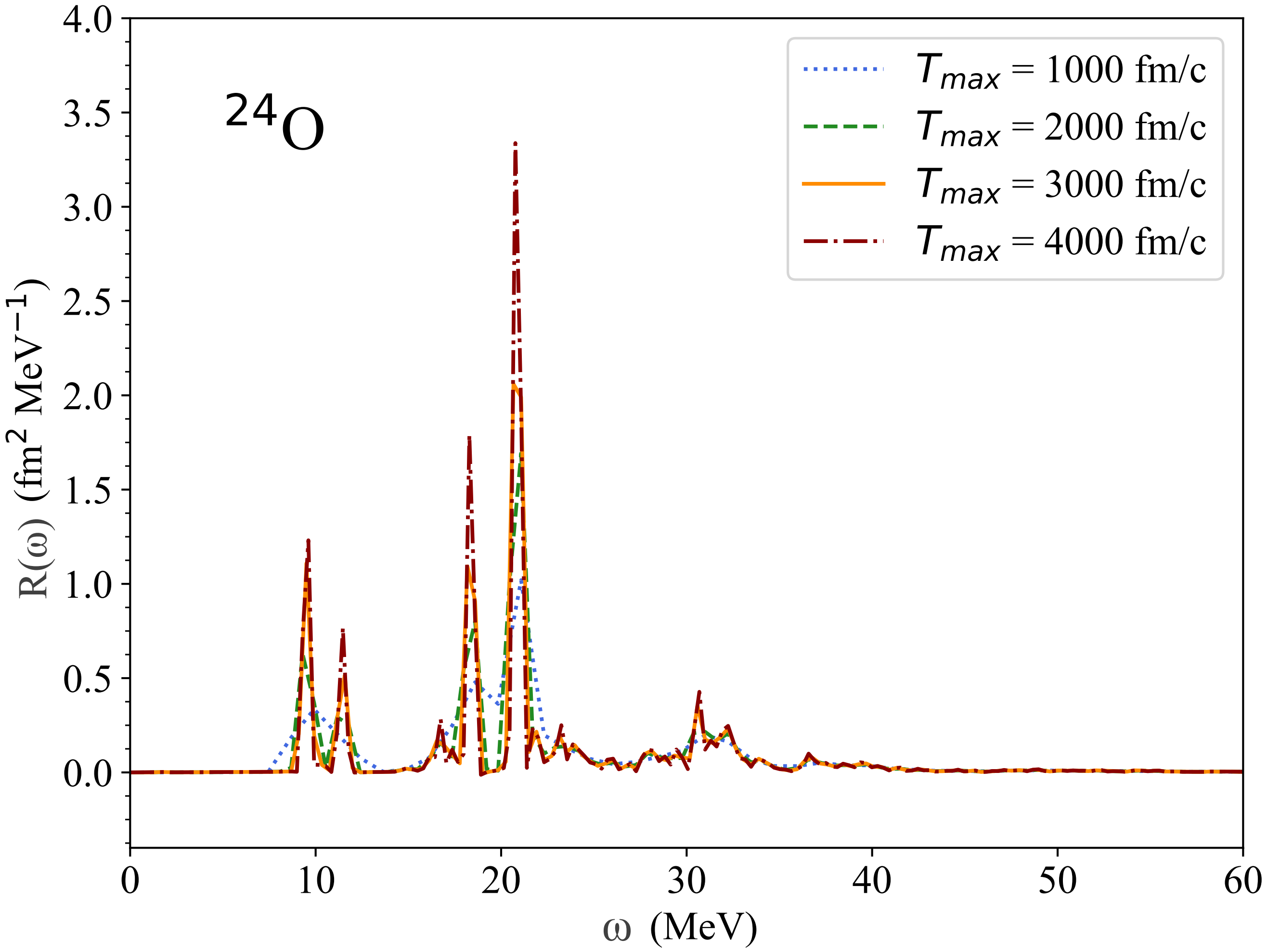

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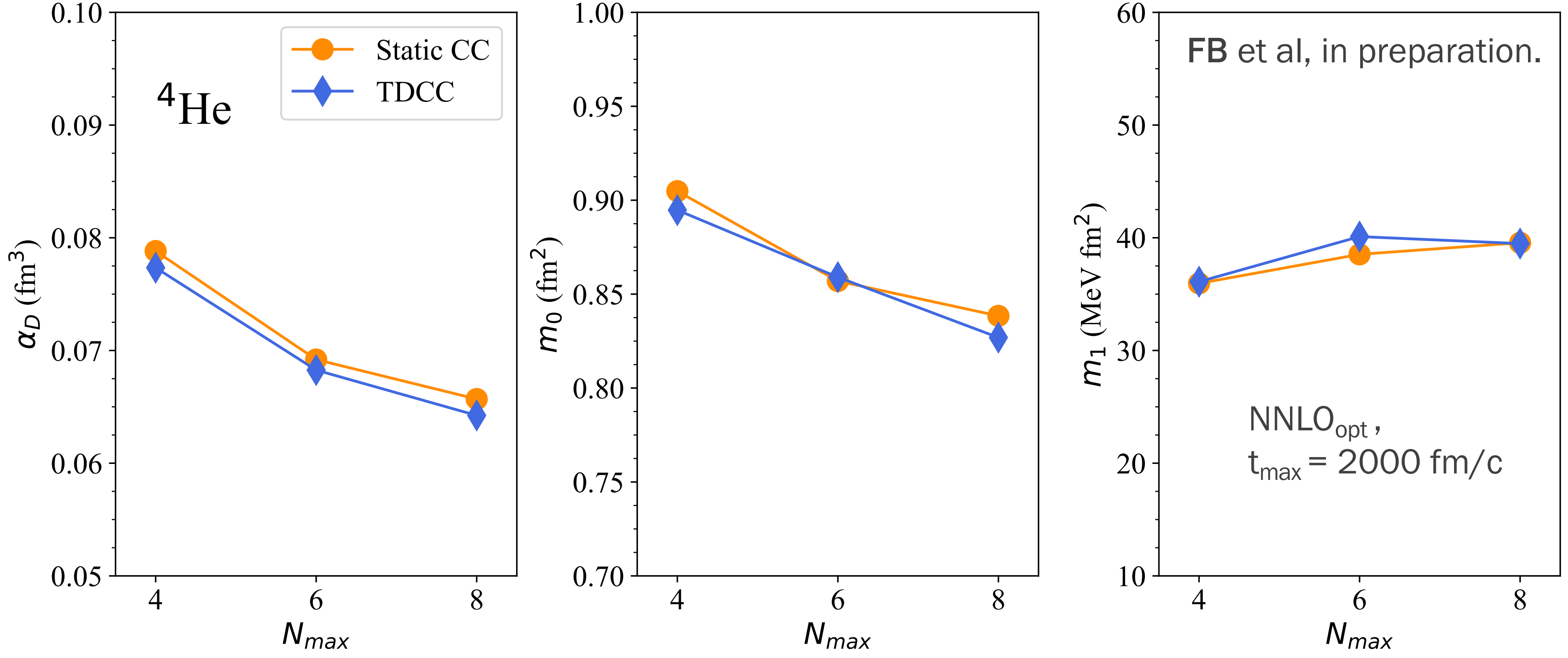
FB et al, in preparation.

