Nuclear dynamics from time-dependent coupled-cluster theory

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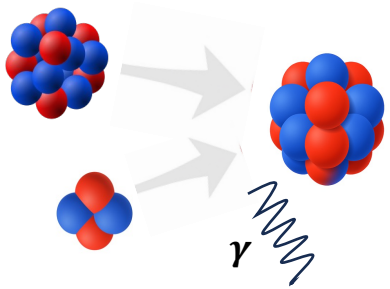
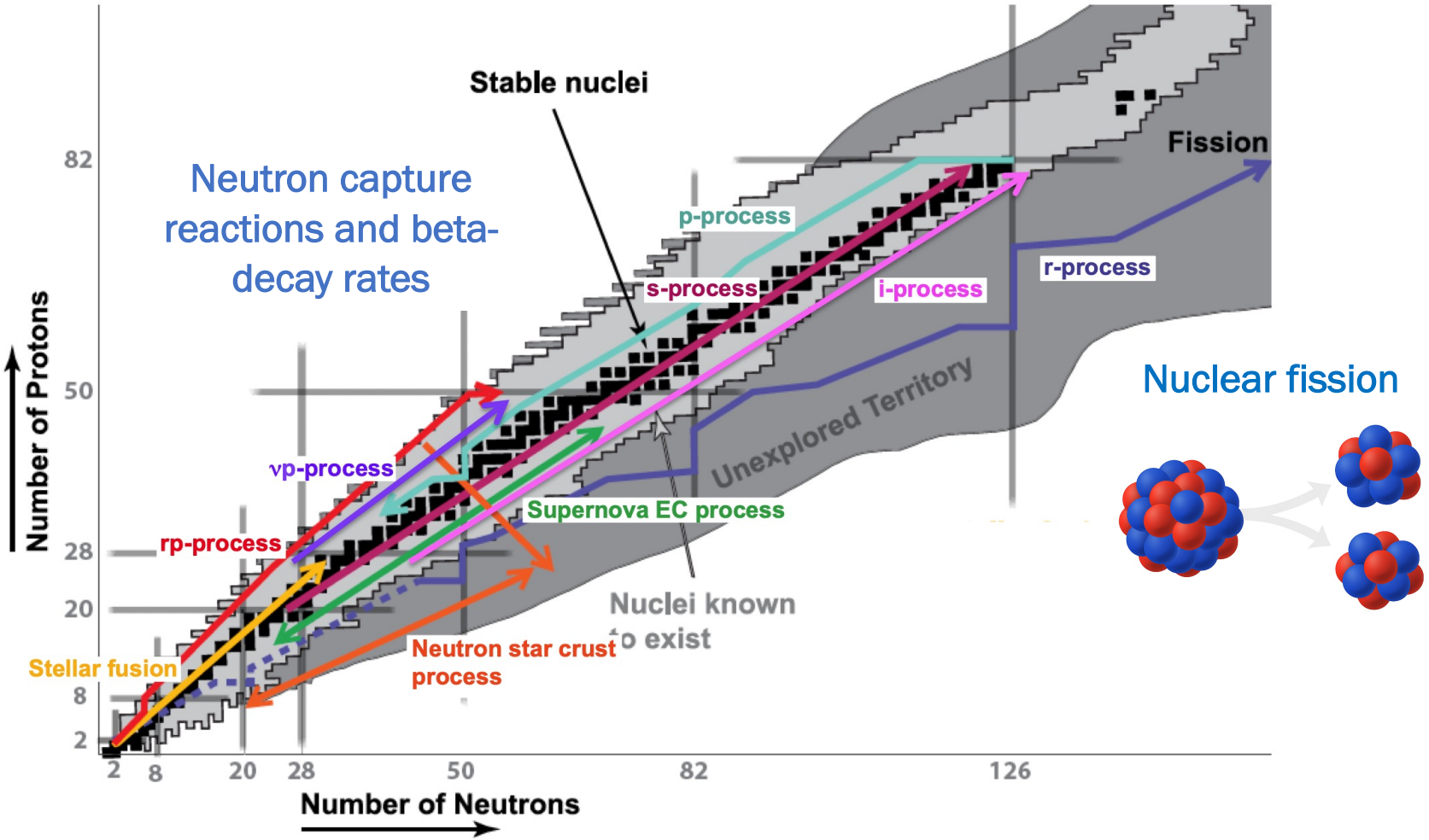
MITP PROGRAM ON «MANY-BODY THEORY: NUCLEAR PHYSICS MEETS QUANTUM CHEMISTRY», MAINZ, GERMANY

SEPTEMBER 1, 2026

Nuclear reactions are key to understand the origin of elements in the Universe

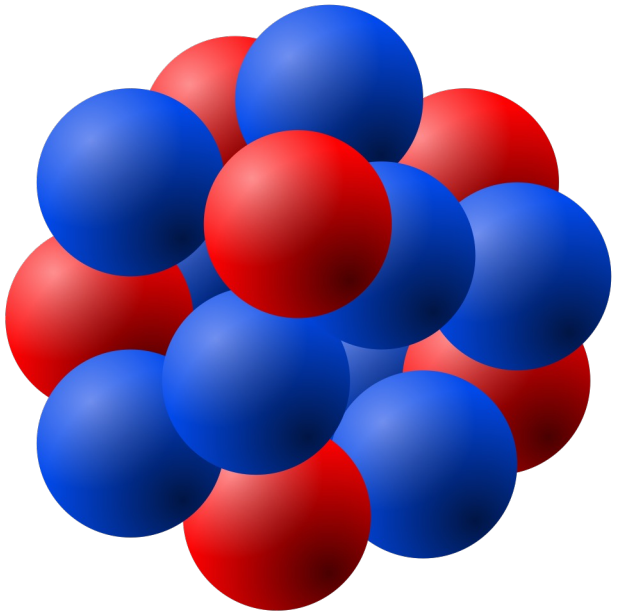
Nuclear fusion in stars





Hendrik Schatz, *J. Phys. G: Nucl. Part. Phys.* **43** 064001 (2016)

Ab initio nuclear theory



- Building blocks: **protons and neutrons.**
- Solve **quantum many-body problem**

$$H\,|\psi\rangle = E\,|\psi\rangle$$
$$H = T + V_{NN} + V_{3N}$$

with **controlled approximations**.

- 2 ingredients: **nuclear interactions** and **many-body solver,**
  in this talk: **nuclear forces** from **chiral EFT** and **coupled-cluster.**

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

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

Time-dependent coupled-cluster theory

- Starting point: harmonic oscillator, Hartree-Fock or lattice reference $|\Phi_0\rangle$

Right time-dependent wf

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

Left time-dependent wf

$$\langle\Psi(t)| = \langle\Phi_0|L(t)e^{-T(t)}$$

S. Kvaal, J. Chem. Phys. 136, 194109 (2012).
D.A. Pigg, G. Hagen, H. Nam, T. Papenbrock, PRC 86, 014308 (2012).

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Right time-dependent wf

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

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

Left time-dependent wf

$$\langle\Psi(t)| = \langle\Phi_0|L(t)e^{-T(t)}$$

$$-i\hbar\dot{l}_0(t) = 0$$
$$-i\hbar\dot{l}_a^i(t) = \langle\Phi_0|L(t)\overline{H}|\Phi_i^a\rangle$$
$$-i\hbar\dot{l}_{ab}^{ij}(t) = \langle\Phi_0|L(t)\overline{H}|\Phi_{ij}^{ab}\rangle$$

- Truncations : CCD, CCSD.

S. Kvaal, J. Chem. Phys. 136, 194109 (2012).
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What do we gain going beyond the mean-field approximation?

- Reactions in medium-mass/heavy nuclei typically modeled with **mean-field approaches** (e.g. TDHF).

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

- We introduce them dynamically and look at **time evolution** of the **time-independent Hamiltonian** starting from **Hartree-Fock reference**.

What do we gain going beyond the mean-field approximation?

- We focus on nuclear radial density, obtained from the one-body density matrix:

$$\rho_{pq}(t) = \langle \Phi_0 | L(t) e^{-T(t)} a_p^\dagger a_q e^{T(t)} | \Phi_0 \rangle$$

- We can look at the typical time scales and amplitudes of nuclear density fluctuations wrt their time average.

FB, G. Hagen, T. Papenbrock, PRL **137**, 072502 (2026).

