New perspectives on the Equation of Motion method for nuclear response functions

Mainz Institute for Theoretical Physics

Many-Body Theory: Nuclear Physics meets Quantum Chemistry

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Based on

Revisiting the Equation-of-Motion Method: A Universal Framework for Correlated Quantum Systems

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A general implementation of the equation-of-motion (EOM) formalism for correlated many-body states is presented and applied to the description of collective excitations in atomic nuclei. While EOM approaches are traditionally formulated on top of independent-particle reference states, the present work extends the method to correlated reference states generated by modern many-body solvers. This formulation enables a consistent treatment of ground-state correlations and excited-state dynamics within a unified framework. Particular emphasis is placed on collective nuclear excitations employing chiral nuclear Hamiltonians in an ab initio context. The approach is motivated by the renewed interest in EOM techniques across several fields, including quantum chemistry and quantum computing, where they provide efficient and systematically improvable descriptions of excitation spectra. The present results demonstrate that the EOM framework offers a flexible and powerful tool for the microscopic description of nuclear spectroscopy beyond the traditional mean-field paradigm.

[arXiv:2607.29396]

Previous developments

PHYSICAL REVIEW C **112**, 054303 (2025)

Editors' Suggestion

Impact of ground-state correlations on the multipole response of nuclei: *Ab initio* calculations of moment operators

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We develop a framework that allows us to calculate integrated properties of the nuclear response from first principles. Using the *ab initio* in-medium similarity renormalization group (IMSRG), we calculate the expectation values of moment operators that are linked to the multipole response of nuclei. This approach is applied to the isoscalar mono- and quadrupole as well as the isovector dipole response of closed-shell nuclei from ^{4}He to ^{78}Ni for different chiral two- and three-nucleon interactions. We find that the inclusion of many-body correlations in the nuclear ground state significantly impacts the multipole response when going from the random-phase approximation to the IMSRG level. Our IMSRG calculations lead to an improved description of experimental data in ^{16}O and ^{40}Ca, including a good reproduction of the Thomas-Reiche-Kuhn enhancement factor. These findings highlight the utility of the moment method as a benchmark for other *ab initio* approaches that describe nuclear response functions through the explicit treatment of excited states.

DOI: 10.1103/1ktc-lknn

Outline

Introduction

- Physics case
- Quantities of interest

The EOM as a dynamical method

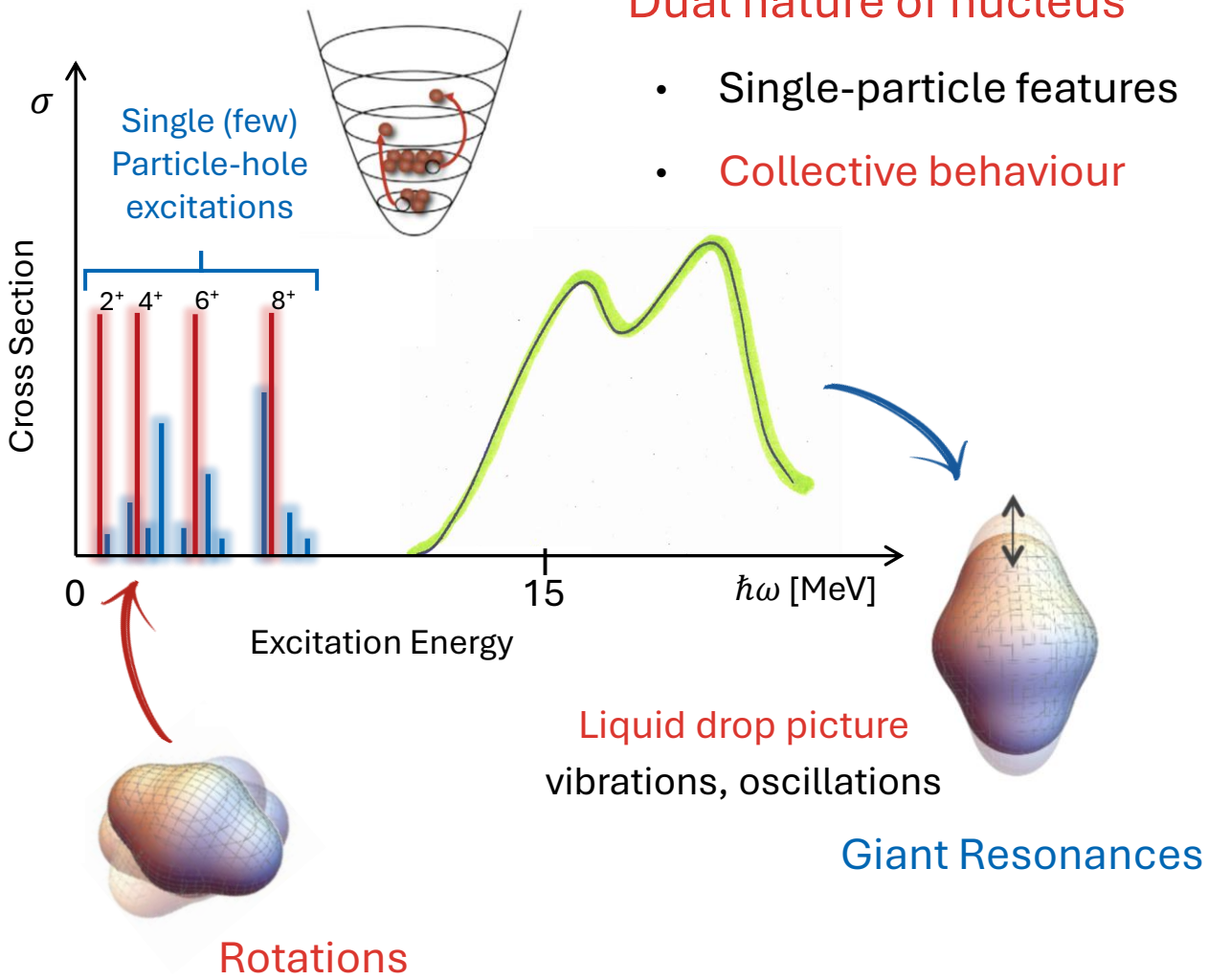
- Theoretical foundations
- Novelty of the present development
- Comparison to existing frameworks