Static CC vs time-dependent CC: ^{4}He

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



Very small deviations between the two completely independent approaches!

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

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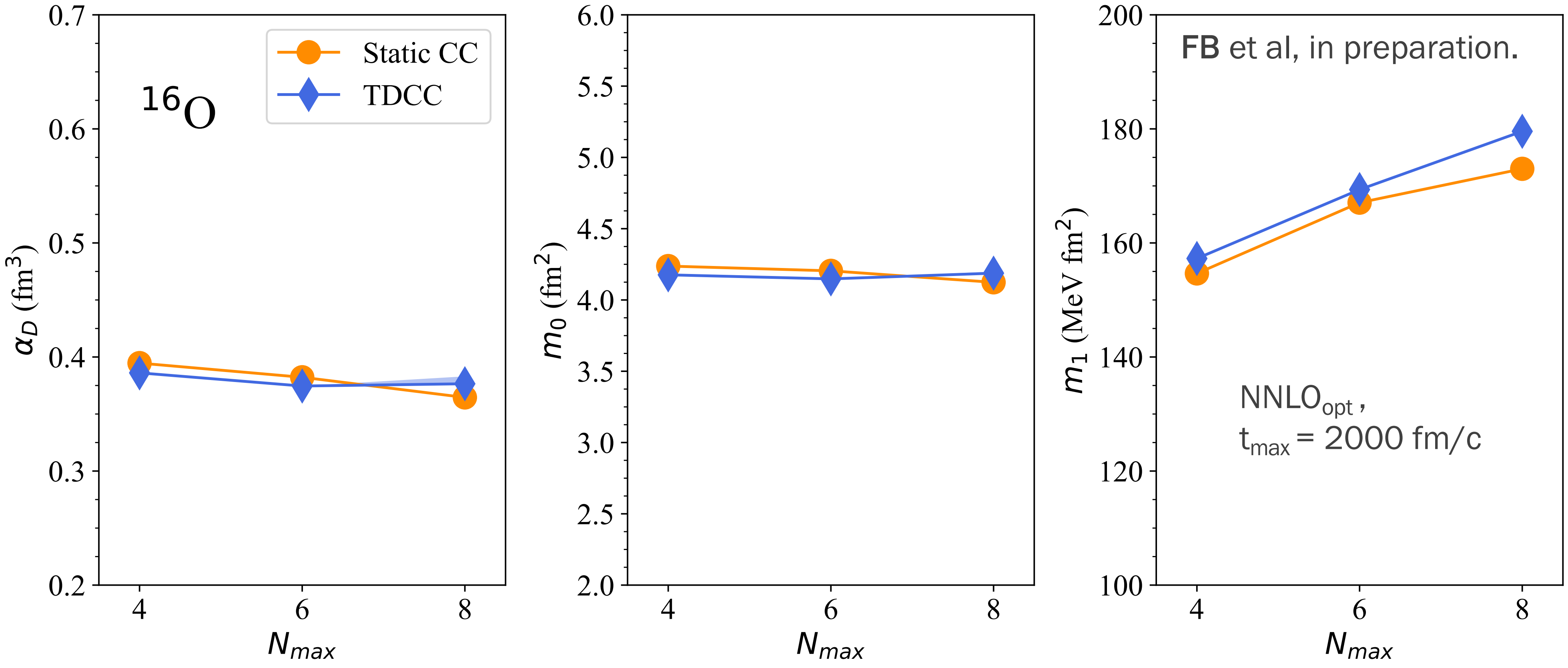