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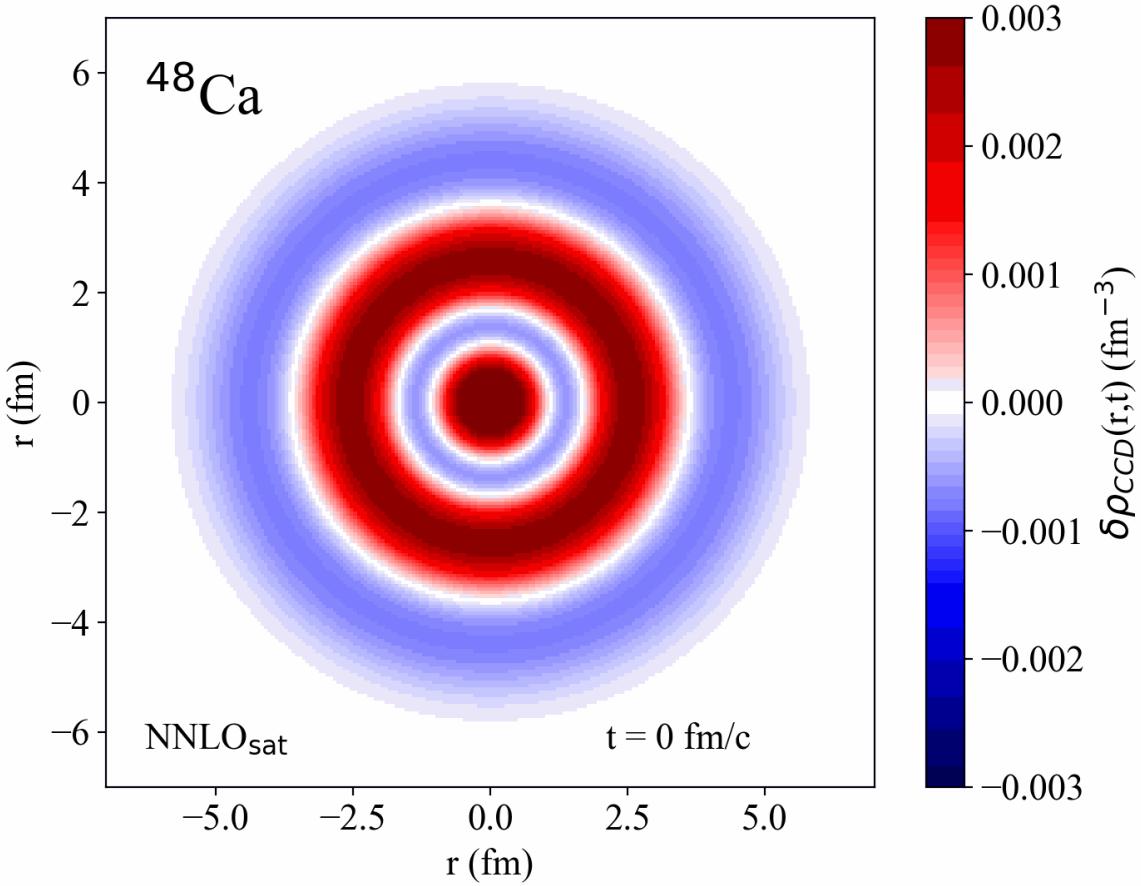
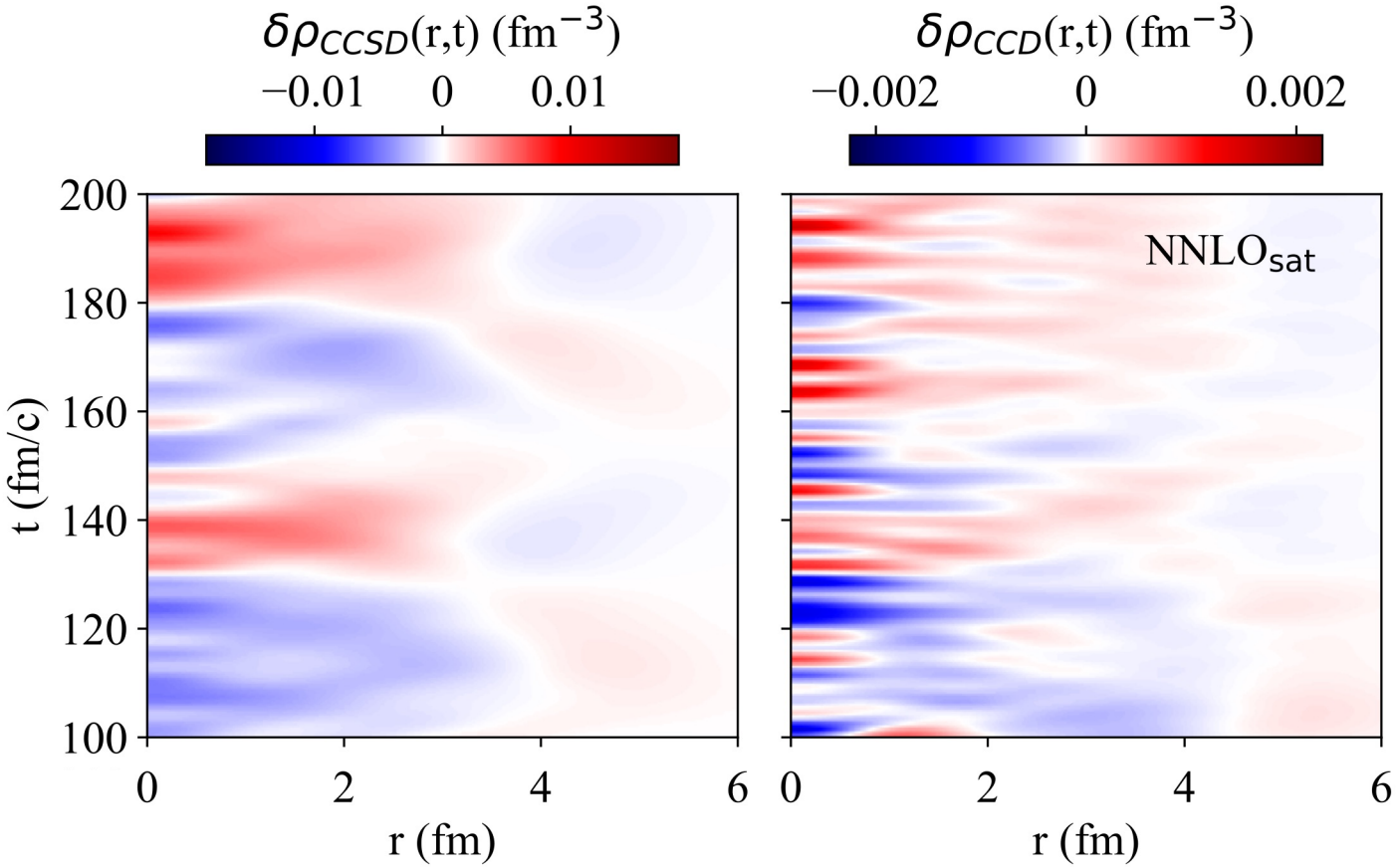
- We can look at the typical **time scales** and **amplitudes** of **nuclear density fluctuations** wrt their **time average**.



FB, G. Hagen, T. Papenbrock, PRL **137**, 072502 (2026).

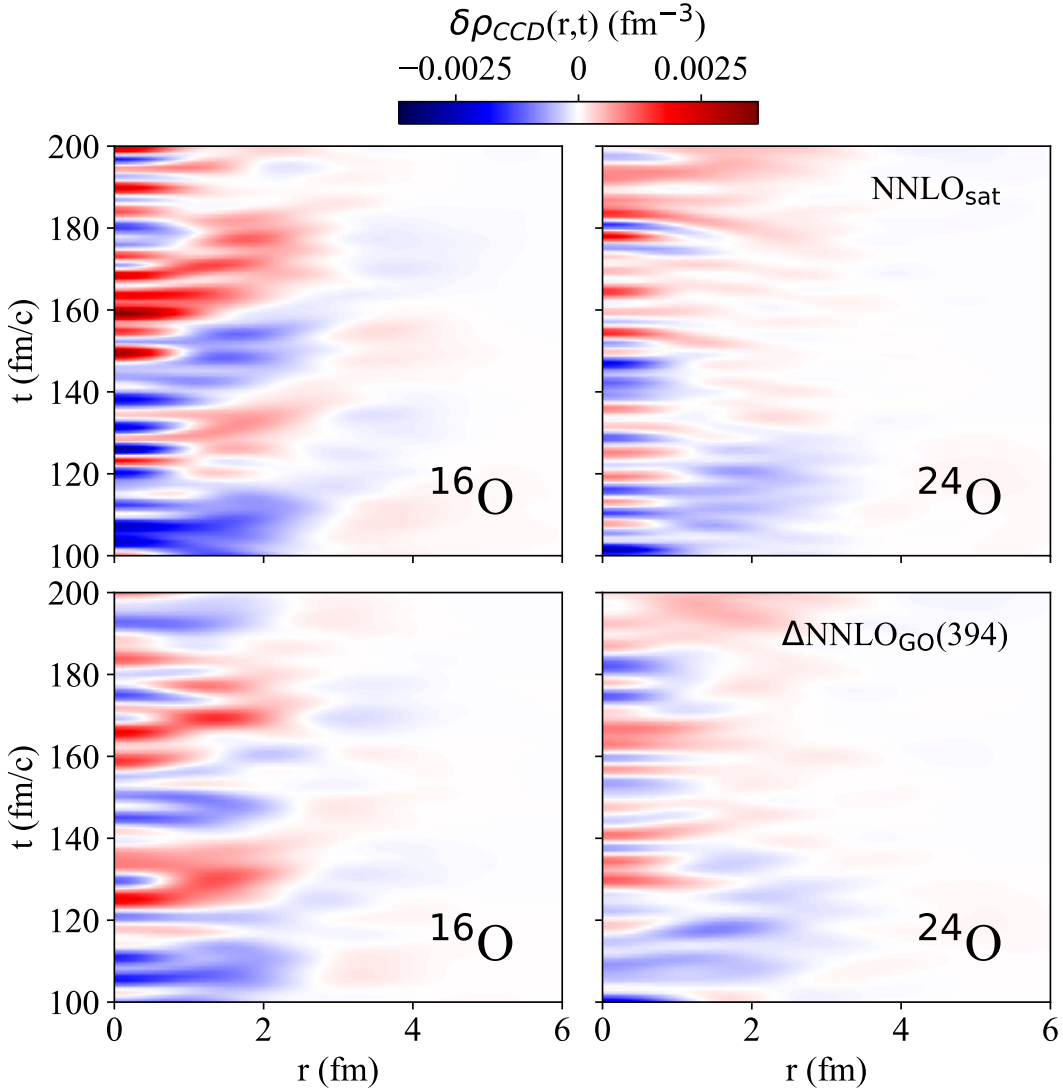
Isolating 2p-2h correlations, we observe fast, short-range fluctuations



NB:
1 fm/c = 3 x 10^{-24} s

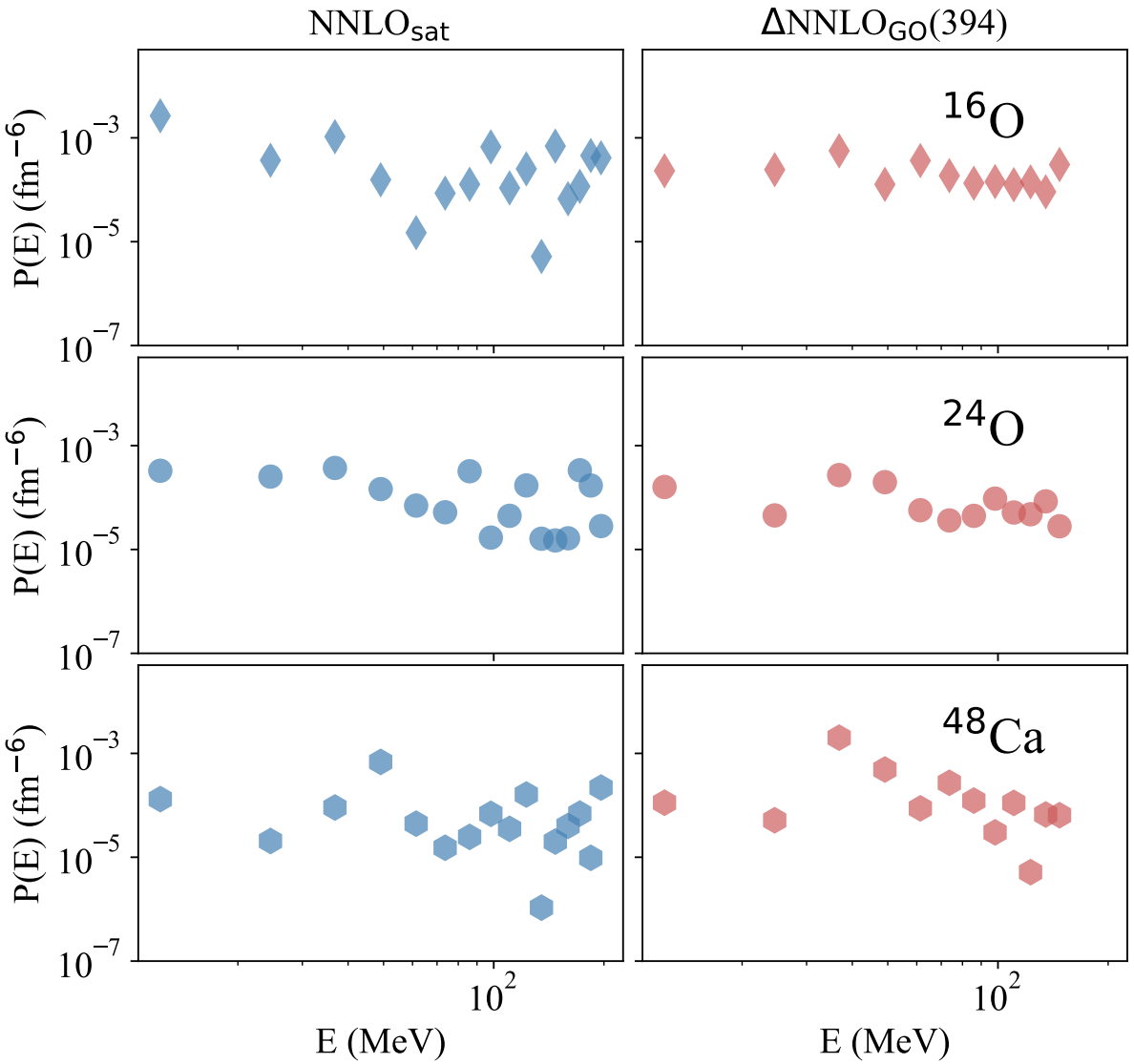
FB et al, PRL **137**, 072502 (2026).

Fast density fluctuations are present across nuclei and nuclear Hamiltonians



FB et al, PRL **137**, 072502 (2026).

Short-range fluctuations are stochastic



FB et al, PRL **137**, 072502 (2026).