Numerical results

- Benchmark and convergence
- Dipole response in oxygen isotopes

Challenges and opportunities

Nuclear spectroscopy



Dual nature of nucleus

- Single-particle features
- Collective behaviour

Response function

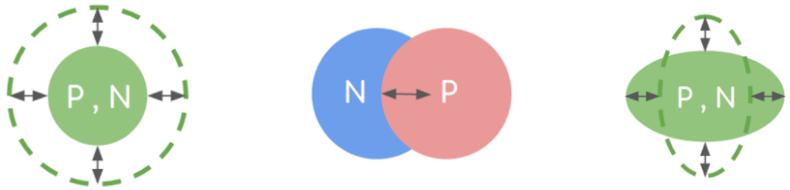
Fully characterise linear response

$$S(Q_\lambda, E) \equiv \sum_{\mu\nu} |\langle \Psi_\nu | Q_{\lambda\mu} | \Psi_0 \rangle|^2 \, \delta(E_\nu - E_0 - E)$$

Transition probability

Excitation energy

Studied quantity: multipole response



[Pictures from Dytrych et al., PRL, 2020]

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Excited states: Where to start from?

Time-Independent Schrödinger Equation

$$H\left|\Psi_\nu\right\rangle = E_\nu\left|\Psi_\nu\right\rangle$$

Variational principle on E

$$\delta E[\tilde{\Psi}] = \delta\frac{\langle\tilde{\Psi}|H|\tilde{\Psi}\rangle}{\langle\tilde{\Psi}|\tilde{\Psi}\rangle} = 0$$

Valid for exact eigenstates

CI-like methods
CI, SM, NCSM, EOM-CC, EOM-IMSRG, etc.

Time-Dependent Schrödinger Equation

$$i\partial_t\left|\Psi(t)\right\rangle = H\left|\Psi(t)\right\rangle$$

Variational principle on action integral

$$\delta\int_{t_0}^{t_1}\left\langle\Psi(t)\right|i\partial_t - H\left|\Psi(t)\right\rangle dt = 0$$

Valid for any state $\left|\Psi\right\rangle$

TD methods,
EOM, RPA and RPA-inspired methods

Contact point: stationary states (eigenstates)

$$\left|\Psi(t)\right\rangle = e^{-iEt}\left|\Psi(0)\right\rangle$$

From TD to EOM (1)

Time-dependent perturbation $H(t) = H_0 + V(t)$

Variational principle on action integral

$$S[\Psi] \equiv \int_{t_0}^{t_1} \langle \Psi(t) \left| i\hbar\partial_t - H(t) \right| \Psi(t) \rangle \, dt \qquad \delta S = 0$$

Treat the problem perturbatively

$$|\Psi(t)\rangle = |\Psi_0(t)\rangle + |\delta\Psi(t)\rangle$$

$$|\delta\Psi(t_0)\rangle = 0$$

Assumed stationary

Stationary perturbation theory

Linear differential equation

$$\boxed{\left(H_0 - i\hbar\partial_t\right) |\delta\Psi(t)\rangle = -V(t) \, |\Psi_0(t)\rangle}$$

Homogeneous Equation

Source term

From TD to EOM (2)

$$\left(H_0 - i\hbar\partial_t\right)|\delta\Psi(t)\rangle = -V(t)\,|\Psi_0(t)\rangle$$

How to solve the homogeneous part ? Ansatz ?