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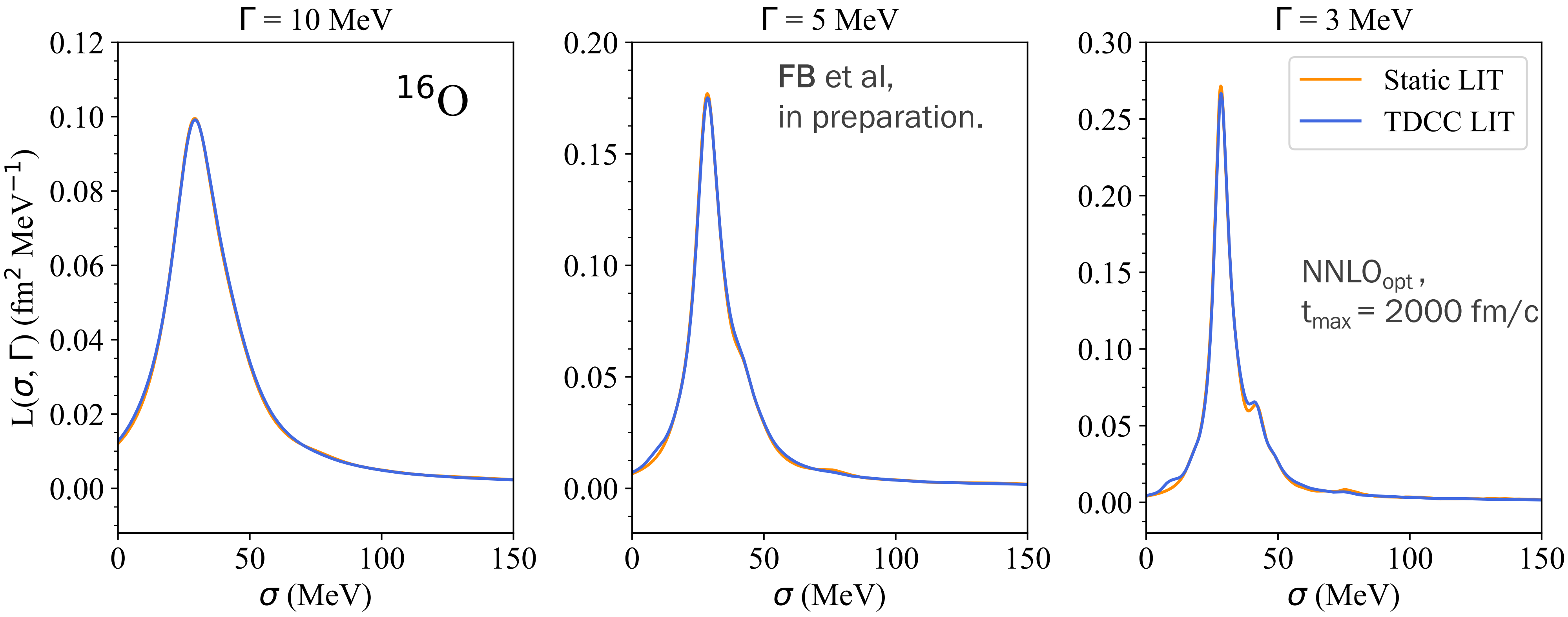

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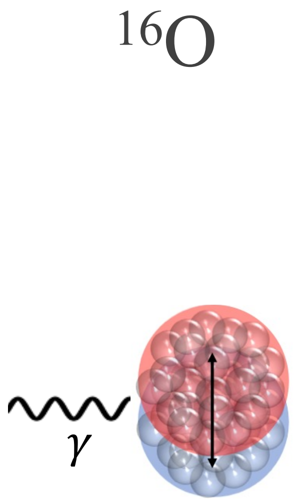
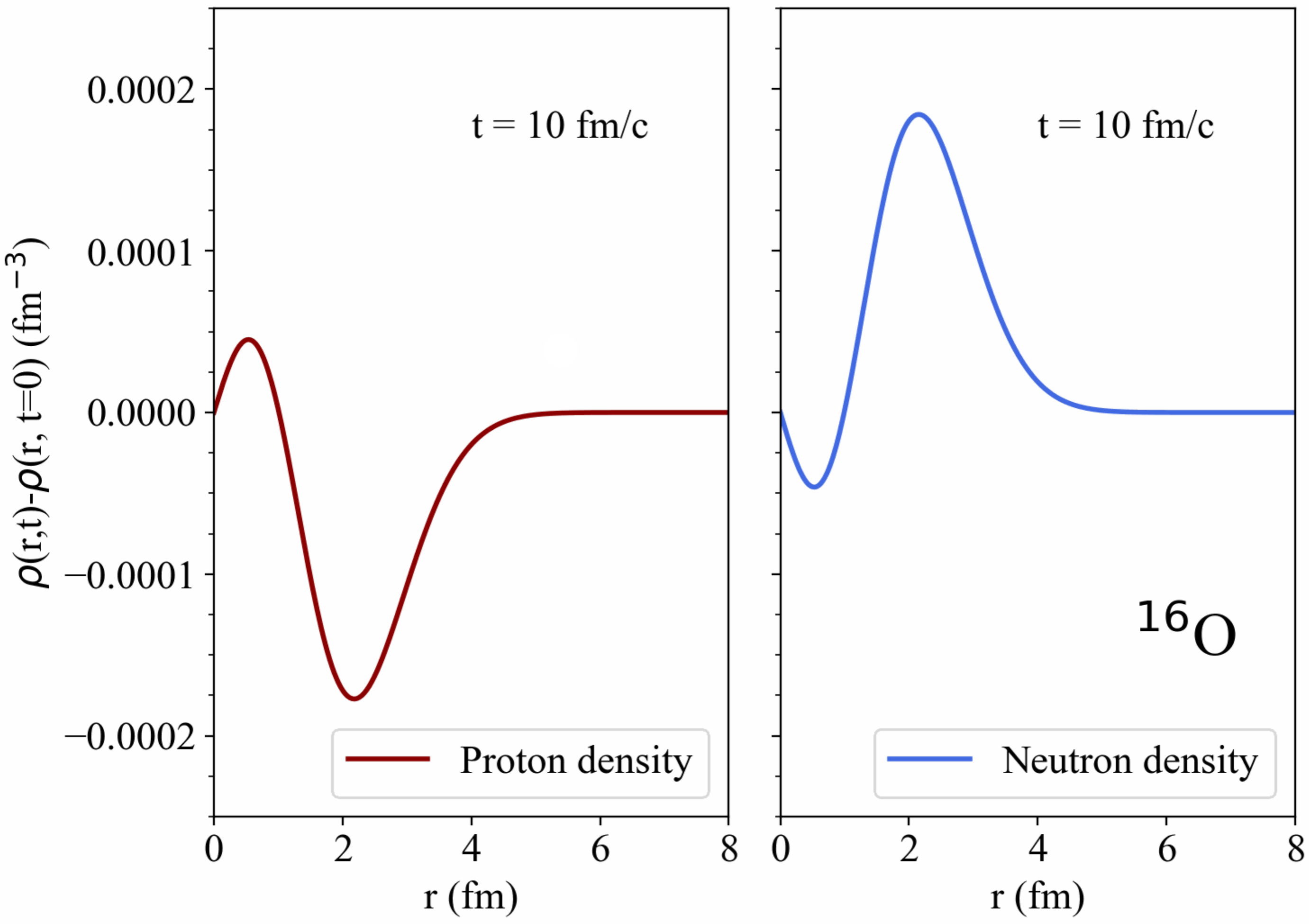
Collective oscillations in real time