How do we compare with exact dynamics?

Survival probabilities

- We consider time evolution of the time-independent Hamiltonian.
- We start from a harmonic oscillator reference state.
- Our observable of interest is the survival probability:

$$P(t) = |\langle \Psi(0) | \Psi(t) \rangle|^2$$

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- Our observable of interest is the survival probability:

$$P(t) = |\langle \Psi(0) | \Psi(t) \rangle|^2$$

As TDCC is a truncated, non-Hermitian framework, P(t) is in general not guaranteed to be real and between 0 and 1.

Biorthogonal vs symmetrized overlap

- We have two ways of computing the survival probability in TDCC.

Biorthogonal overlap

$$P(t) = \langle \Psi(0)|\Psi(t)\rangle \langle \Psi(t)|\Psi(0)\rangle$$
$$= e^{t_0(t)} \langle \Phi_0|L(t)e^{-T(t)}|\Phi_0\rangle$$

Analogous to the expression we use to compute transition strengths

$$\left|\langle b|\hat{O}|a\rangle\right|^2 \leftarrow \langle \tilde{a}|\hat{O}|b\rangle\langle \tilde{b}|\hat{O}|a\rangle$$

Biorthogonal vs symmetrized overlap

- We have **two ways** of computing the **survival probability** in TDCC.

Biorthogonal overlap

$$P(t) = \langle\Psi(0)|\Psi(t)\rangle\,\langle\Psi(t)|\Psi(0)\rangle$$
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Analogous to the expression we use to compute transition strengths

$$\left|\langle b|\hat{O}|a\rangle\right|^2 \leftarrow \langle\widetilde{a}|\hat{O}|b\rangle\langle\widetilde{b}|\hat{O}|a\rangle$$

Symmetrized overlap

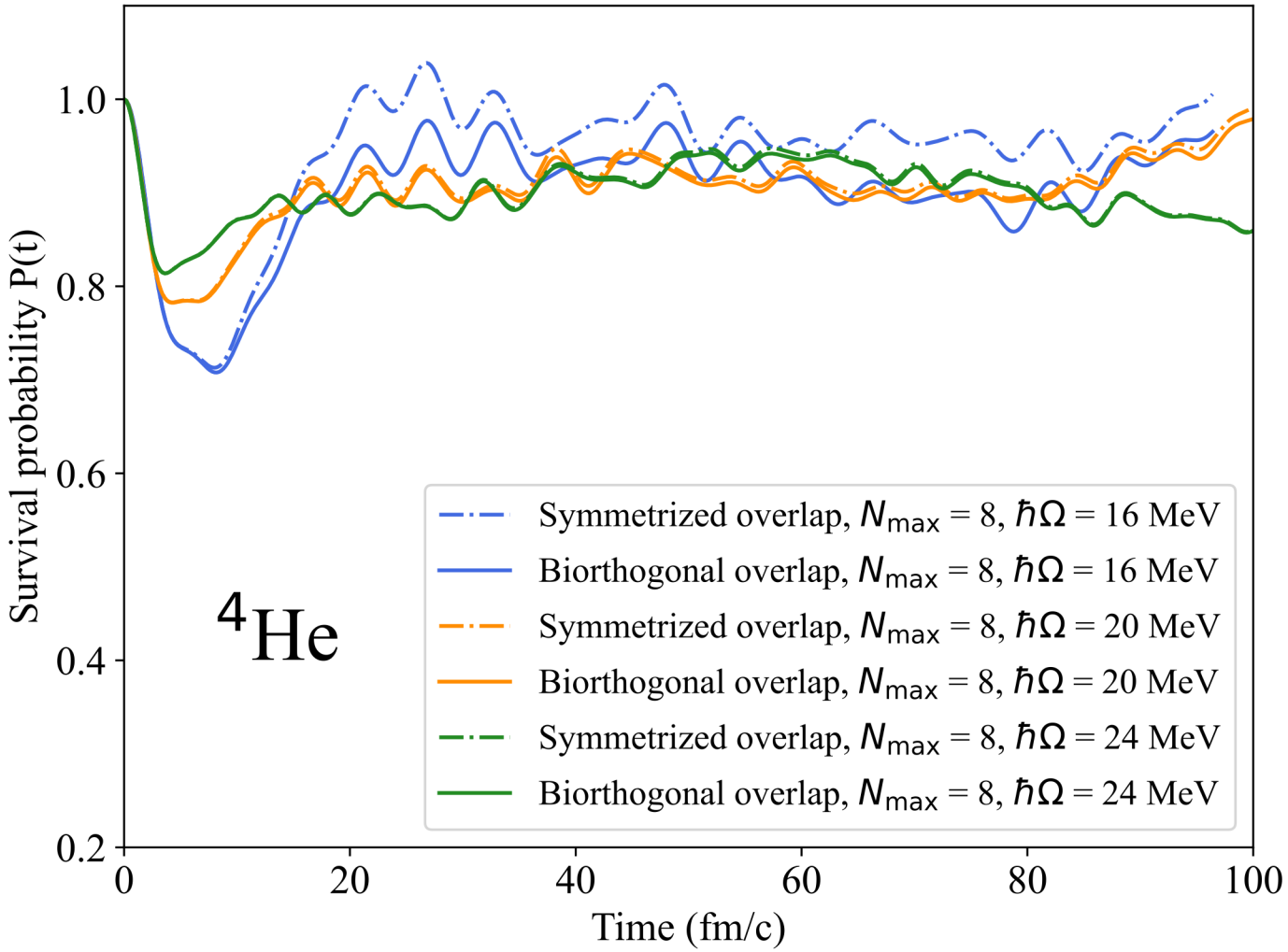
One can also take the absolute square of the symmetrized overlap

$$\frac{1}{2}\left(\langle\widetilde{\Psi}(0)|\Psi(t)\rangle + \langle\widetilde{\Psi}(t)|\Psi(0)\rangle^*\right)$$

Used in quantum chemistry to compute autocorrelation functions.

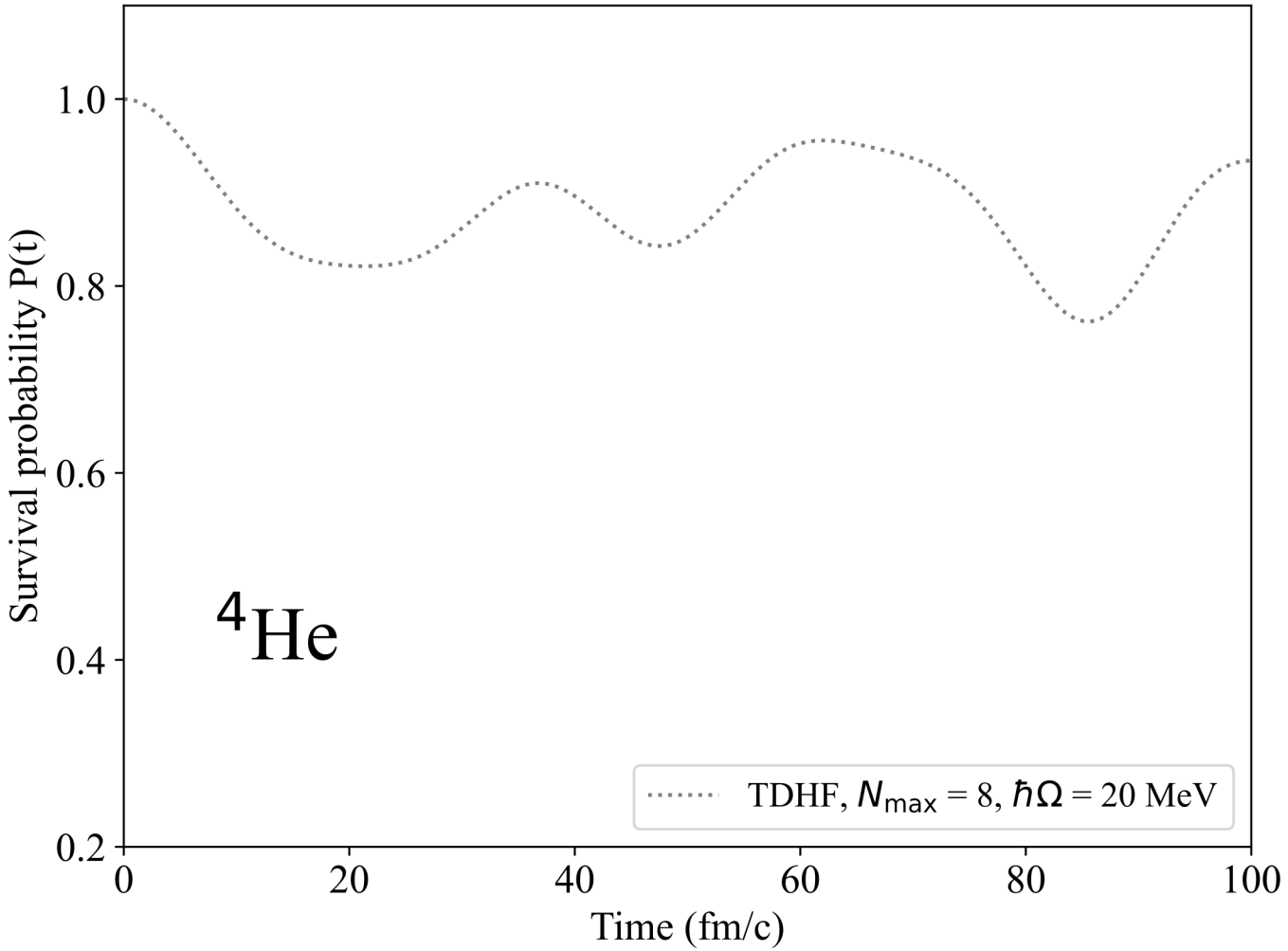
T. B. Pedersen and S. Kvaal,
J. Chem. Phys. 150, 144106 (2019).

