Impact of ground-state correlations on the nuclear response

Porro, Schwenk and Tichai, Phys. Rev. C 112, 054303 (2025)

EMMI Workshop – Hirschegg

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Outline

Introduction

- Physics case
- Quantities of interest

IMSRG multipole moments

- Strategy
- Model-space convergence
- Numerical results

New perspectives on the EOM

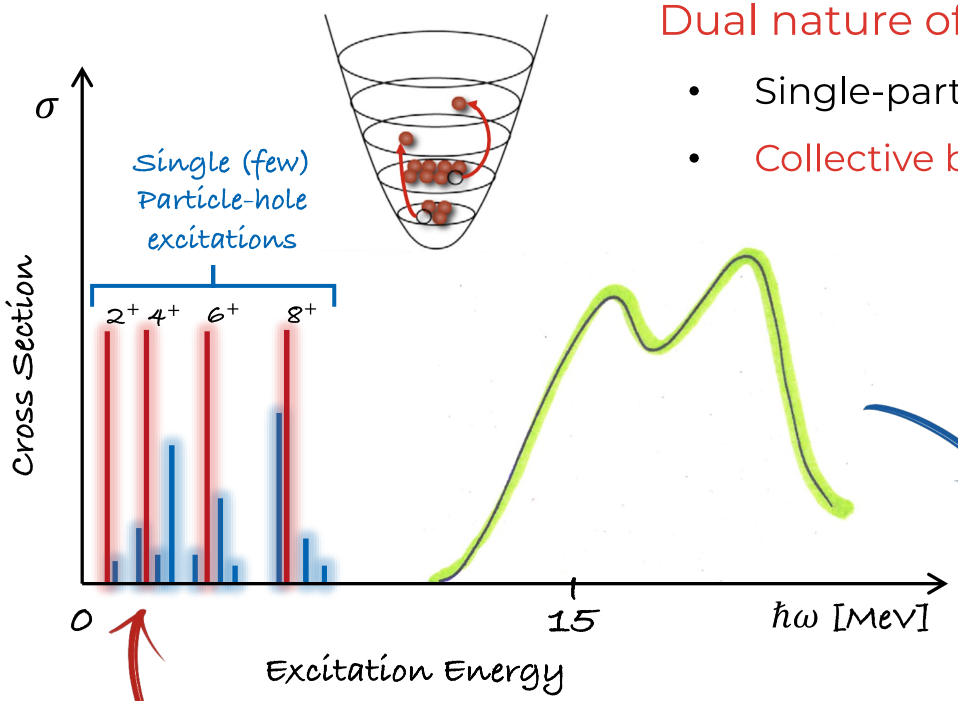
- Formal development
- Numerical results