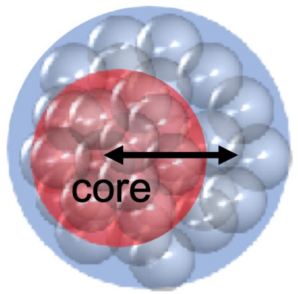




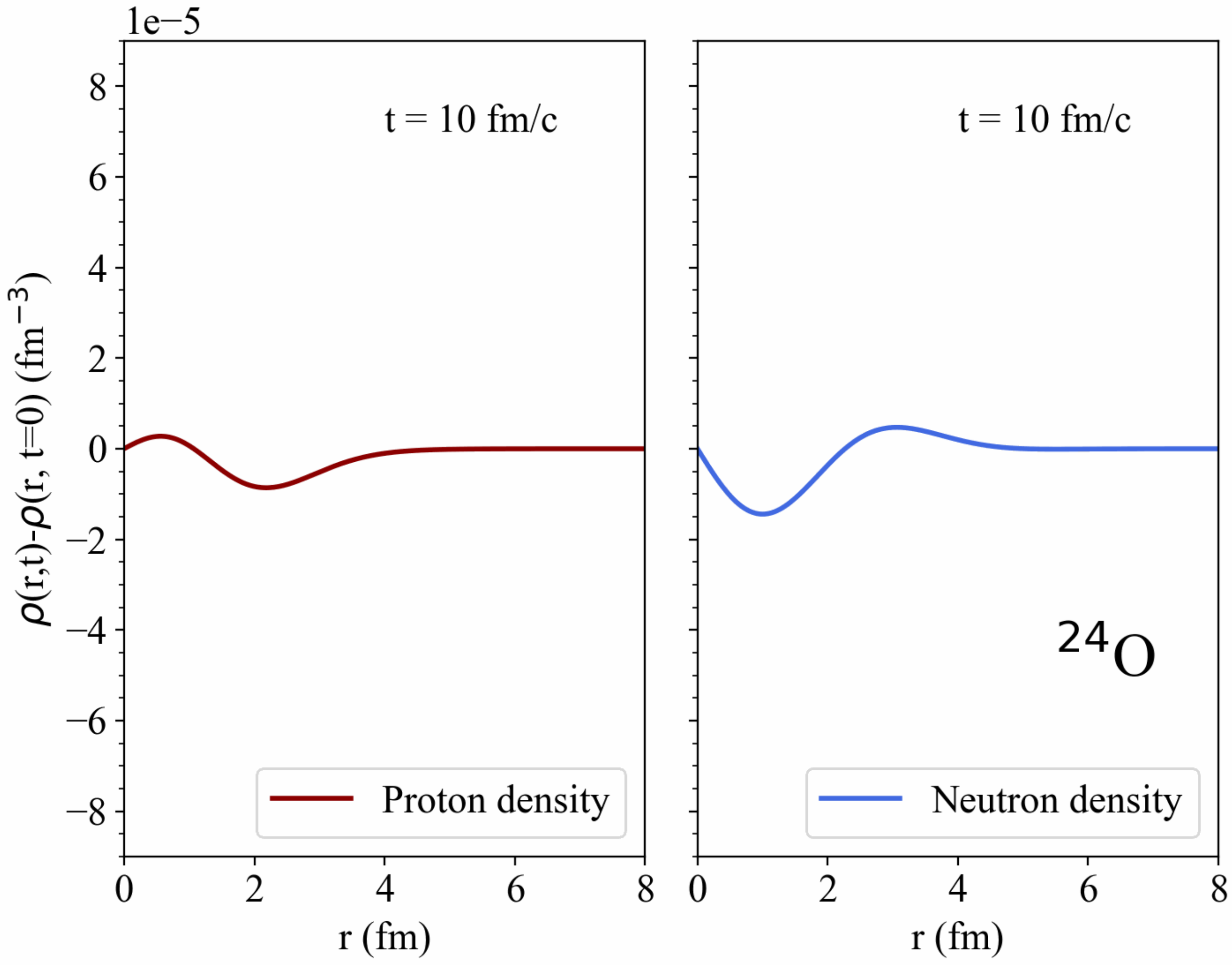
FB et al, in preparation.

Collective oscillations in real time

^{24}O



isolating
soft dipole mode
at low-energy



FB et al, in preparation.

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, $B(E1)^{1/2} \sim 0.01$ e fm [TUNL database], so we need ε = 100 MeV/fm to get a perturbation ~ MeV.