Biorthogonal vs symmetrized overlap



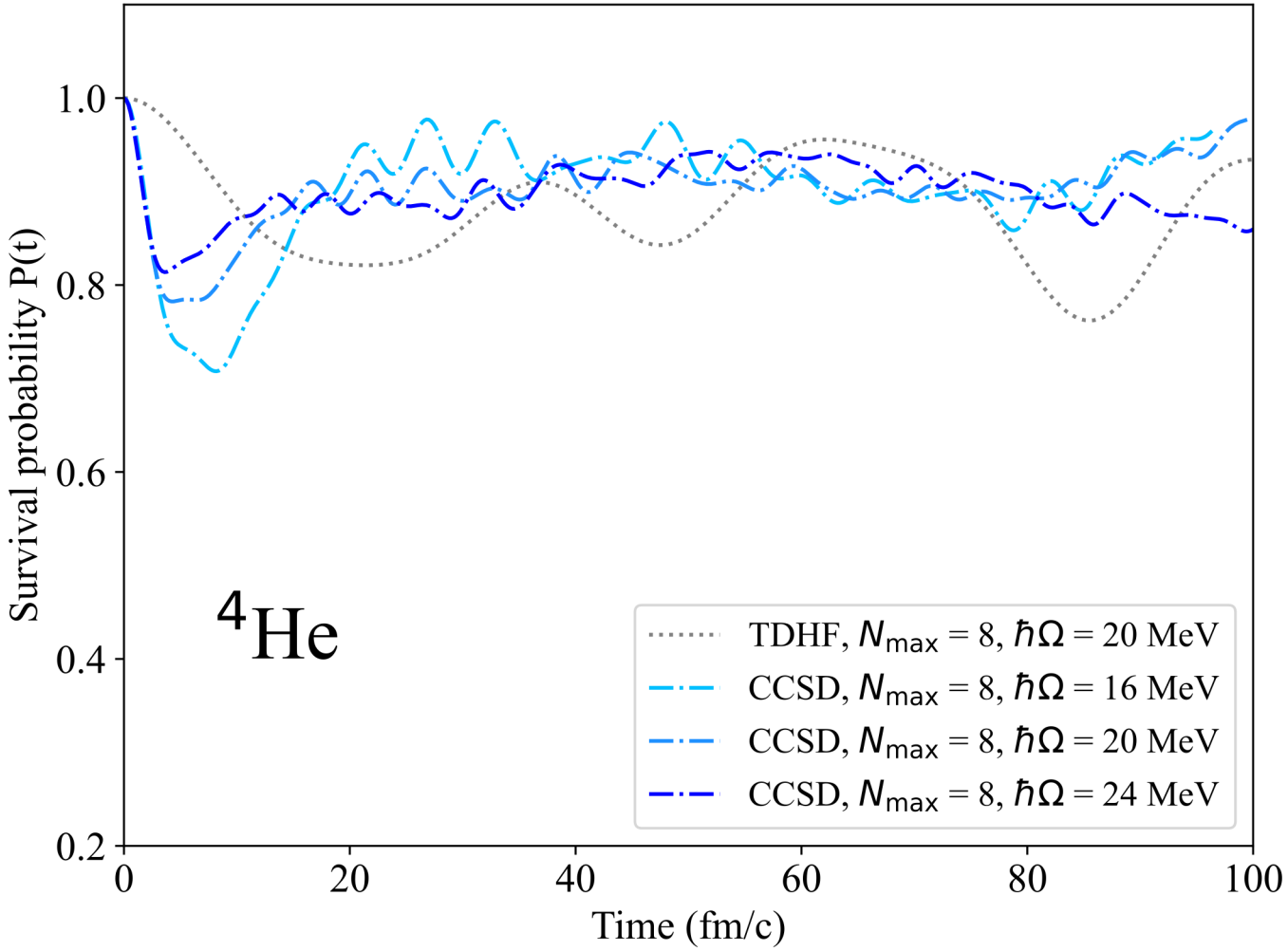
C. Forssén, FB, G. Hagen, T. Papenbrock, in preparation.

From the mean field …



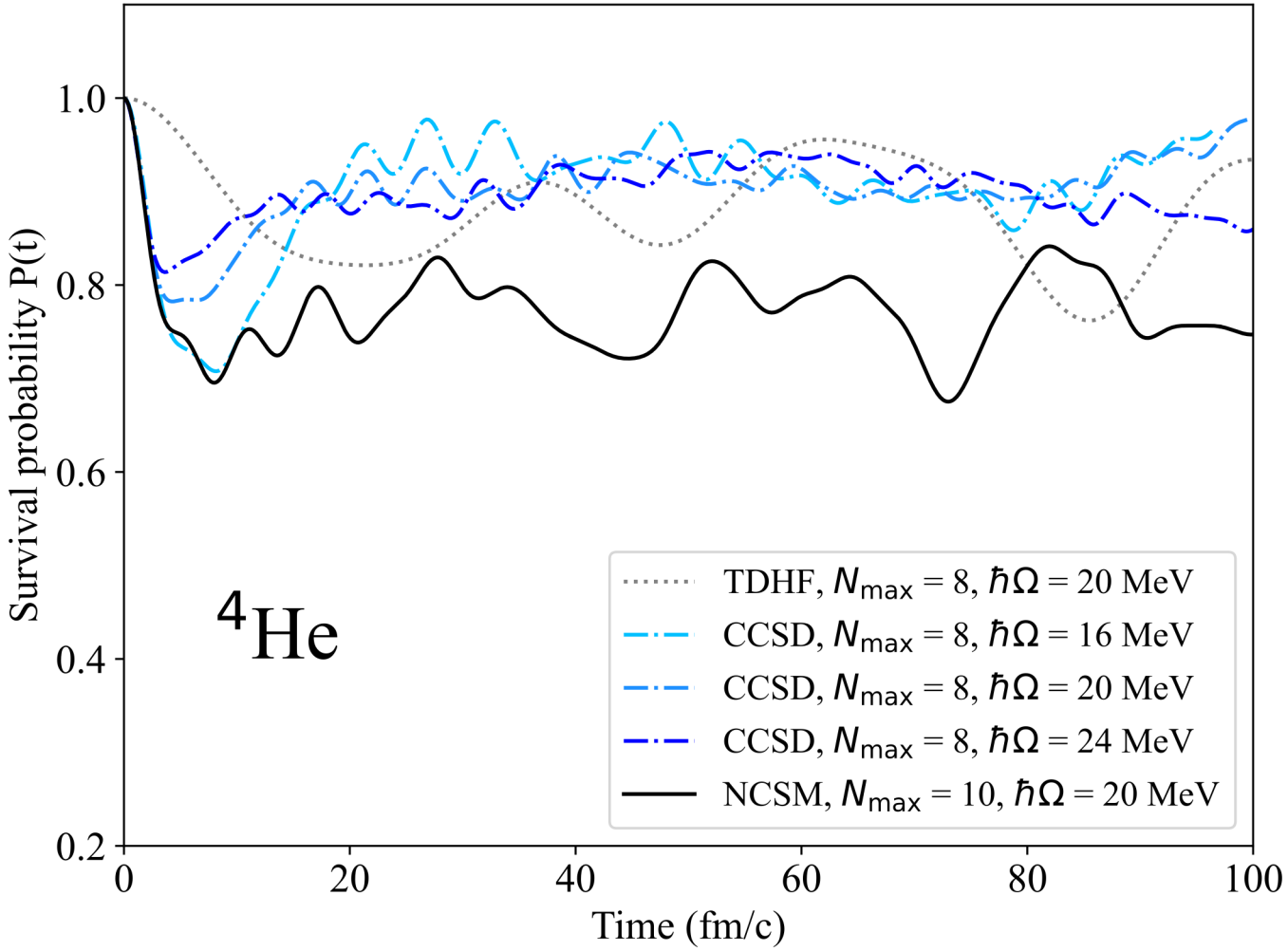
C. Forssén, **FB**, G. Hagen, T. Papenbrock, in preparation.

From the mean field to TDCC …



C. Forssén, FB, G. Hagen, T. Papenbrock, in preparation.

From the mean field to TDCC and TD-NCSM

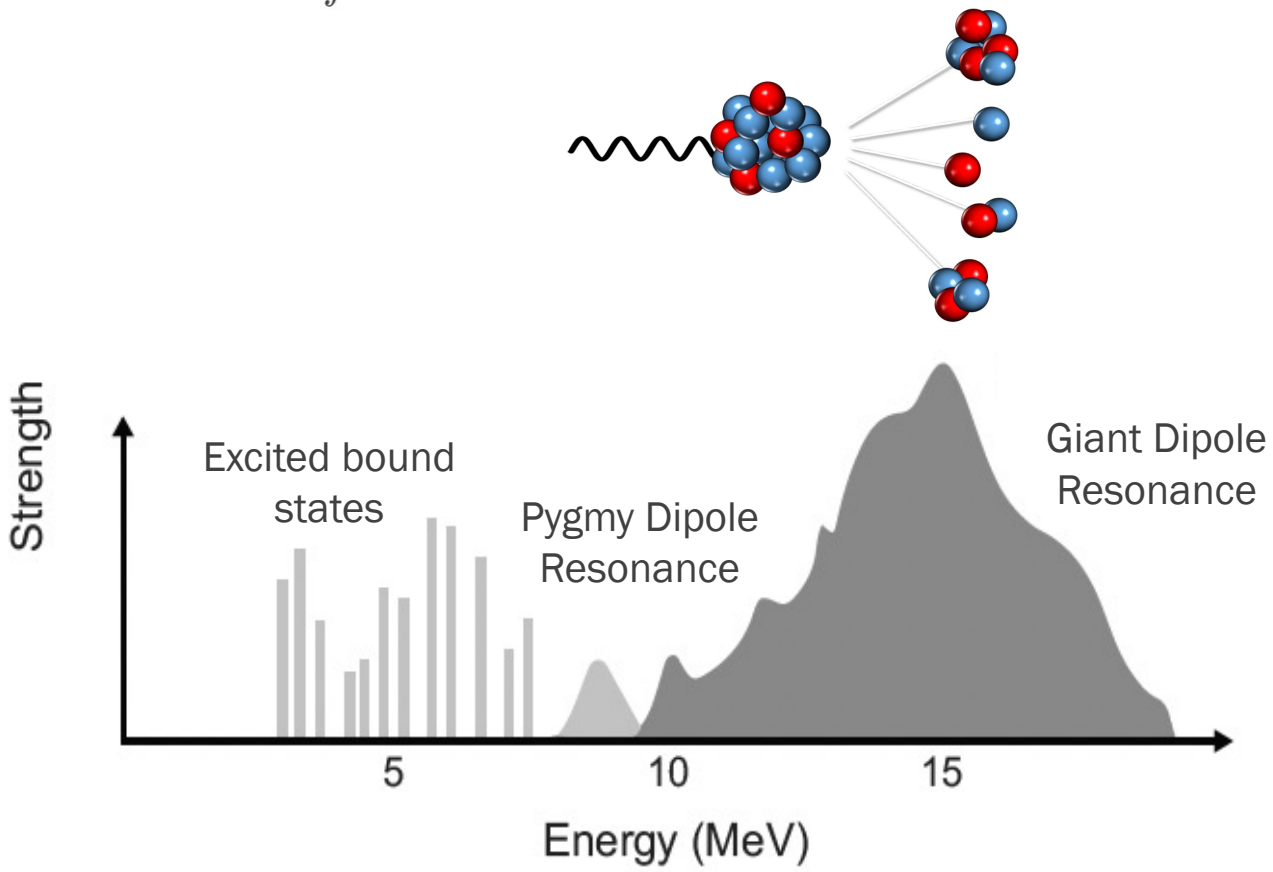


C. Forssén, **FB**, G. Hagen, T. Papenbrock, in preparation.

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

Nuclear response functions

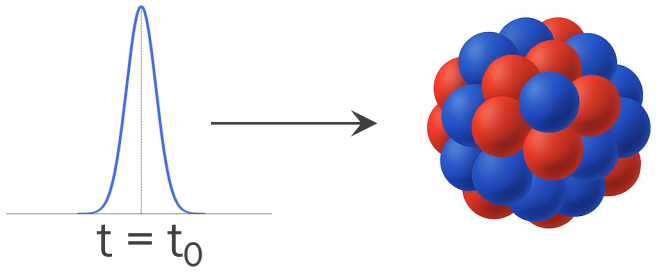
$$R(\omega) = \sum\!\!\!\!\!\!\int_f |\langle \Psi_f | \Theta | \Psi_0 \rangle|^2 \delta(E_f - E_0 - \omega)$$



Responses in a time-dependent approach

Goal: solving

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



with

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

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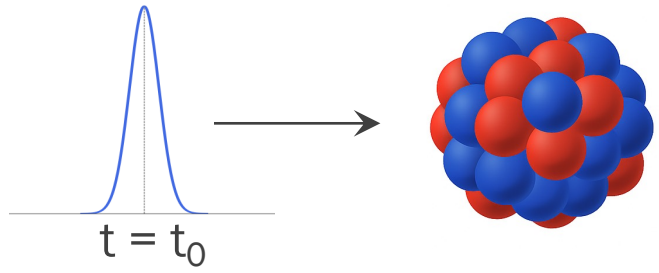

with

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

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

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

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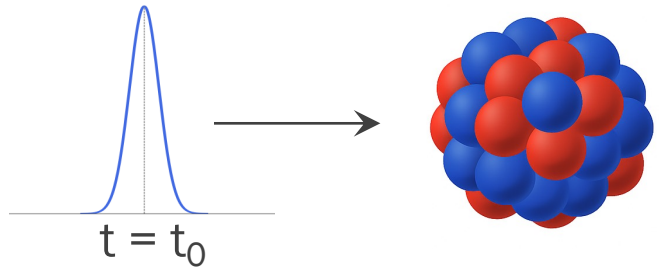