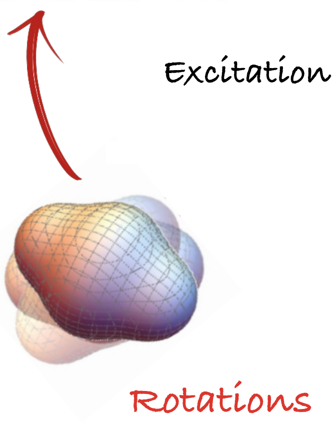
Challenges and opportunities

Nuclear spectroscopy

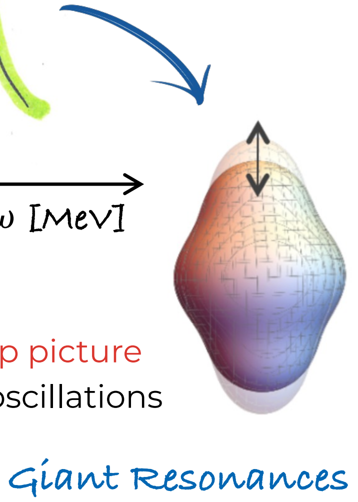
Dual nature of nucleus

- Single-particle features
- Collective behaviour





Liquid drop picture
vibrations, oscillations



Response function

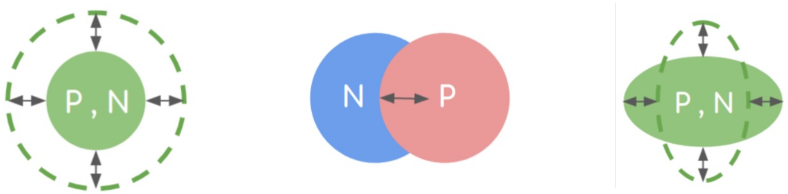
Fully characterise linear response

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

Transition probability

Excitation energy

Studied quantity: multipole response



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

Moments of the strength

Studied quantity: multipole response

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

Related moments

$$m_k(Q_\lambda) \equiv \int_0^\infty E^k S(Q_\lambda, E) dE$$

$$= \sum_{\mu\nu} (E_\nu - E_0)^k |\langle \Psi_\nu | Q_{\lambda\mu} | \Psi_0 \rangle|^2$$

Integrated properties

→ Must know excited states

→ Ground state only ← Identity resolution

$$\mathbb{1} = \sum_\nu |\Psi_\nu\rangle \langle \Psi_\nu|$$

Complexity shifted to operator structure

$$M_0(Q_\lambda) \equiv \sum_\mu (-1)^\mu Q_{\lambda,-\mu} Q_{\lambda\mu}$$

$$M_1(Q_\lambda) = \frac{1}{2} \sum_\mu (-1)^\mu [Q_{\lambda,-\mu}, [H, Q_{\lambda\mu}]]$$

Exact implementation up to m_1

Effective two-body Hamiltonian

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

Spherical tensor operators

$$Q^\dagger_{\lambda\mu} = (-1)^\mu Q_{\lambda,-\mu}$$

- Exact treatment for exc states
- Many-body truncation only GS

"Exact sum rules with approximate ground states"

[Johnson et al. , JPG, 2020]

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Previous PGCM study

I. [EPJA (2024) 60, 133]
II. [EPJA (2024) 60, 134]
III. [EPJA (2024) 60, 155]
IV. [EPJA (2024) 60, 233]

Eur. Phys. J. A (2024) 60:155
https://doi.org/10.1140/epja/s10050-024-01377-5

THE EUROPEAN PHYSICAL JOURNAL A

Check for updates

Regular Article - Theoretical Physics

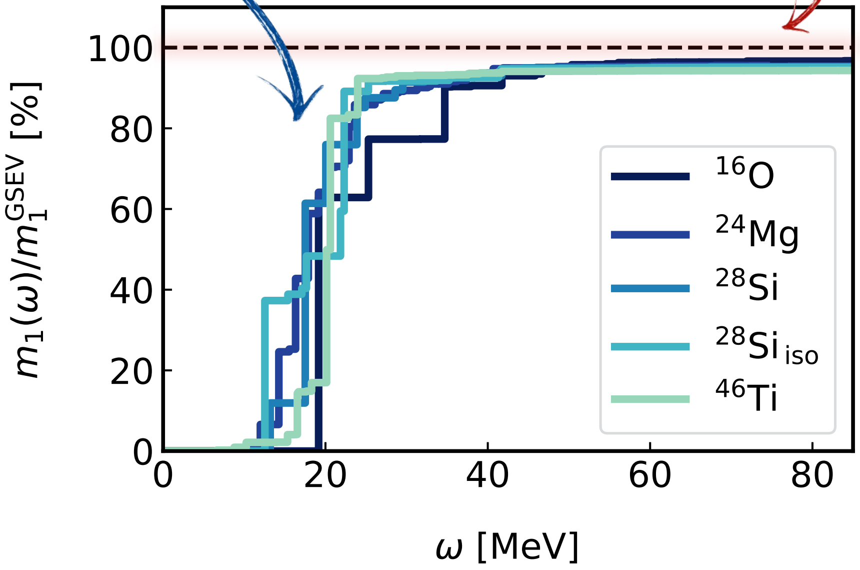
Ab initio description of monopole resonances in light- and medium-mass nuclei

III. Moments evaluation in ab initio PGCM calculations

A. Porro[1,2,3,a], T. Duguet[3,4], J.-P. Ebran[5,6], M. Frosini[7], R. Roth[1,8], V. Somà[3]

$$m_1(\omega) = \int_0^{\omega} d\tilde{\omega}\, S(r^2, \tilde{\omega})\tilde{\omega}$$

$$m_1^{\mathrm{GSEV}} = \frac{1}{2}\langle \Psi_0 | [r^2, [H, r^2]] | \Psi_0 \rangle$$



Based on

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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(Received 28 July 2025; accepted 23 September 2025; published 5 November 2025)

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.