Perturbative expansion (Dyson)

$$|\delta\Psi(t)\rangle = -\frac{i}{\hbar}e^{-iH_0(t-t_0)/\hbar}\int_{t_0}^{t} dt' V_I(t')\,|\Psi_0\rangle + \dots$$

The DOF are chosen by the perturbation itself !

$$V(t) \to V(t) + \delta V(t) \qquad V(t) = \sum_a f_a(t) X_a$$

[Rowe, Nucl. Phys. A107 (1968) 99-105]

[Rowe, Rev. Mod. Phys. 40, 1 (1968)]

If the perturbation timescale is fast

$$\sum_b \langle\Psi_0|[X_a, H_0, X_b]|\Psi_0\rangle\, f_b(t) = i\hbar \sum_b \langle\Psi_0|[X_a, X_b]|\Psi_0\rangle\, \frac{df_b(t)}{dt}$$

EOM-equations by Rowe

+ periodic $\sum_b \langle\Psi_0|[X_a, H_0, X_b]|\Psi_0\rangle\, c_b = i\hbar\omega \sum_b \langle\Psi_0|[X_a, X_b]|\Psi_0\rangle\, c_b$

This work

Expand on a many-body basis

$$\begin{pmatrix} A & B \\ B^* & A^* \end{pmatrix} \begin{pmatrix} \mathcal{X}_\nu \\ \mathcal{Y}_\nu \end{pmatrix} = \hbar\omega_\nu \begin{pmatrix} U & V \\ -V^* & -U^* \end{pmatrix} \begin{pmatrix} \mathcal{X}_\nu \\ \mathcal{Y}_\nu \end{pmatrix}$$

$$A_{ab} \equiv \langle\Psi|[\eta_a, H, \eta_b^\dagger]|\Psi\rangle \qquad U_{ab} \equiv \langle\Psi|[\eta_a, \eta_b^\dagger]|\Psi\rangle$$
$$-B_{ab} \equiv \langle\Psi|[\eta_a, H, \eta_b]|\Psi\rangle \qquad -V_{ab} \equiv \langle\Psi|[\eta_a, \eta_b]|\Psi\rangle$$

Develop commutators as operators
J-coupled scheme

[Lu and Johnson, PRC 97 (2018) 3, 034330]

Expectation value over correlated states

Universal strategy for modern many-body solvers

Correlation in the GS propagates to exc. States
(no consistency problems)

Generalised Eigenvalue Problem

$$\mathrm{H}\,\mathrm{X} = \mathrm{N}\,\mathrm{X}\,\Omega$$

Hessian at $|\Psi\rangle$ — Norm matrix

Full basis give the exact normal modes

Theoretical comparison

	Hamiltonian	Ground state $\lvert\Psi_0\rangle$	Excited states $\lvert\Psi_n\rangle$
This work	H	$\lvert\Phi(s)\rangle = U^\dagger(s)\lvert\Phi\rangle$	$\sum_{ab} X^{ab} c_a^\dagger c_b \lvert\Phi(s)\rangle$
EOM-IMSRG	$H(s) = U(s)HU^\dagger(s)$	$\lvert\Phi\rangle$	$\sum_{php'h'} X^{php'h'} c_{p'}^\dagger c_{h'} c_p^\dagger c_h \lvert\Phi\rangle$
EOM-CC	$\bar{H} = e^{-T} H e^T$	$\lvert\Phi\rangle$	$\sum_{php'h'} X^{php'h'} c_{p'}^\dagger c_{h'} c_p^\dagger c_h \lvert\Phi\rangle$

Approximations introduced here:

- IMSRG(2) ground state
- One-body perturbation

Physical motivation
1B transition operators dominant
(e.g. electromagnetic)

N.B.: 1B wrt correlated GS

Easy interpretation of physics input

All methods are exact (and equivalent) in the full space

Different computational (cost) schemes

TI vs TD ? When to truncate ? Still fully dynamical ?

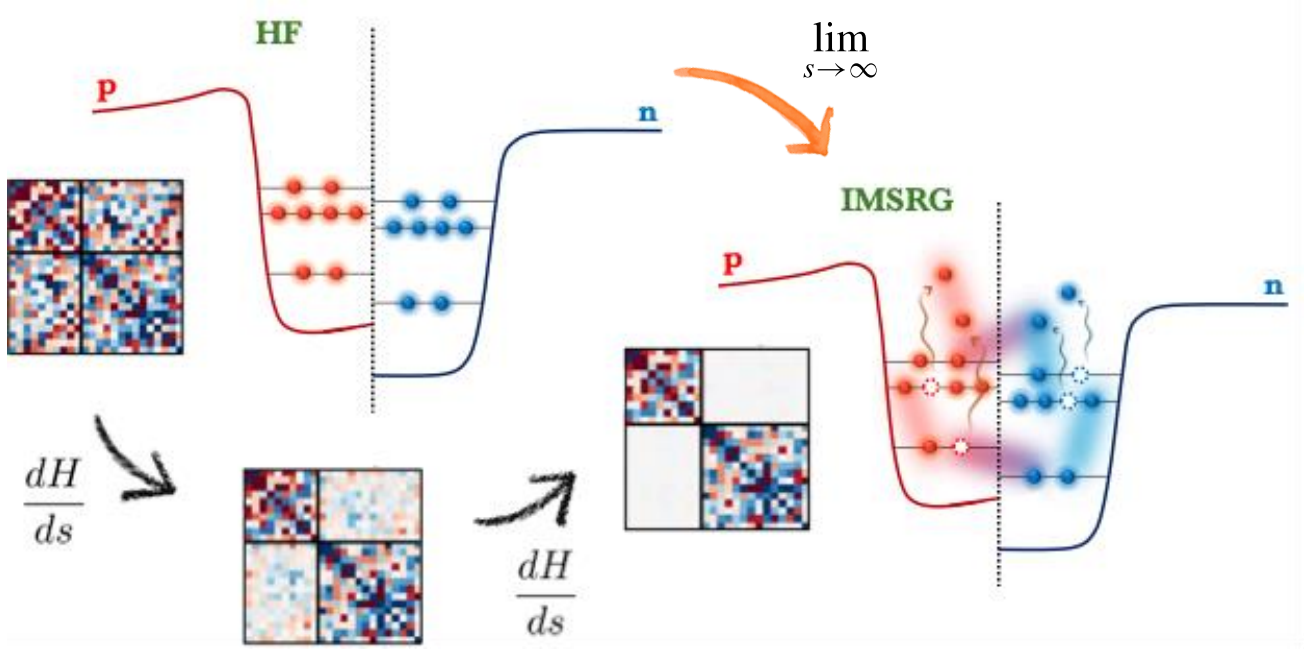
How this formulation differ from existing methods ?