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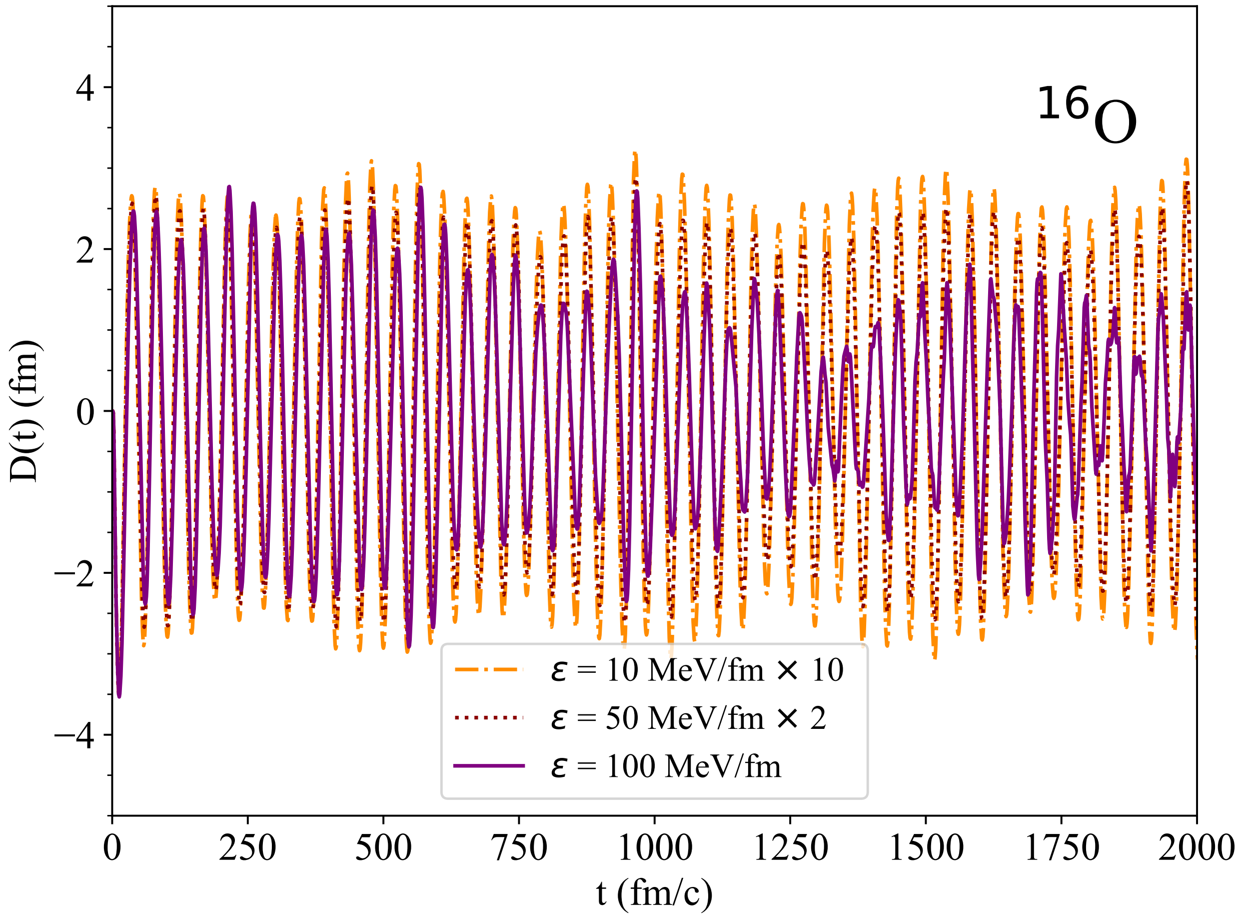
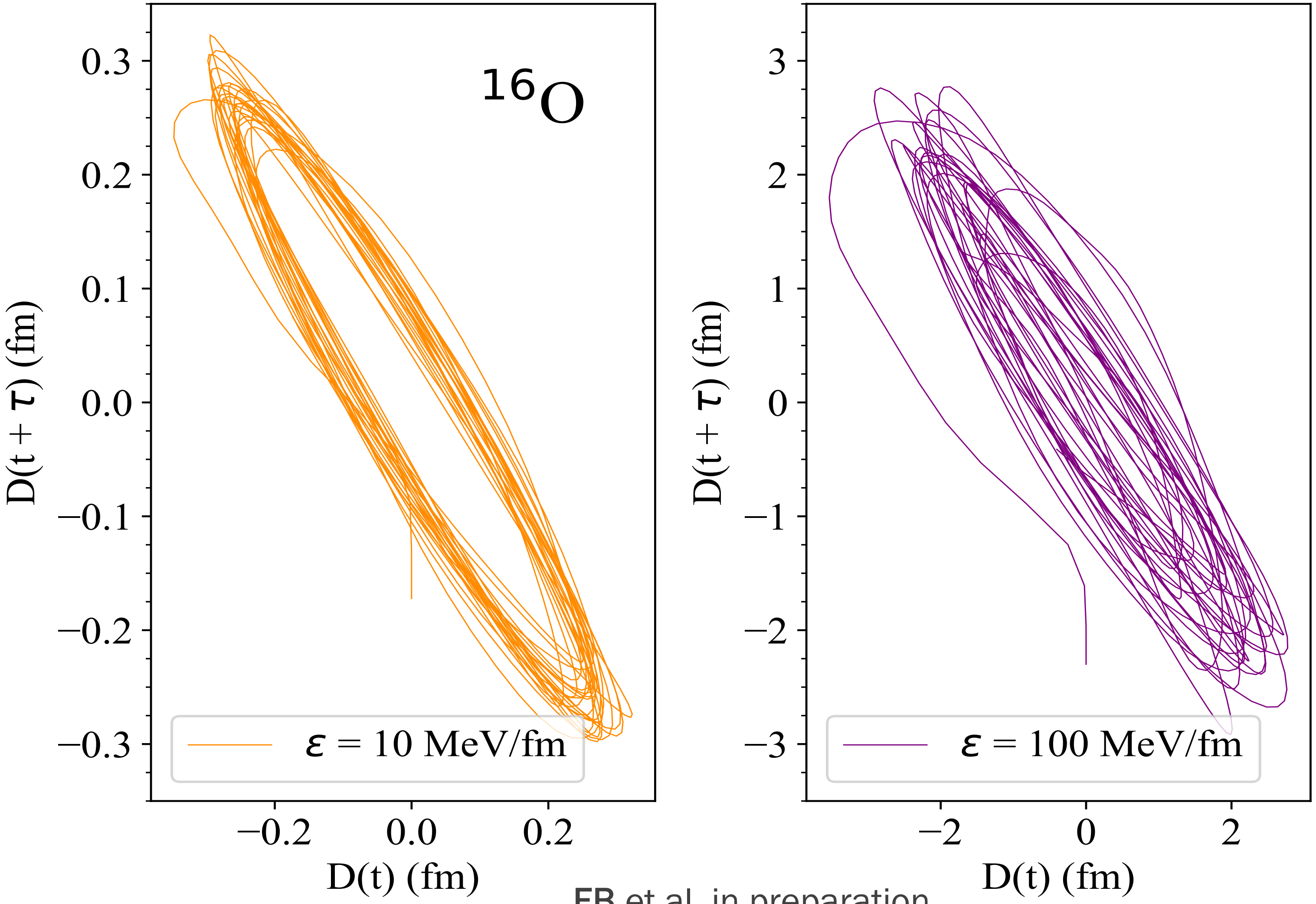