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Fourier transform

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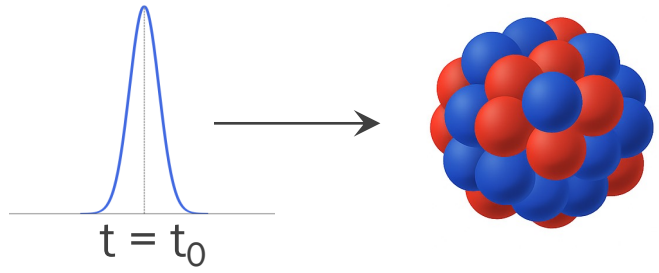

with

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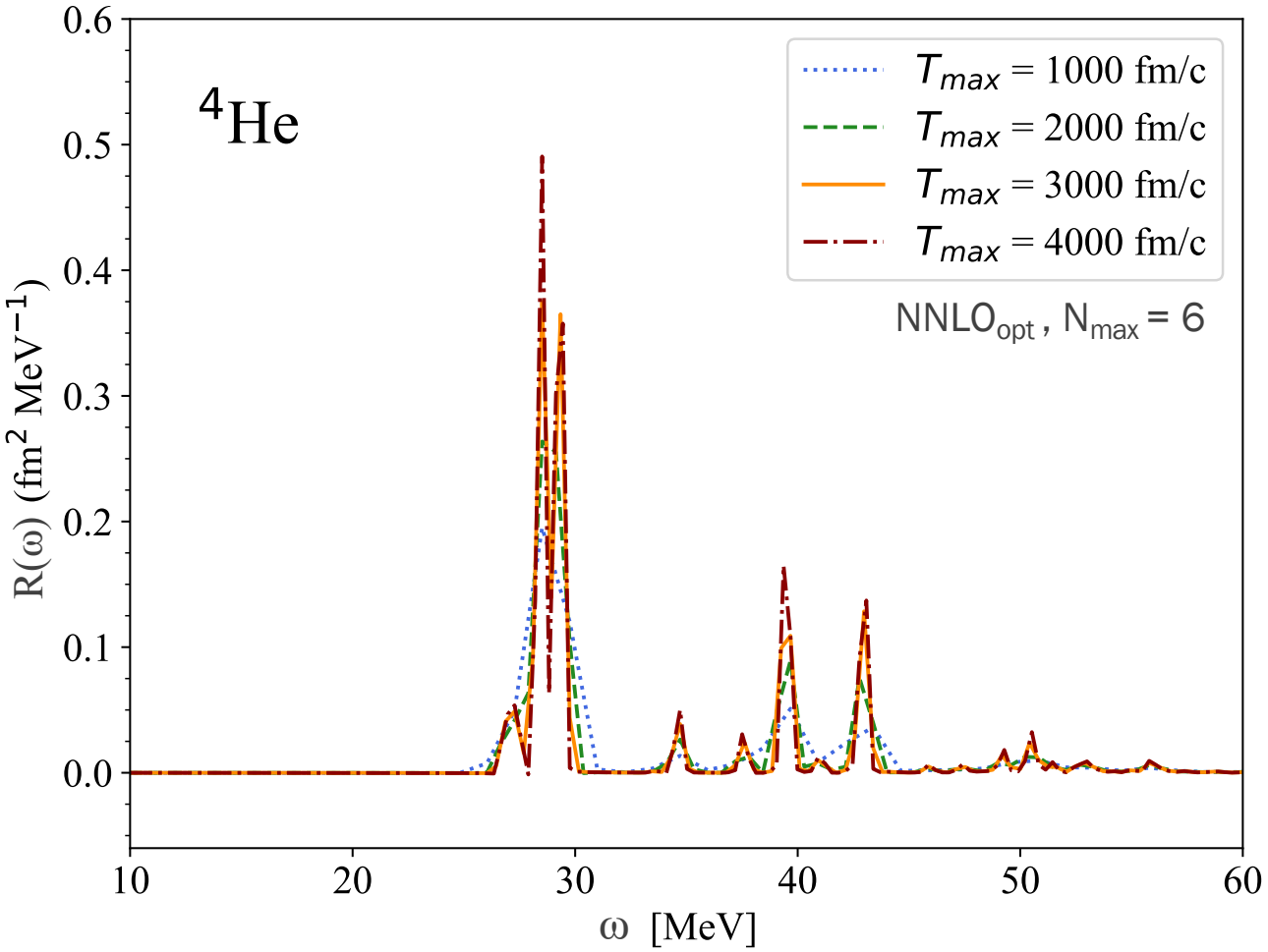
For small ε, first-order time-dependent perturbation theory yields:

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

Fourier transform

Simulation time and resolution



Resolution

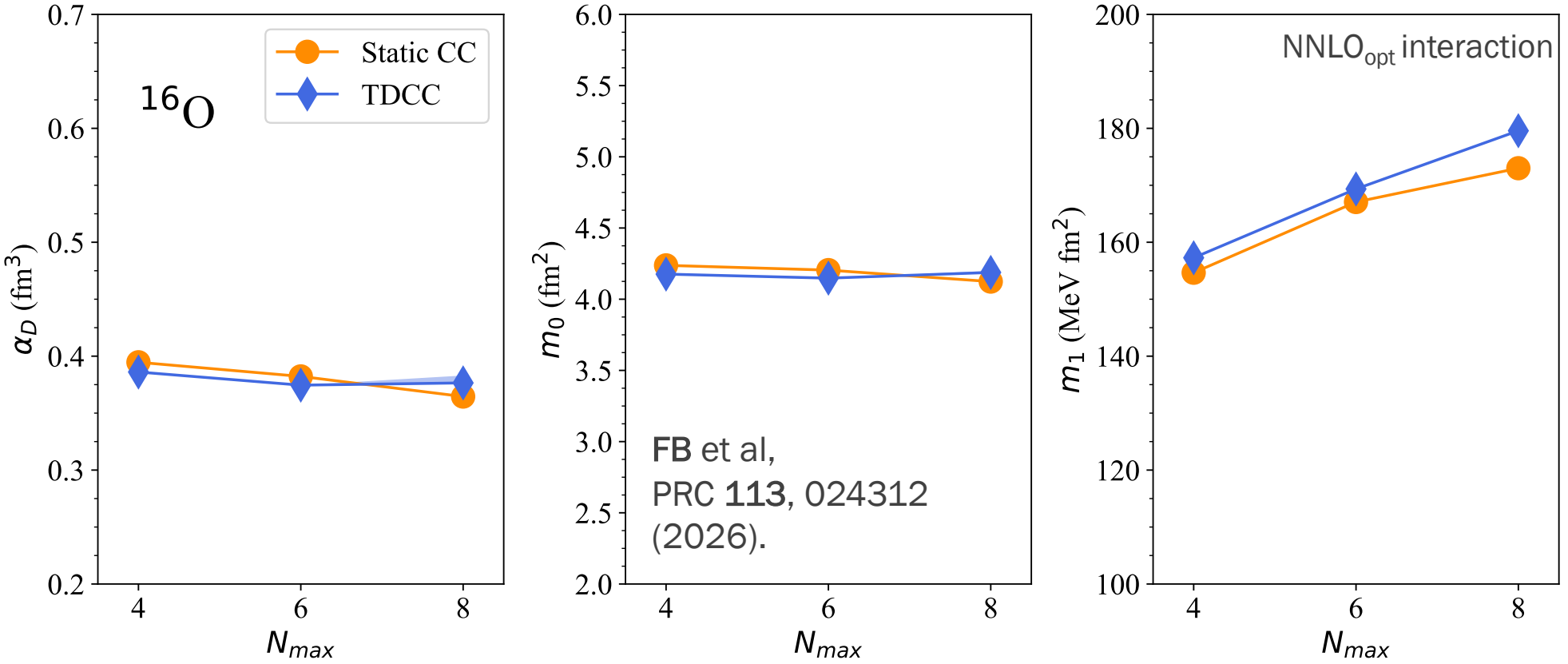
$$\Delta\omega = \frac{2\pi\hbar c}{t_{max}}$$

Maximum simulation time

FB, C. Balos, K. Godbey, G. Hagen, T. Papenbrock, C. Woodward, PRC **113**, 024312 (2026).

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

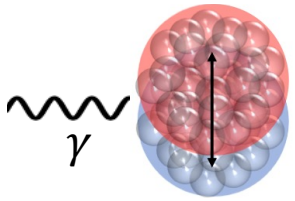
$$\alpha_D = 2\alpha \int d\omega\, \omega^{-1} R(\omega) \qquad m_0 = \int d\omega R(\omega) \qquad m_1 = \int d\omega\, \omega R(\omega)$$

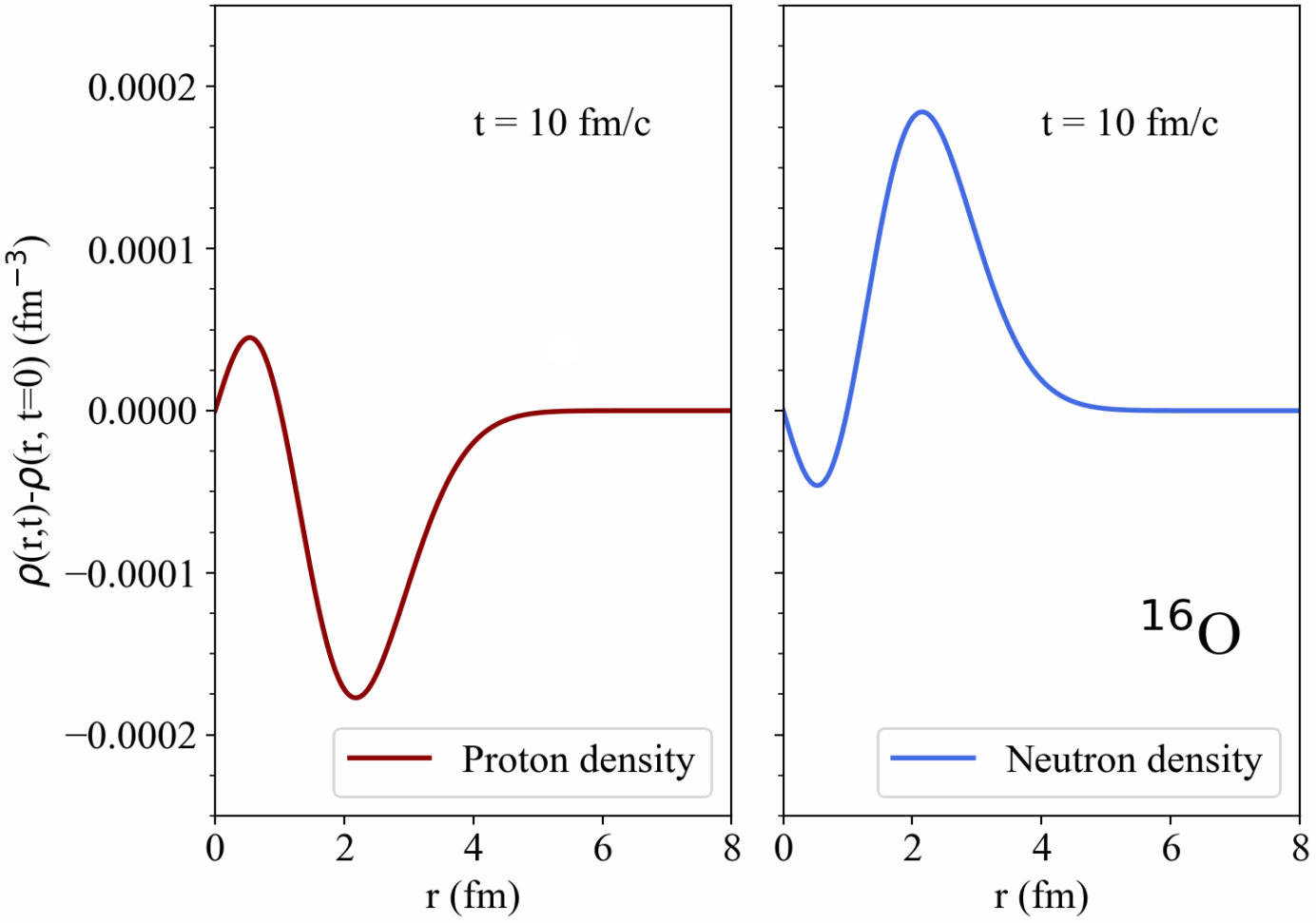


Very small deviations between the two completely independent approaches!