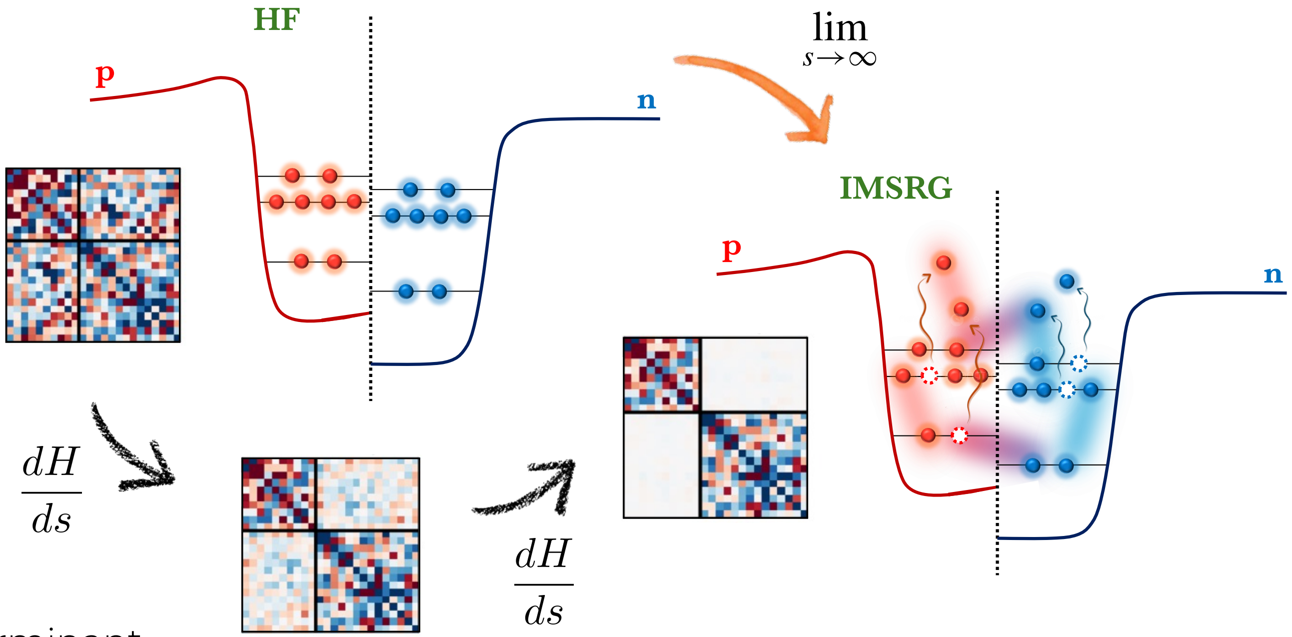
DOI: 10.1103/1ktc-lknn

Strategy in the IMSRG framework

Unitary transformation

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

Diagonal Off-diagonal



$$E_{\mathrm{gs}} = \lim_{s\to\infty} E_0(s) = \langle \Phi | H(s) | \Phi \rangle$$

Slater determinant

Steps

- Start from the moment operator in the HO basis
- Perform an IMSRG(2) calculation
- Evolve moment operators using Magnus

$$U(s) \equiv e^{\Omega(s)}$$

$$M_0(Q_\lambda) \equiv \sum_\mu (-1)^\mu Q_{\lambda,-\mu} Q_{\lambda\mu}$$

$$M_1(Q_\lambda) = \frac{1}{2} \sum_\mu (-1)^\mu [Q_{\lambda,-\mu}, [H, Q_{\lambda\mu}]]$$