FB et al, in preparation.

From order to chaos



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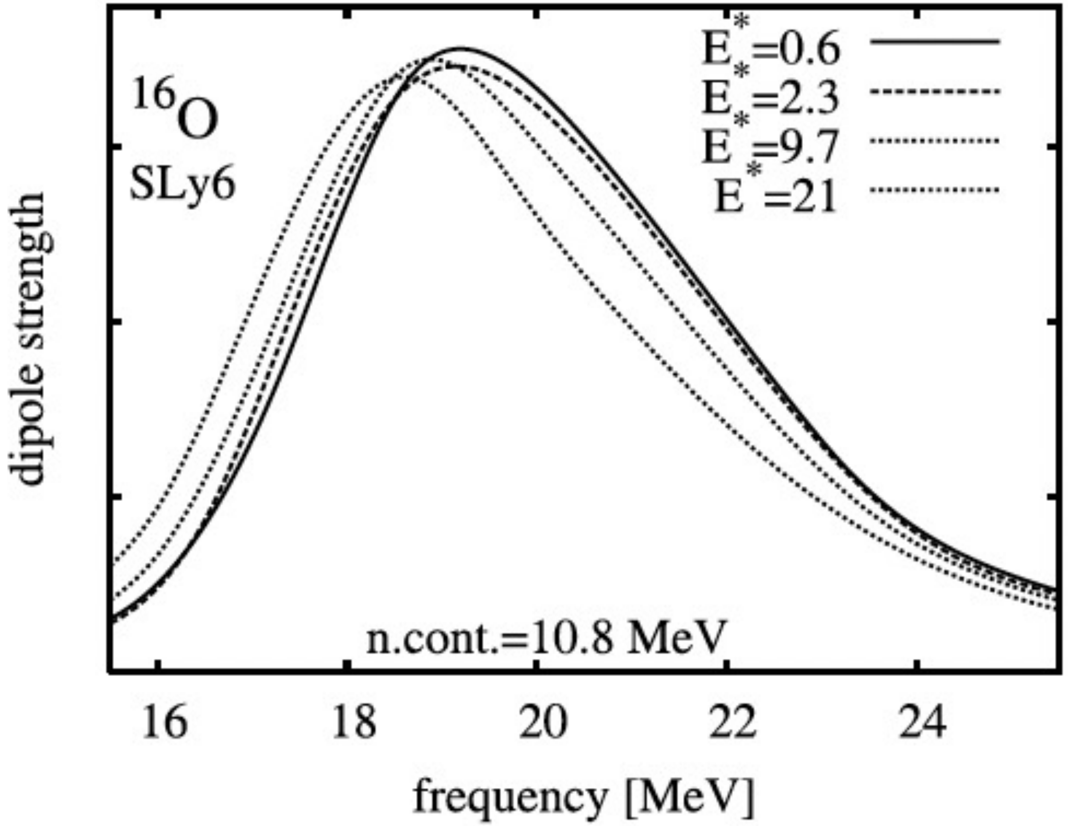
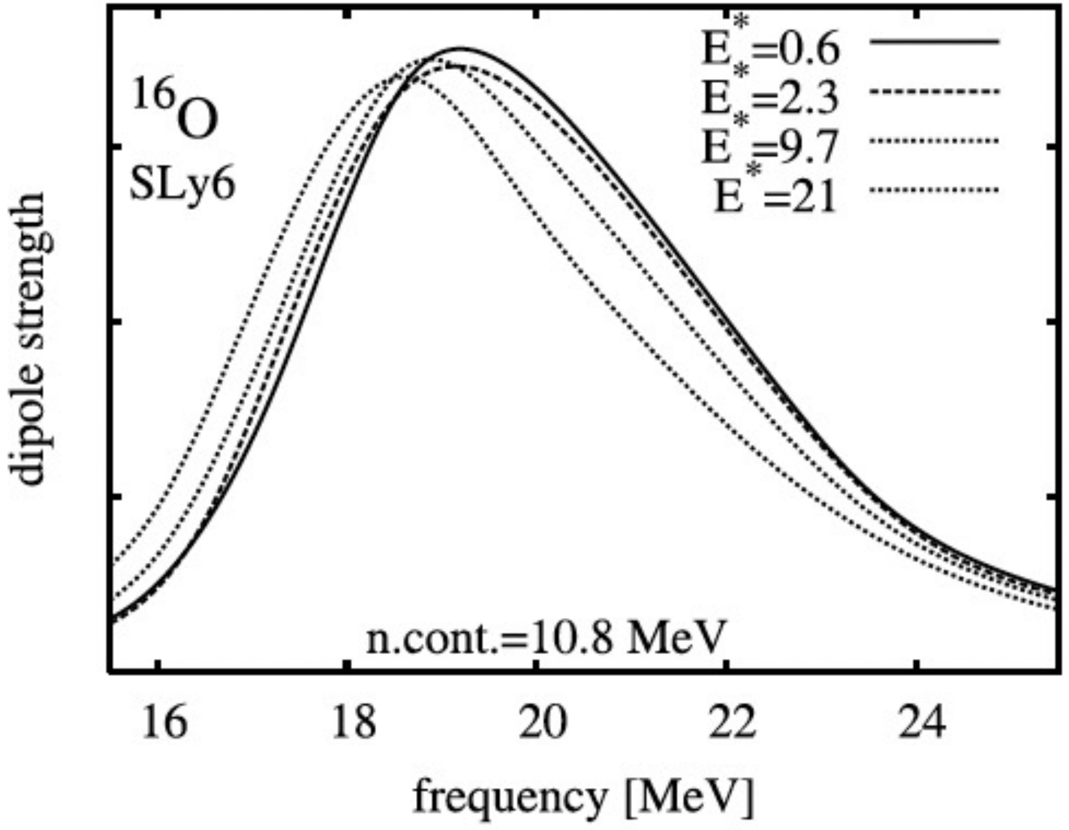