Collective oscillations in real time

^{16}O





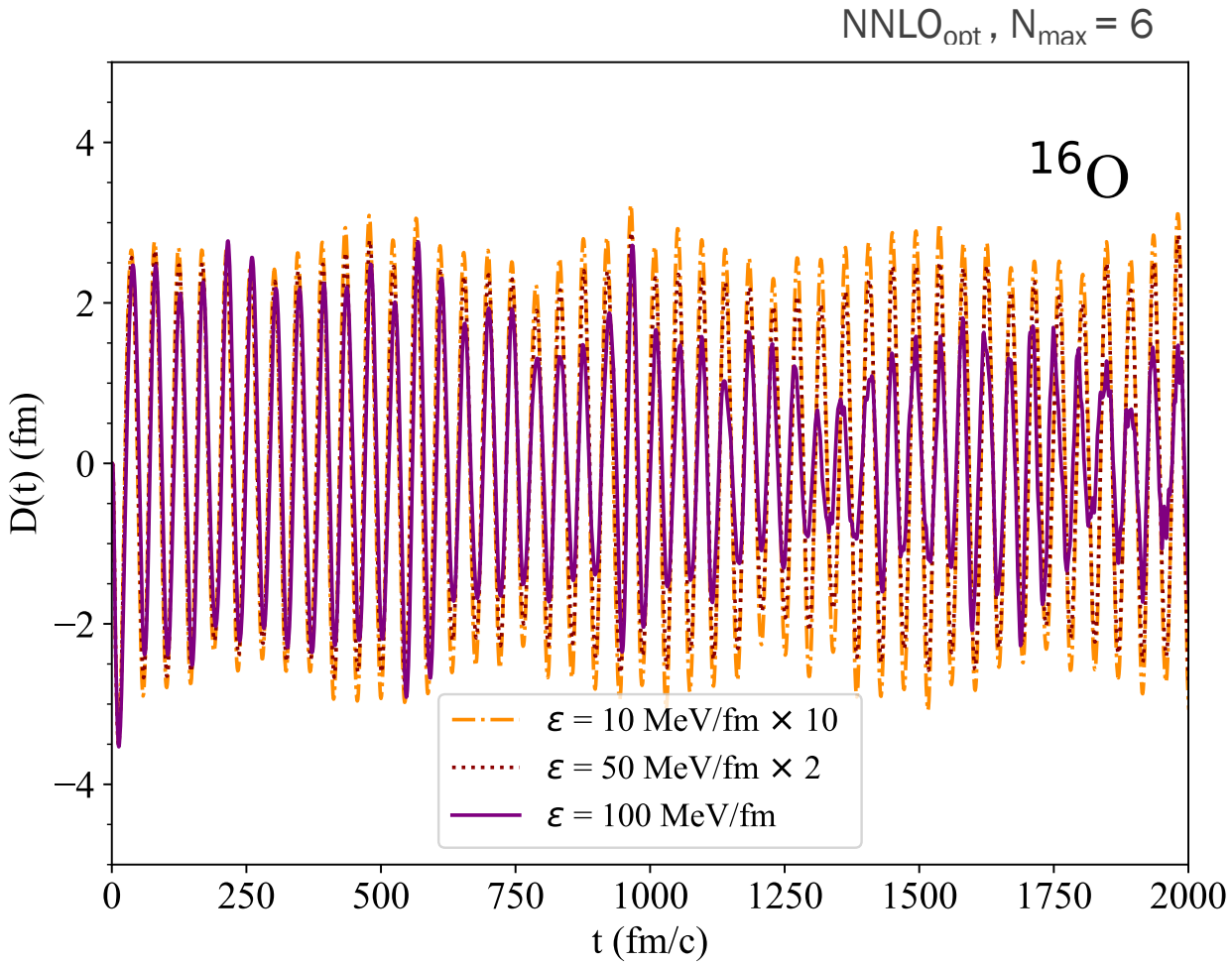
$NNLO_{opt}$,
$N_{max} = 6$

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

What happens when we increase ε?

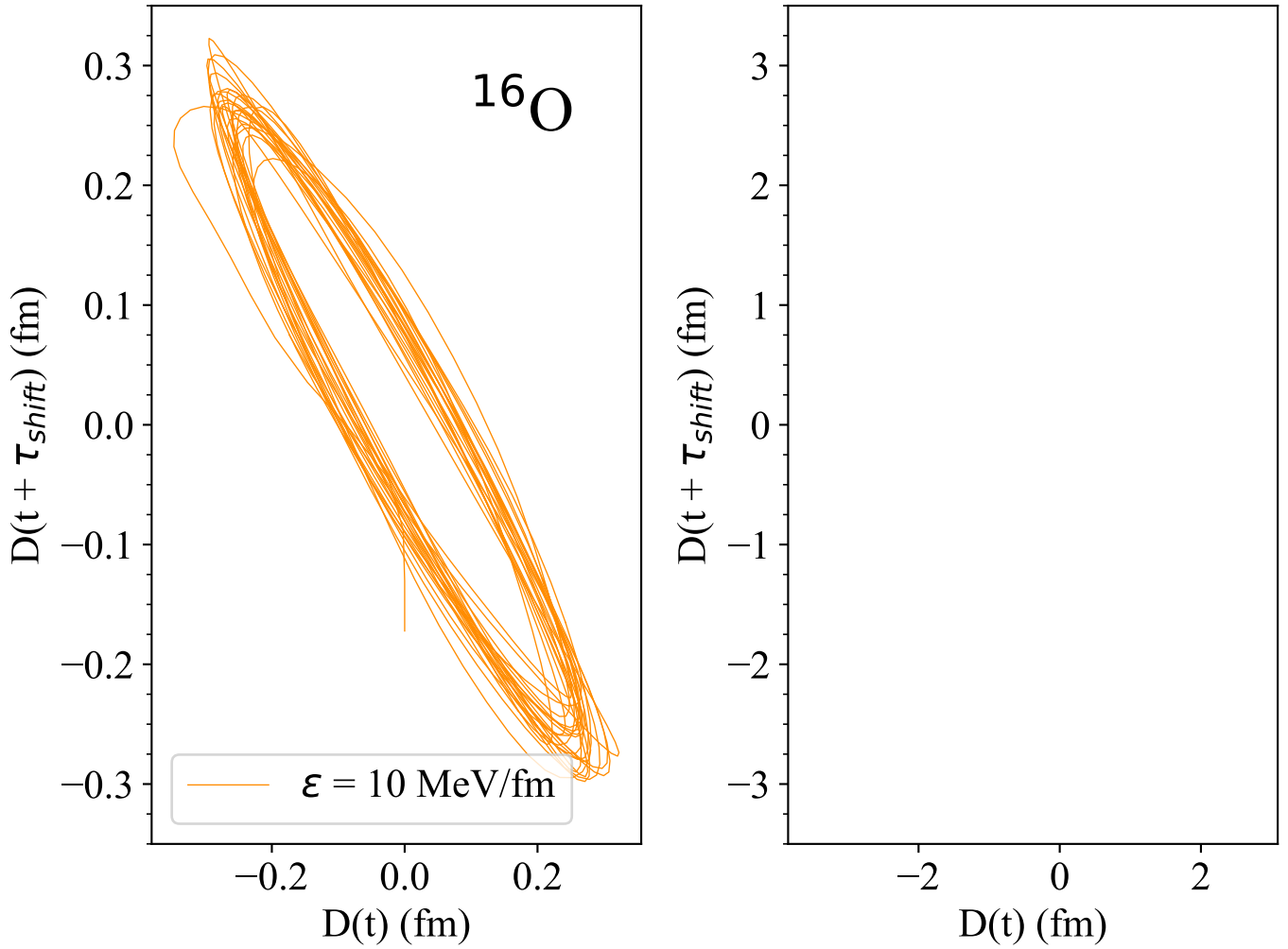
$$\hat{H}(t) = \hat{H}_0 + \epsilon f(t)\hat{D}$$

- 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.



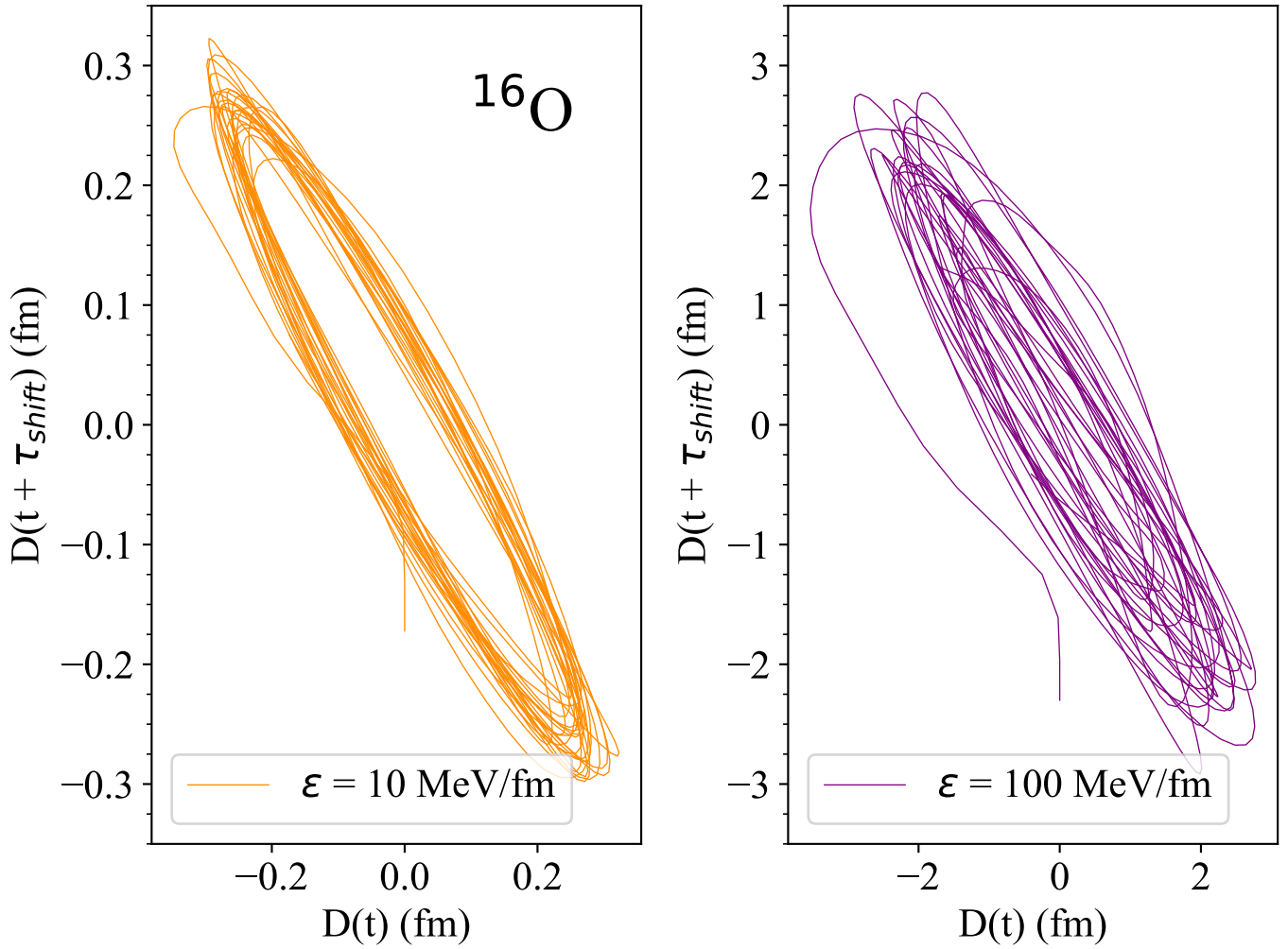
FB et al, PRC **113**, 024312 (2026).