Strategy in the IMSRG framework

Unitary transformation

$$H(s) = U(s)HU^\dagger(s)$$
$$\equiv H^{\rm d}(s) + H^{\rm od} \to H^{\rm d}(\infty)$$

Diagonal Off-diagonal



Effective two-body Hamiltonian

$$H = H^{[1]} + H^{[2]}$$

Steps

- Start from the commutator operator in the HF basis
- Perform an IMSRG(2) calculation
- Evolve commutators using Magnus $U(s) \equiv e^{\Omega(s)}$

[Tsukiyama, Bogner and Schwenk, PRL, 2011]

[Hergert, Bogner, Morris, Schwenk, Tsukiyama, Phys. Rept., 2016]

$$A_{ab} \equiv \langle\Psi|[\eta_a, H, \eta_b^\dagger]|\Psi\rangle$$
$$-B_{ab} \equiv \langle\Psi|[\eta_a, H, \eta_b]|\Psi\rangle$$

J-coupled scheme

[Lu and Johnson, PRC 97 (2018) 3, 034330]

Implemented within imsrg++ code

[github.com/ragnarstroberg/imsrg]

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Benchmark and convergence

Studied quantity

$$Q^{\mathrm{IV}}_{1\mu} = \frac{N}{A}\sum_{i=1}^{Z} r_i Y_{1\mu}(\hat{r}_i) - \frac{Z}{A}\sum_{i=1}^{N} r_i Y_{1\mu}(\hat{r}_i)$$

Response function

$$R(Q^{\mathrm{IV}}_1, \omega) \equiv \sum_{\mu\nu} \frac{|\langle \Psi_\nu | Q^{\mathrm{IV}}_{1\mu} | \Psi_0 \rangle|^2}{\omega - \omega_\nu}$$

Spectral function

$$S(Q^{\mathrm{IV}}_1, \omega) = -\frac{1}{\pi}\mathrm{Im}\, R(Q^{\mathrm{IV}}_1, \omega)$$