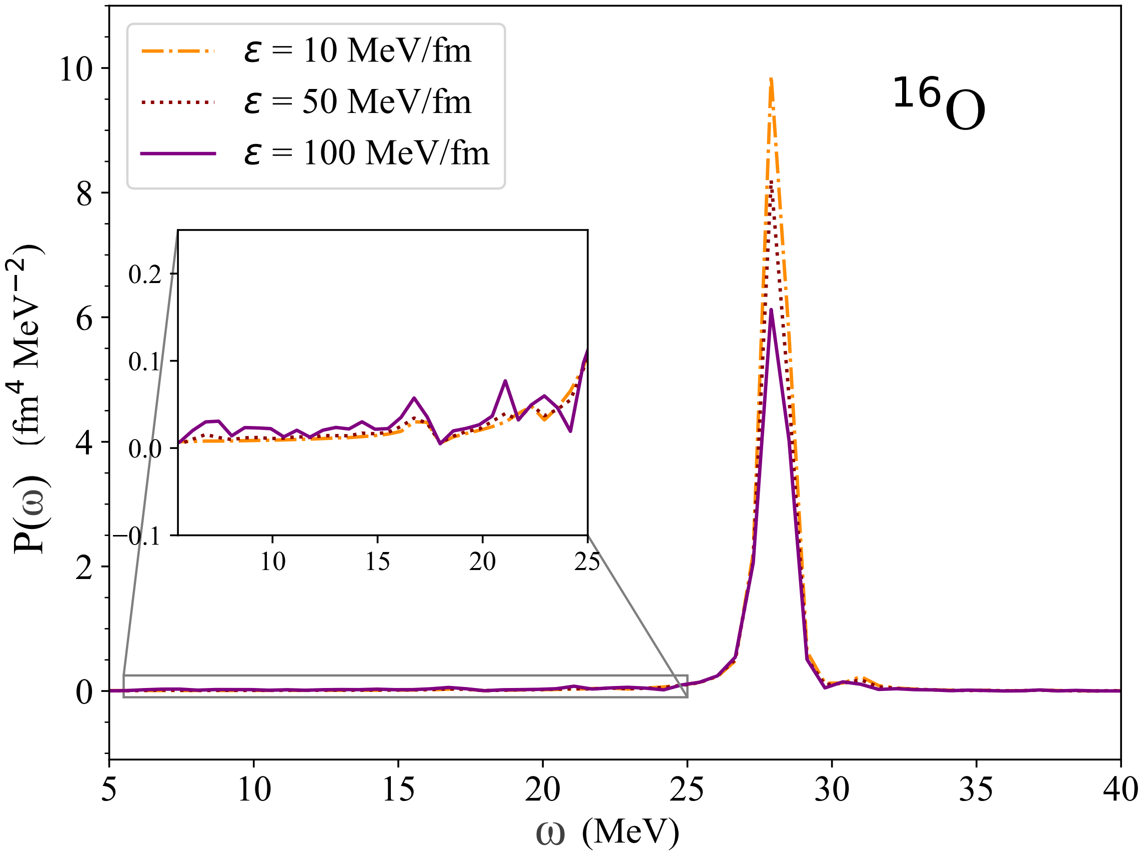
P.-G. Reinhard et al, Eur. Phys. J. A 32, 19–23 (2007).

What happens when we increase ε?



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

NNLO$_{opt}$, N$_{max}$ = 6, t$_{max}$ = 2000 fm/c



FB et al, in preparation.