J-scheme expressions of m_0 and m_1

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

Implemented within imsrg++ code

[github.com/ragnarstroberg/imsrg]

Benchmarks

- HF value of m_0 against TDA
- HF value of m_1 against RPA

[Tsukiyama, Bogner and Schwenk, PRL, 2011]

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

Model-space convergence

Dipole response

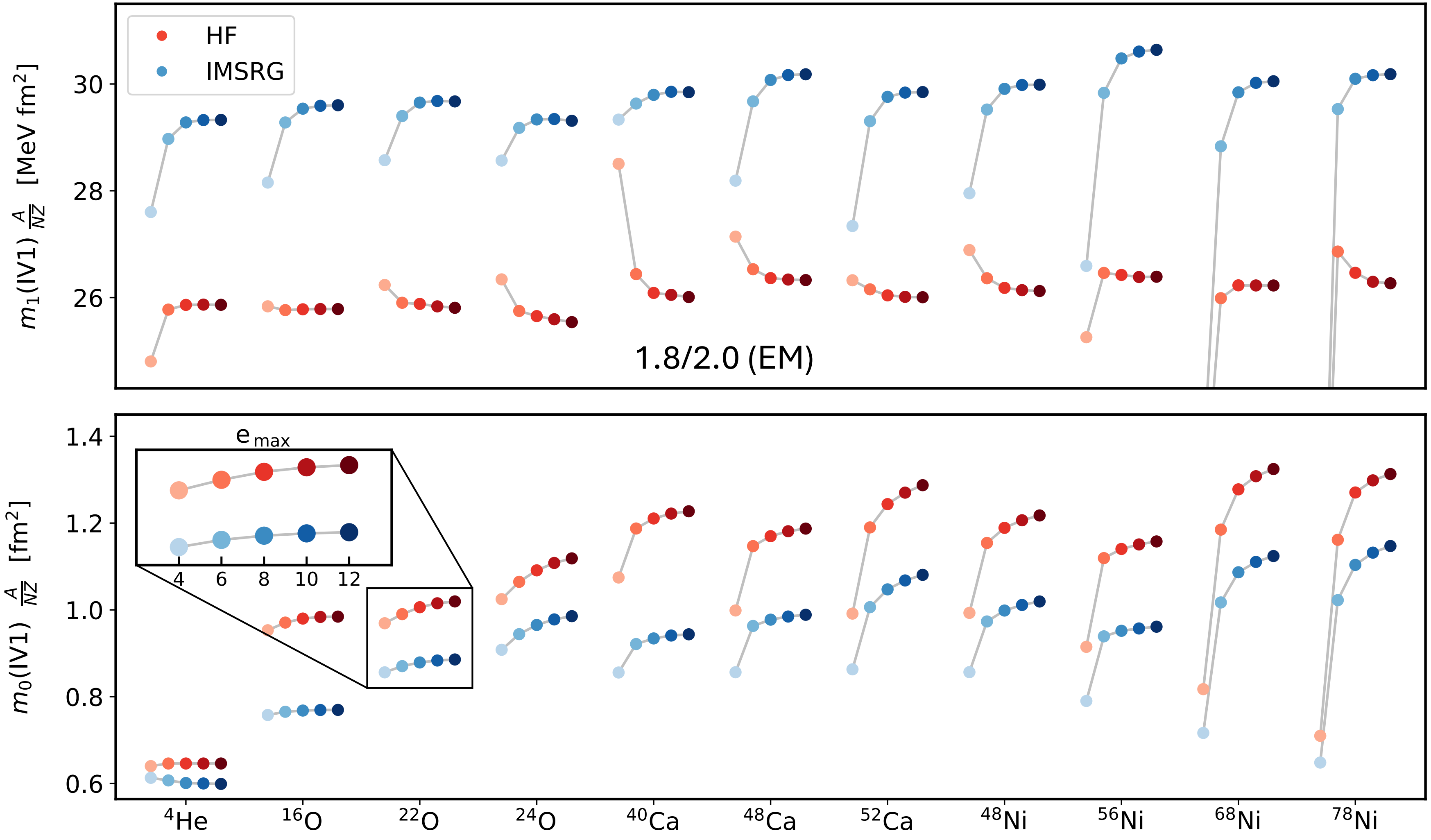
$$Q_{1\mu}^{\mathrm{IV}} = \frac{N}{A}\sum_{i=1}^{Z} r_i Y_{1\mu}(\hat{r}_i) - \frac{Z}{A}\sum_{i=1}^{N} r_i Y_{1\mu}(\hat{r}_i)$$