From order…



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

From order to chaos



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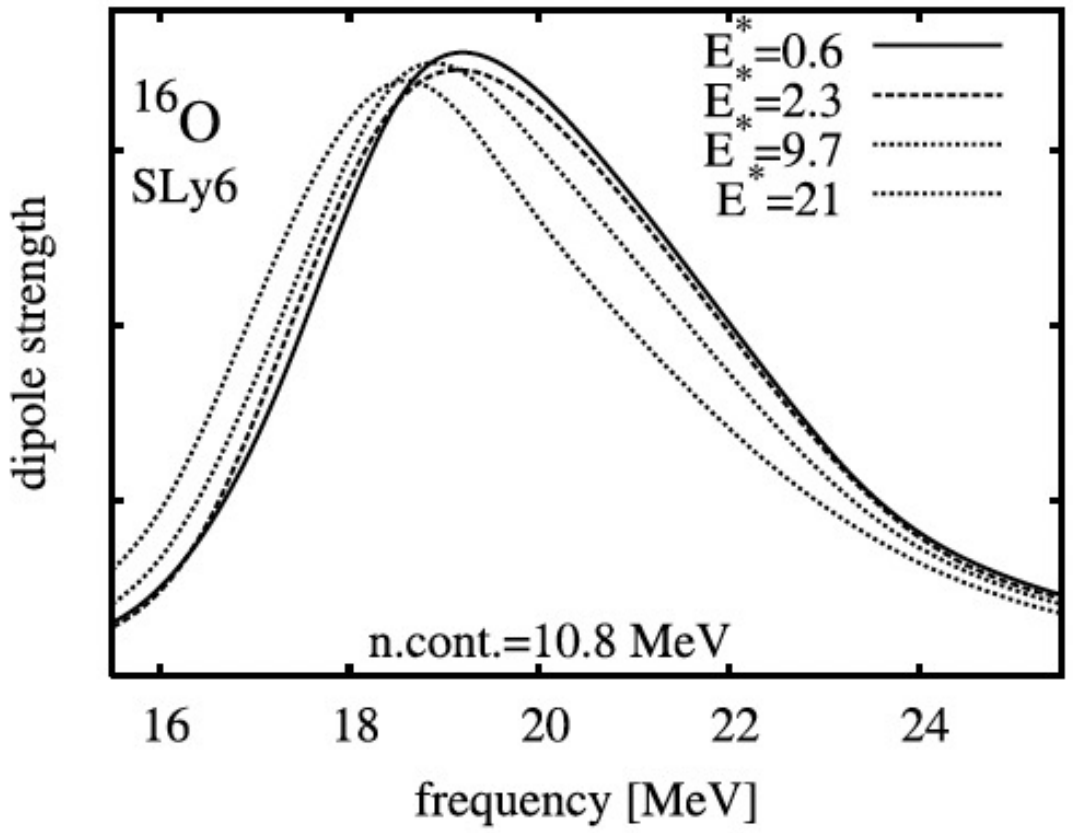

P.-G. Reinhard et al, Eur. Phys. J. A 32, 19–23 (2007).

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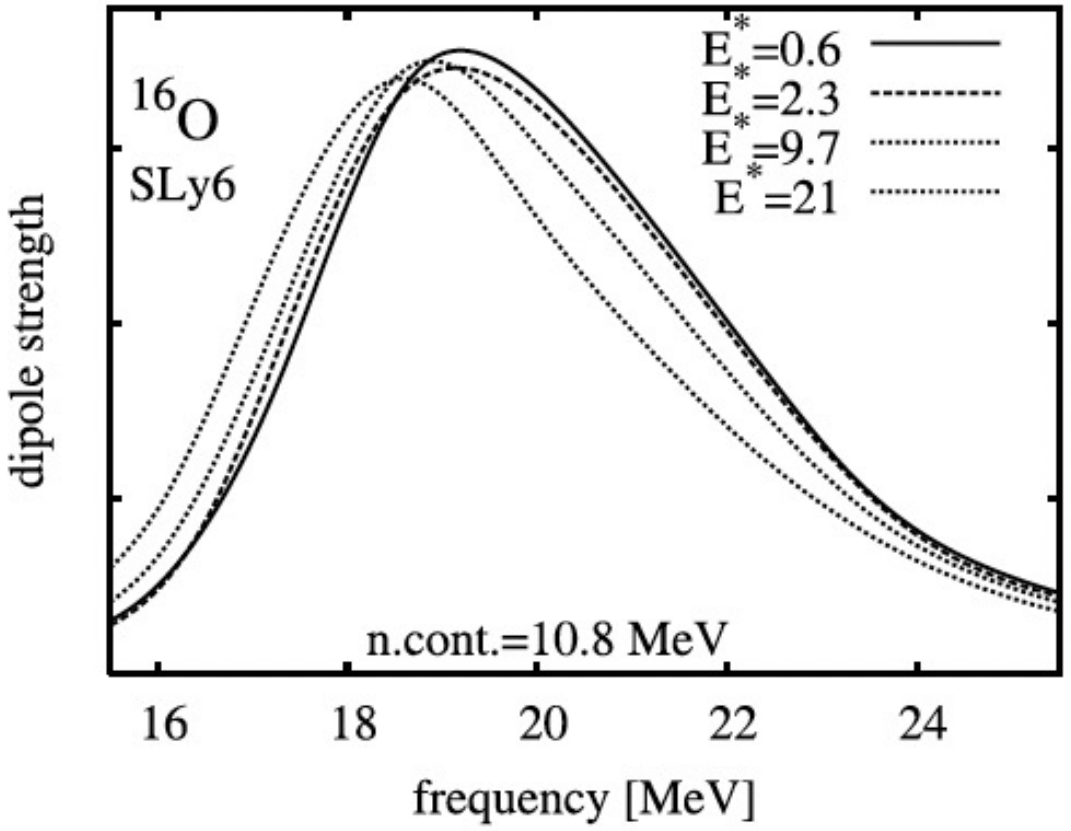

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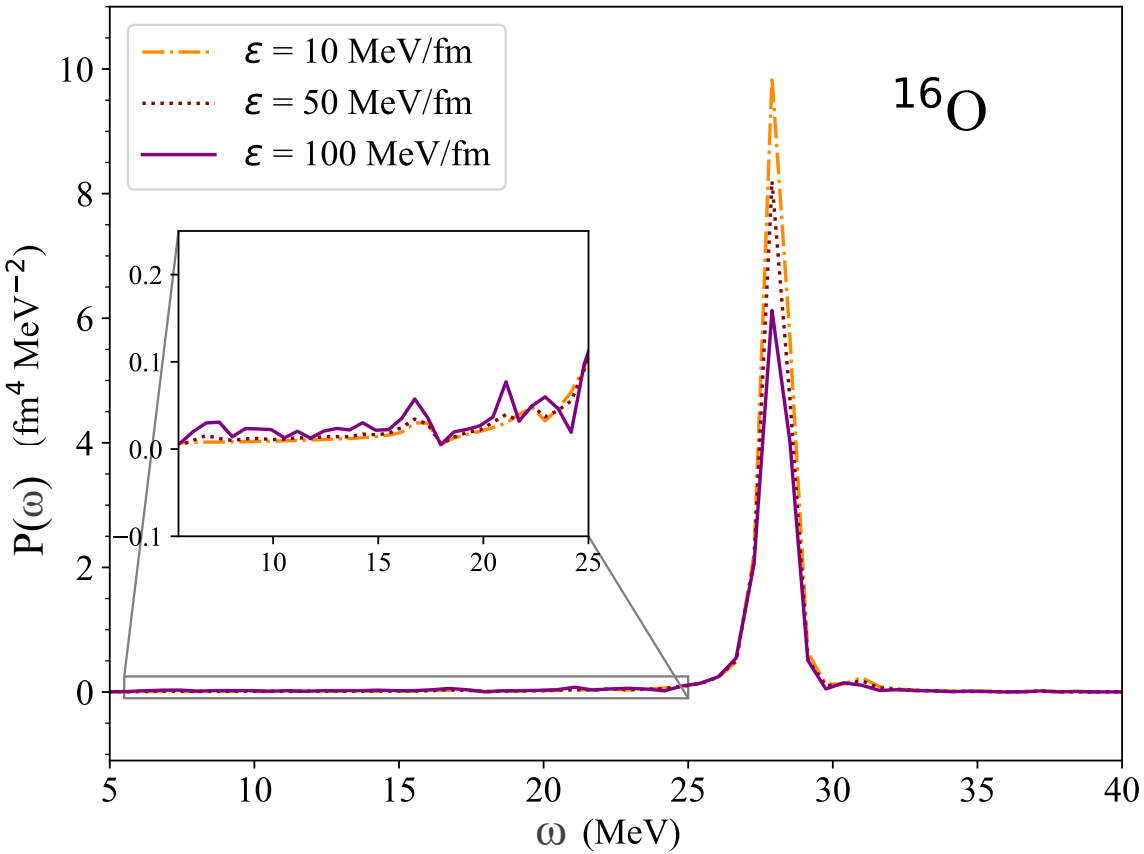
NNLO$_{opt}$, N$_{max}$ = 6