Γ = 1 MeV

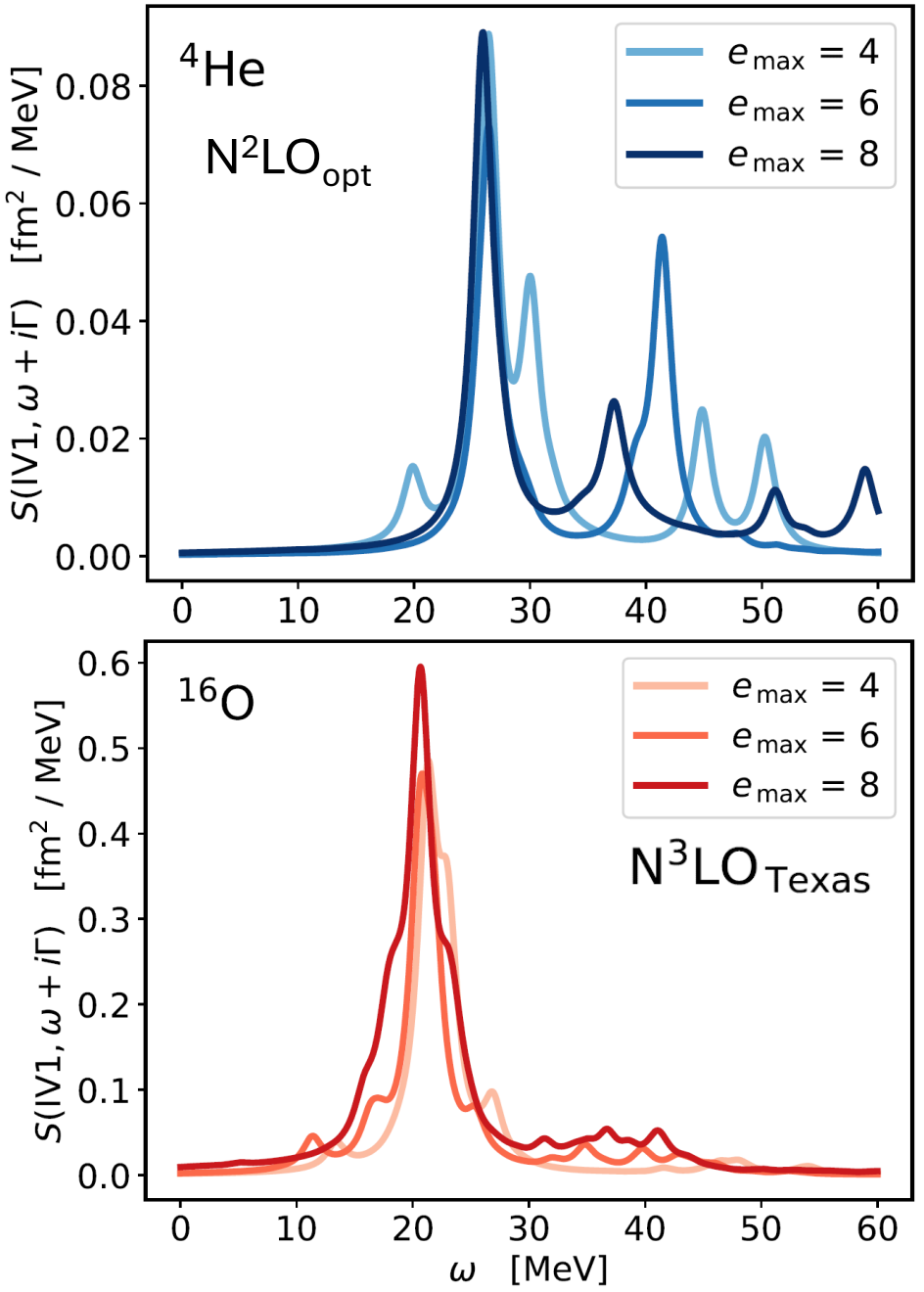
Basis size for 1^- response

e_{max}	# of states
4	66
6	180
8	380

^{4}He benchmark
Main peak 26 MeV (NCSM 26.5 MeV)

^{16}O convergence study
Fast convergence (similar to TD-CC)

Is convergence faster for dynamical calculations ?



Correlation impact

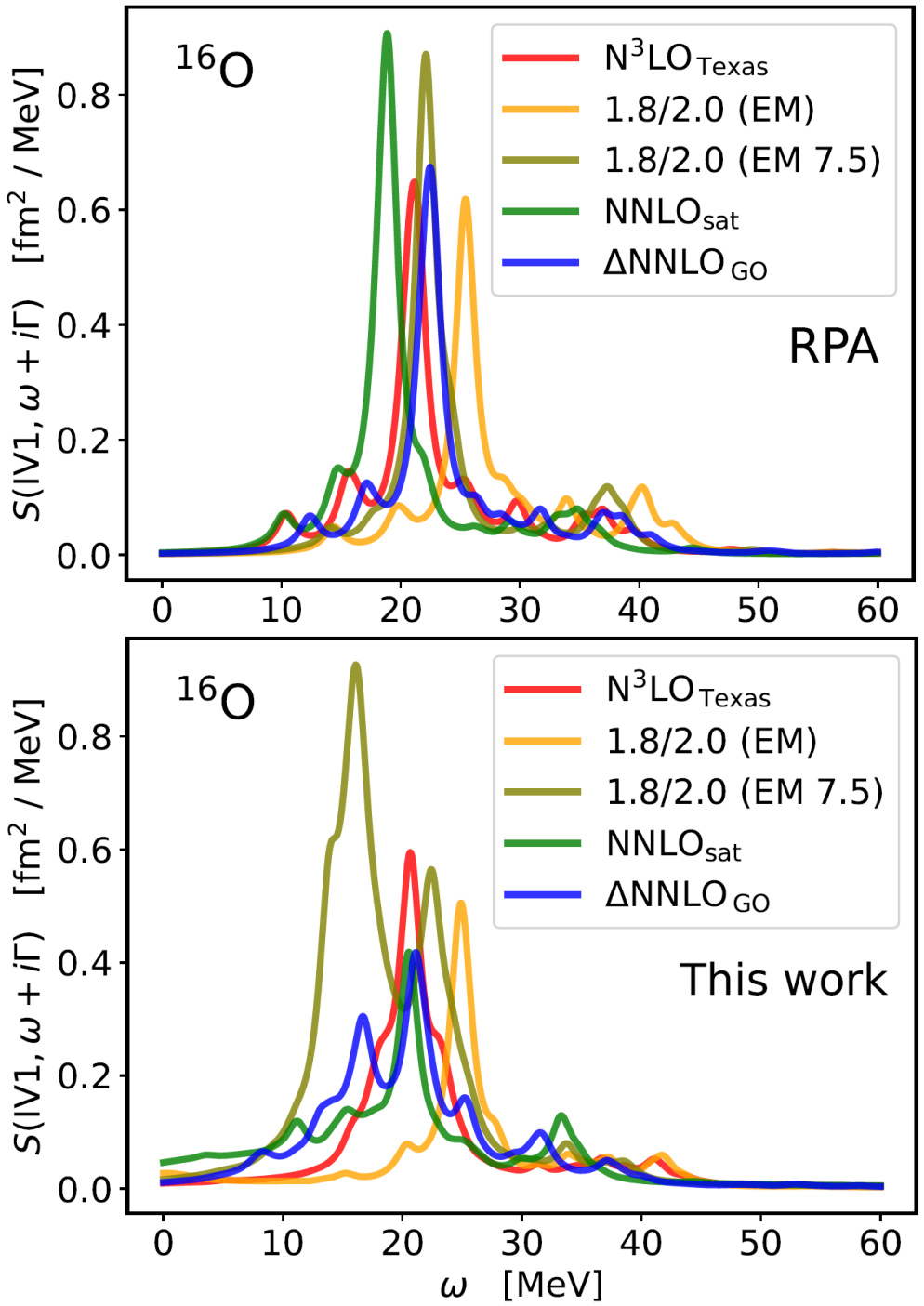
Compare calculations based on HF and IMSRG