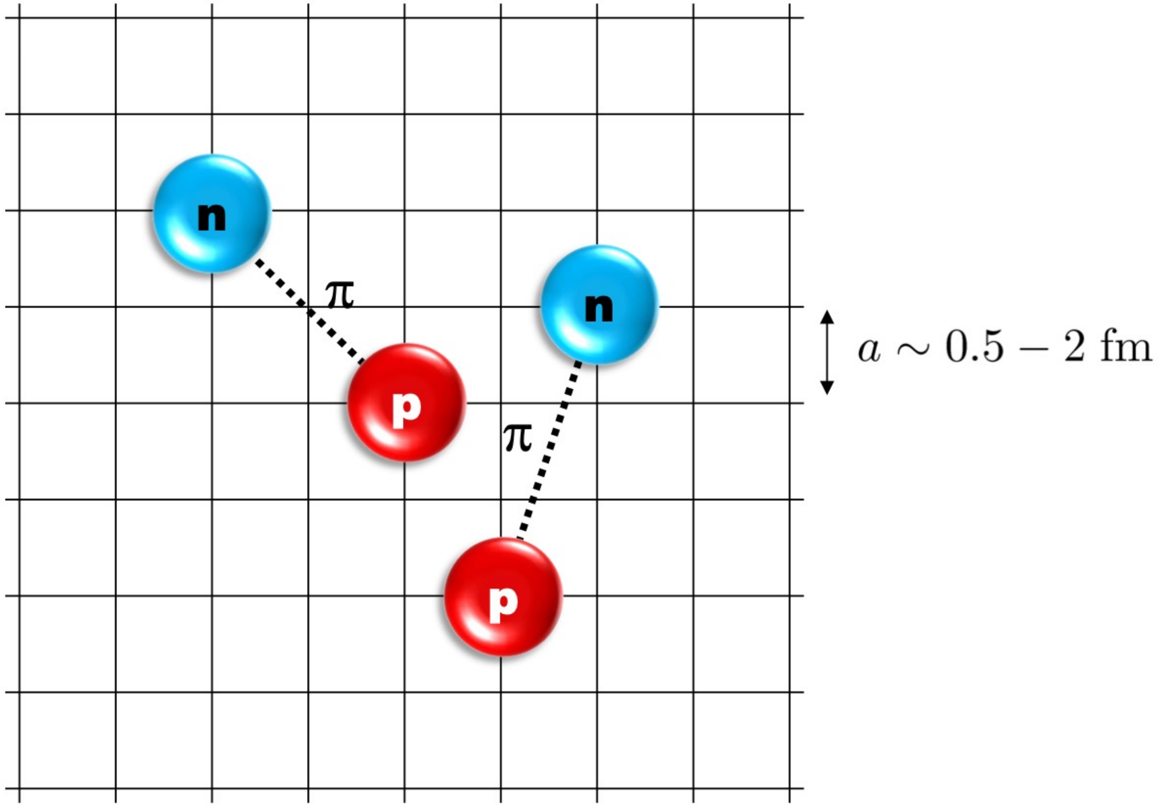
How do we go from this to
a microscopic description
of nuclear reactions?

A natural framework: nuclei on the lattice

- We can exploit the short-range nature of the nuclear force! Correlations are only between neighbours.

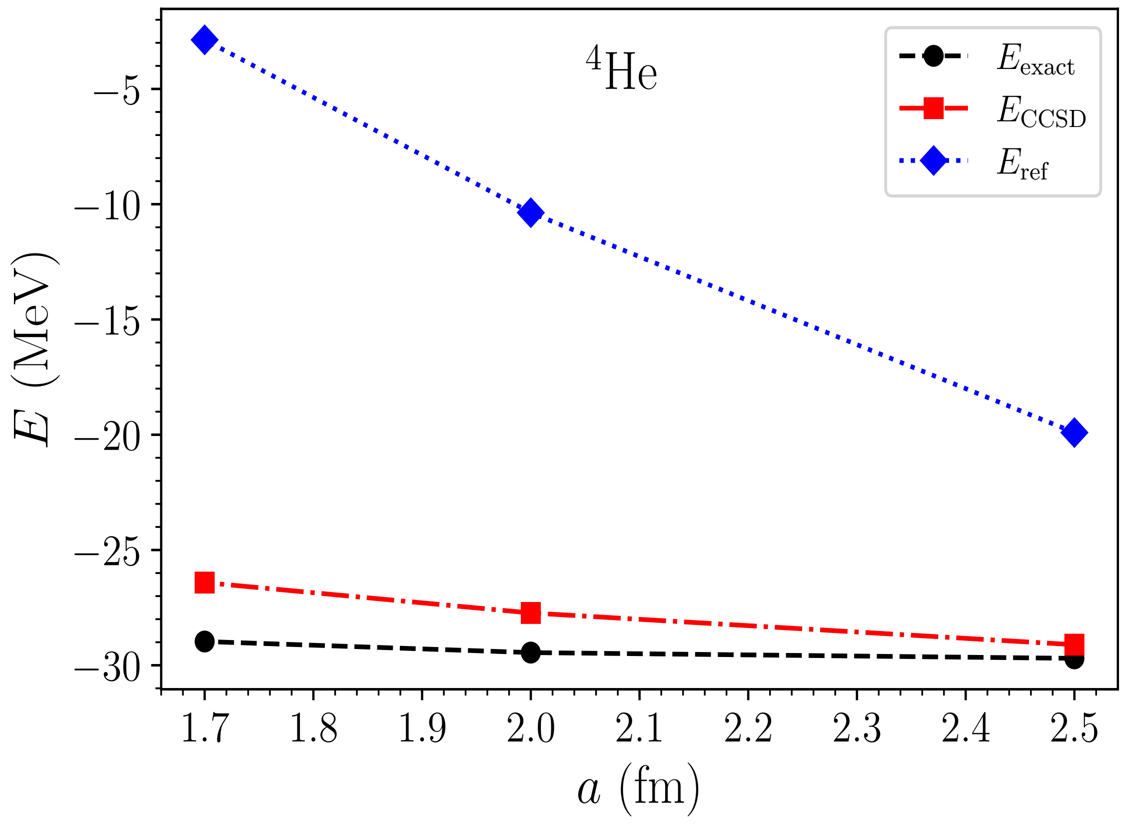
- Computational cost scales with volume → problem becomes sparse and we can do calculations on a laptop!

- 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}He



M. Rothman, B. Johnson-Toth, **FB**, G. Hagen, M. Heinz, T. Papenbrock, arXiv:2508.01507 [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, a natural framework where to achieve a microscopic description of nuclear dynamics.

Stay tuned!

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FRIB Theory Alliance

NUCLEI Nuclear Computational Low-Energy Initiative