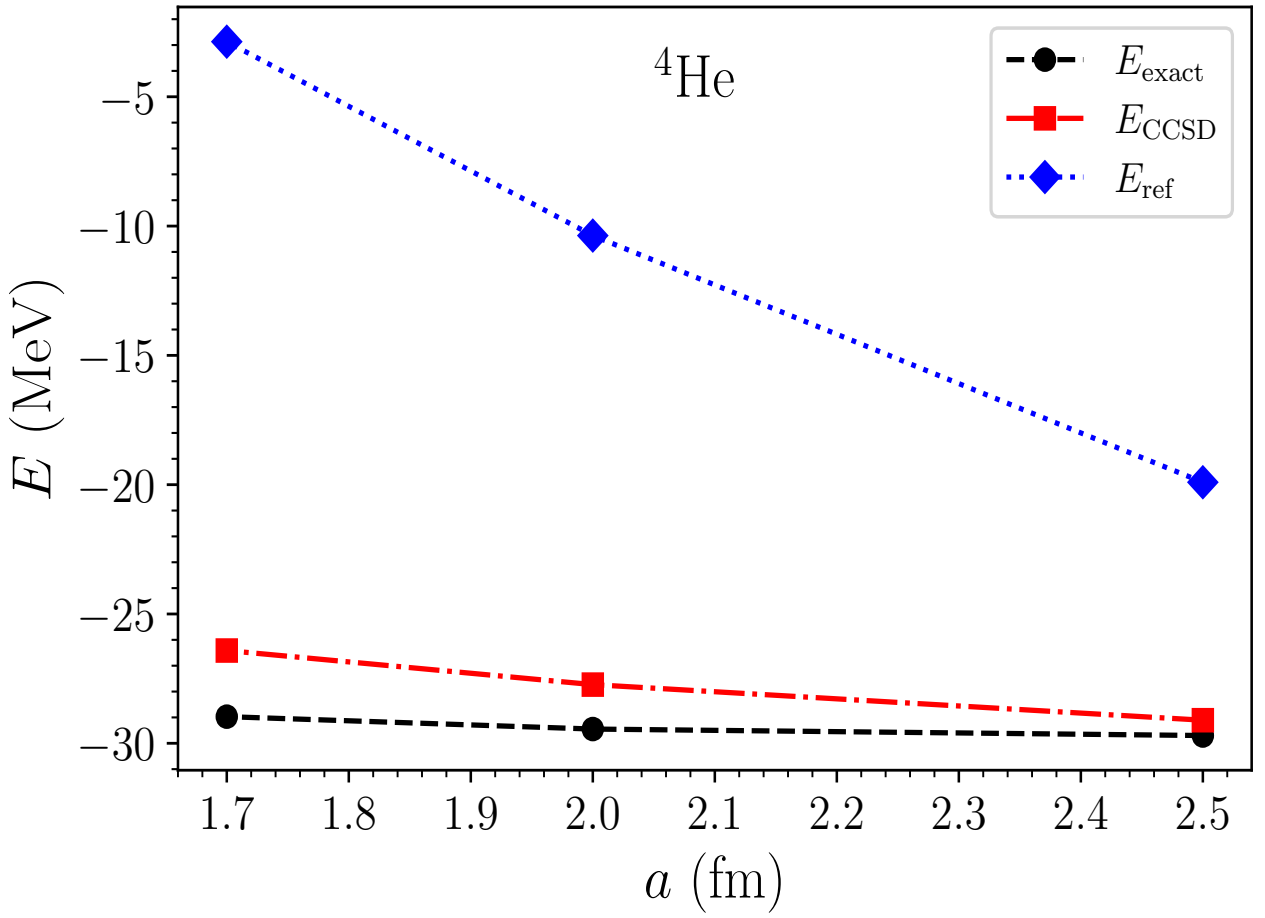
FB et al, PRC **113**, 024312 (2026).

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

A natural framework for reactions: the lattice

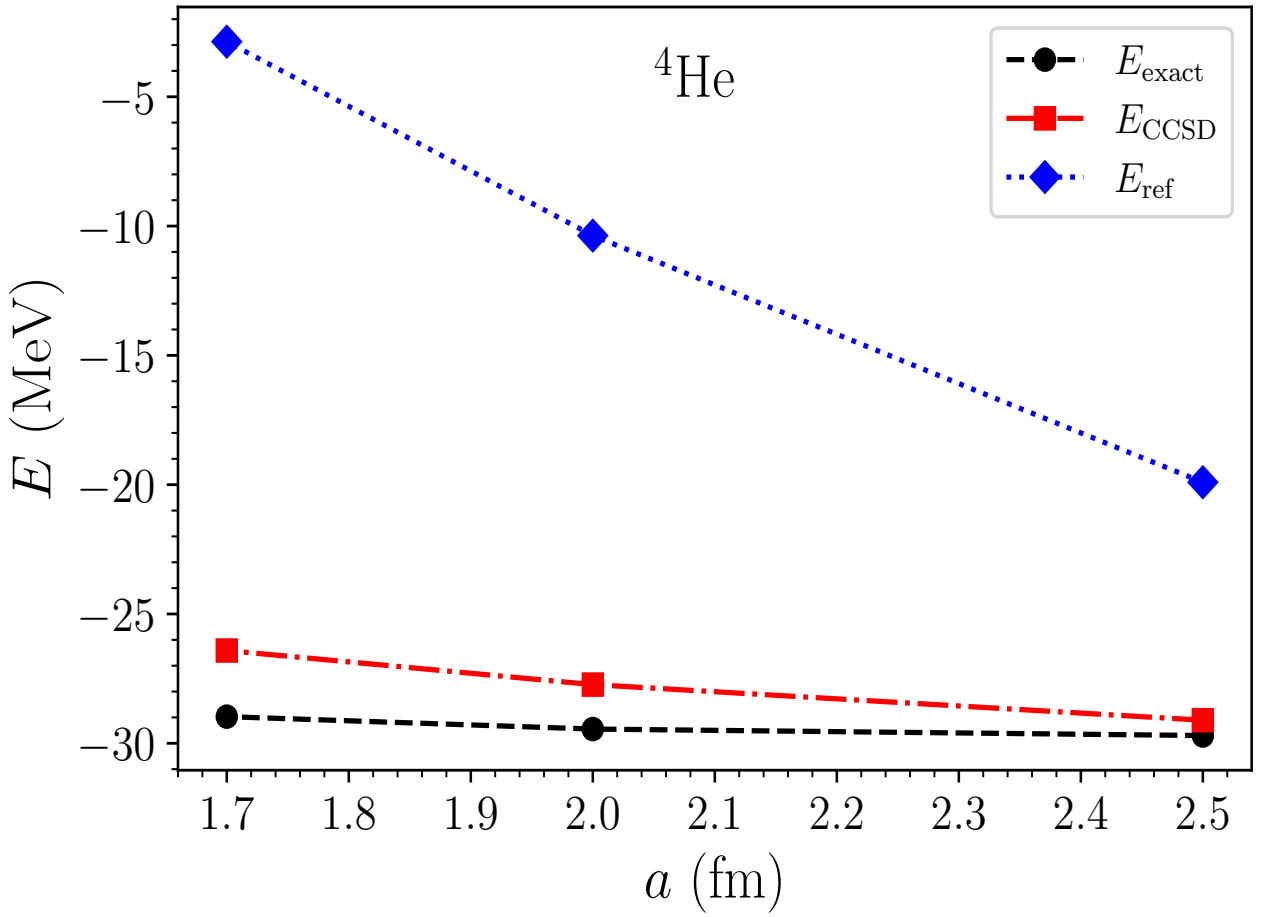
- We can exploit the short-range nature of the nuclear force! Correlations are only between neighbours.
- Computational cost scales with volume → problem becomes sparse and in some cases we can do calculations on a laptop!
- How far can we go with coupled-cluster on the lattice?

Benchmark on ground-state energies



M. Rothman, B. Johnson-Toth, **FB** et al, PRC **112**, L051301 (2025).

Benchmark on ground-state energies



NuLattice: Python package for **ab initio computations on lattices**

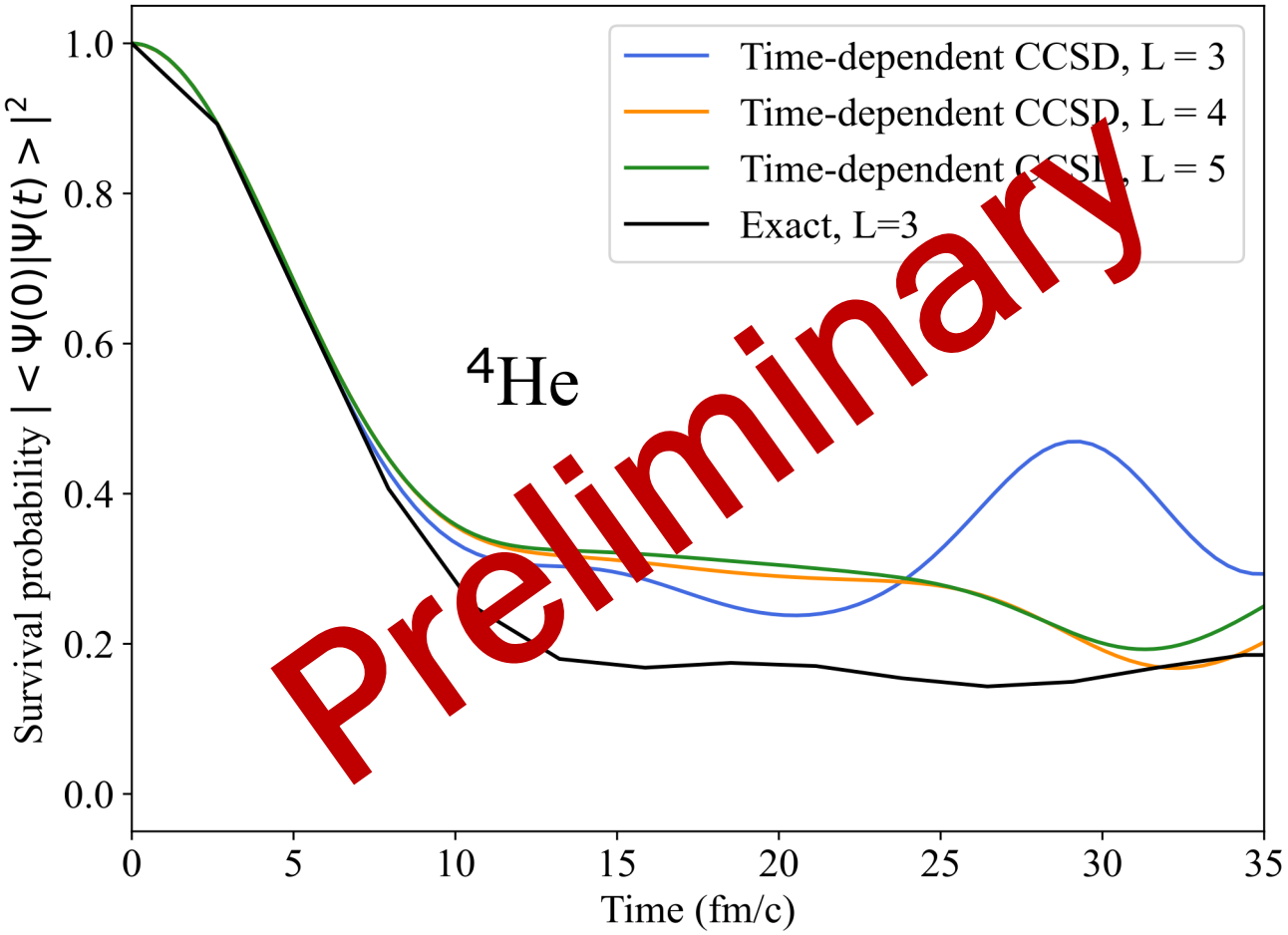
Try it out!

M. Rothman, B. Johnson-Toth et al, EPJA 62, 28 (2026).

M. Rothman, B. Johnson-Toth, **FB** et al, PRC **112**, L051301 (2025).

First dynamical simulations on the lattice: survival probabilities

based on NuLattice



Conclusions

We are putting the foundations for **simulating nuclear reactions** as **fusion** and **fission** in **medium-mass** and **heavy nuclei** from **first principles**.

To connect with the quantum chemistry community:

- ❑ Have **many-body truncation effects** in dynamics been explored?
- ❑ Test of TDCC approaches in **strong fields**?

Stay tuned!

Thanks to my collaborators:

@ORNL/UTK: Gaute Hagen, Matthias Heinz, Ben Johnson-Toth, Thomas Papenbrock, Maxwell Rothman
@FRIB/MSU: Kyle Godbey (now at NVIDIA)
@Chalmers: Christian Forssèn
@LLNL: Cody Balos, Carol Woodward

and to you for your attention!

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FRIB Theory Alliance

NUCLEI Nuclear Computational Low-Energy Initiative