HF-based calculations = RPA
(useful to benchmark implementation)

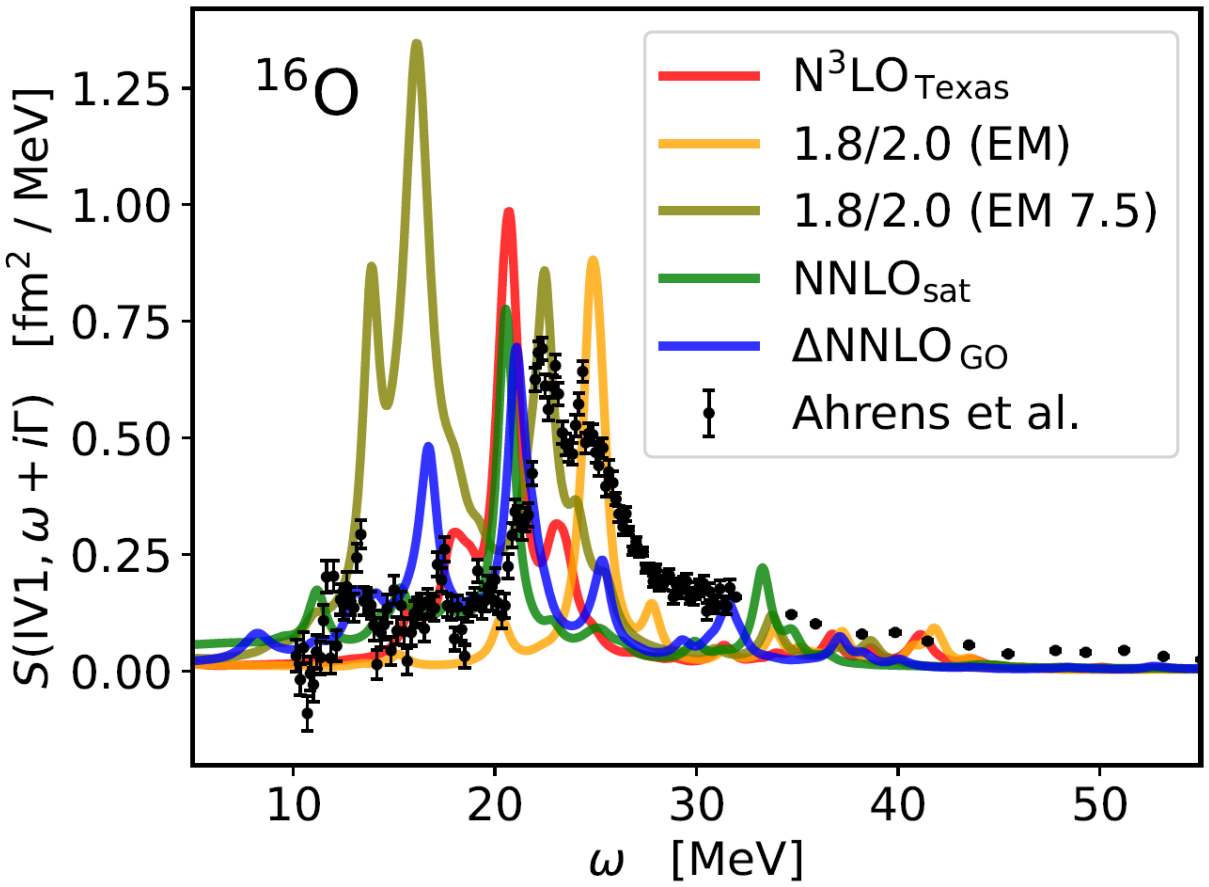
Reduced main resonance spread
(different interactions)

Correlation increases fragmentation

Small impact on soft interactions



Comparison to experimental data



Higher spectral resolution

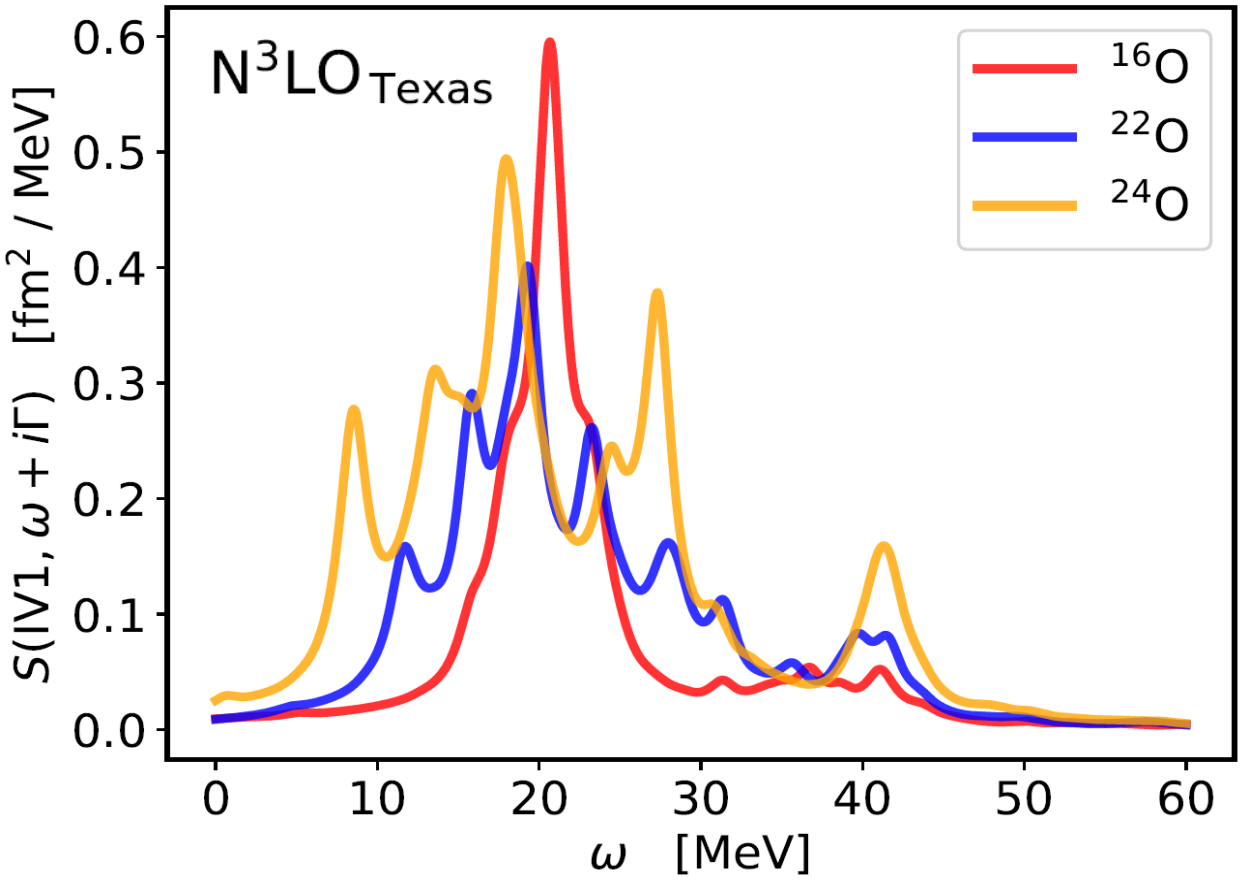
Γ = 0.5 MeV

1.8/2.0 (EM) overpredicts GDR
(known to give bad radii)

Texas, Sat and GO give similar GDR
(slightly lower energy)

1.8/2.0 (EM 7.5) very good GDR
Lower strength exaggerated

Neutron-rich oxygen isotopes



Spherical code allows other closed-shell

More neutron-rich oxygen isotopes

Lower strength increases with N excess

Agrees with phenomenology
Better convergence study needed

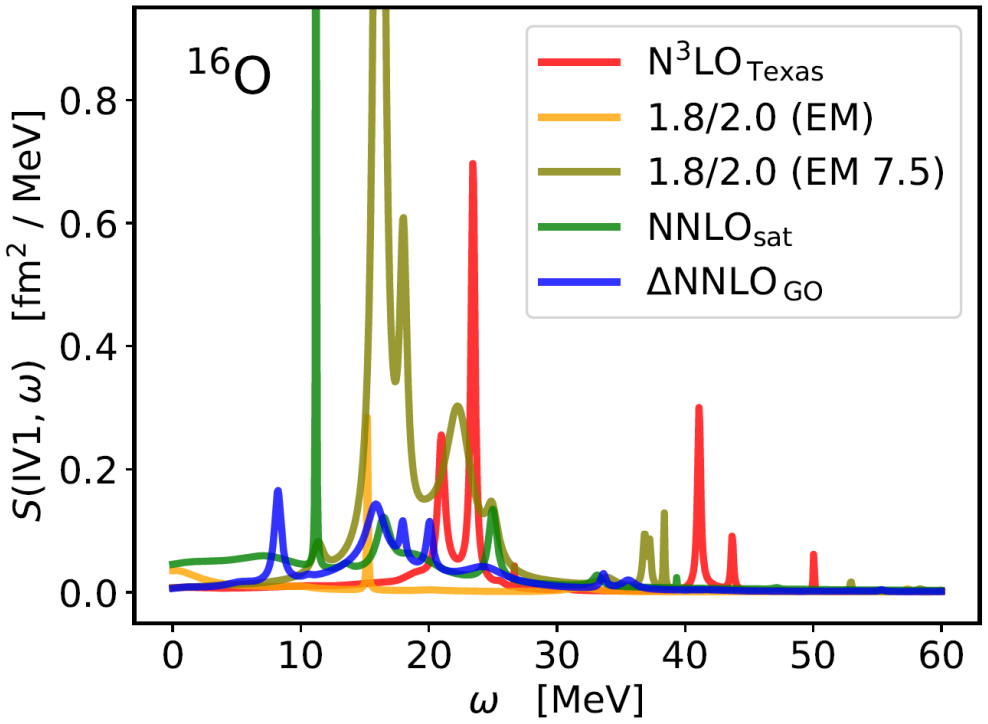
Complex eigenvalues

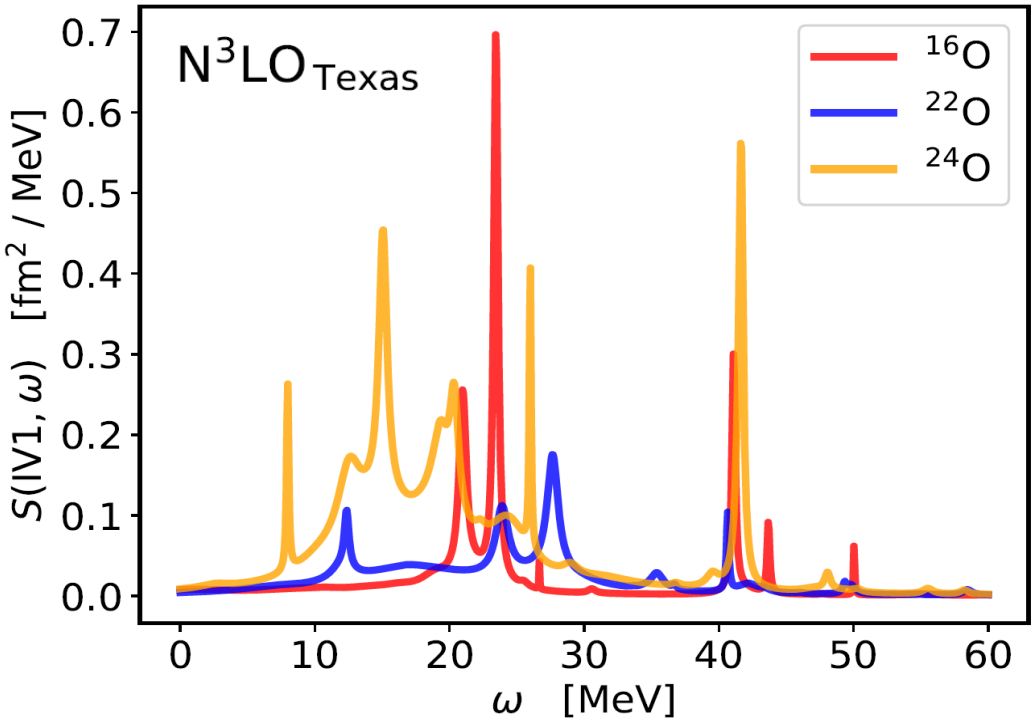
When using IMSRG state complex eigenvalues appear

Let show them separately $\Gamma = 0$ MeV

Why ?

Strong dependence on interaction and nucleus





Complex eigenvalues

$$\mathbf{H}\,\mathbf{X} = \mathbf{N}\,\mathbf{X}\,\Omega$$

Hessian at $|\Psi\rangle$ — Norm matrix

Both Hermitian (by construction)

Most general solutions of the EOM equation

- Real pairs
- Imaginary pairs
- Complex quartets

If H is not positive definite → Complex solutions appear

→ The energy at $|\Psi\rangle$ is not a minimum in the 1B op. space !

Known in CC (chemistry) → Iterative scheme to improve GS

→ Orbital optimization
(variational principle wrt 1B rotation)

Subtraction techniques (Feshbach projection)

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Summary

EOM is a dynamical framework giving the normal modes of the system

Universal implementation for modern many-body solvers

Propagate correlations from ground to exc. states

Fast model-space convergence and good agreement with NCSM

Embarrassingly parallel

Challenges and opportunities

Further numerical optimisation for larger model spaces

Study other systems, other multipoles, charge exchange, etc.

Combine with other WF (CC, symmetry-breaking and restoration, QVE, NNQS, etc.)

Use for new GS optimisation strategies

Thank you for the attention

Thomas Duguet
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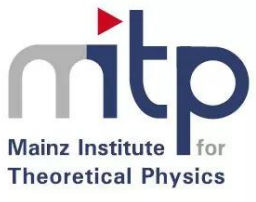

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