$$M_1(Q_\lambda) = \frac{1}{2}\sum_{\mu}(-1)^{\mu}[Q_{\lambda,-\mu},[H,Q_{\lambda\mu}]]$$

- Large correlation impact
- Relative difference ~0.2%
- Similar error for $\hbar\omega$ variations

$$M_0(Q_\lambda) \equiv \sum_{\mu}(-1)^{\mu}Q_{\lambda,-\mu}Q_{\lambda\mu}$$

- Slower convergence
- Relative difference ~1.3%
- 2% error for $\hbar\omega$ variations



Another example: Kumar invariants

0th quadrupole moment

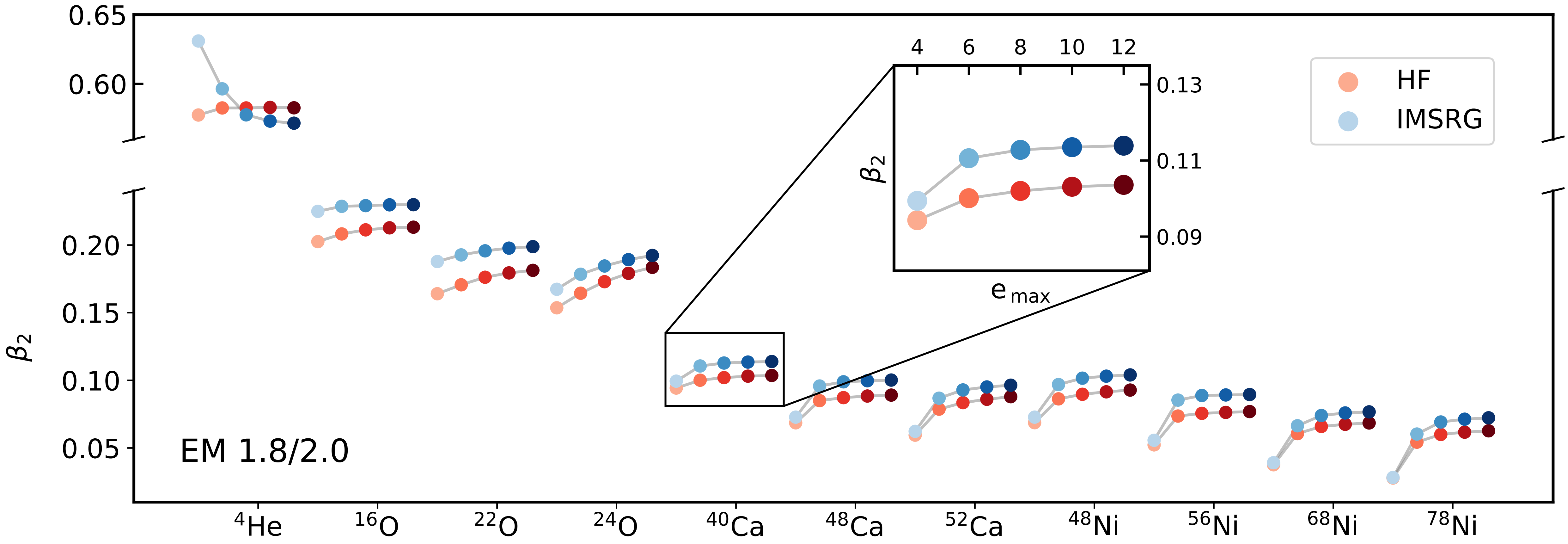
$$m_0(Q_2) = \langle Q_2 \cdot Q_2 \rangle$$

Model-independent deformation «measure»

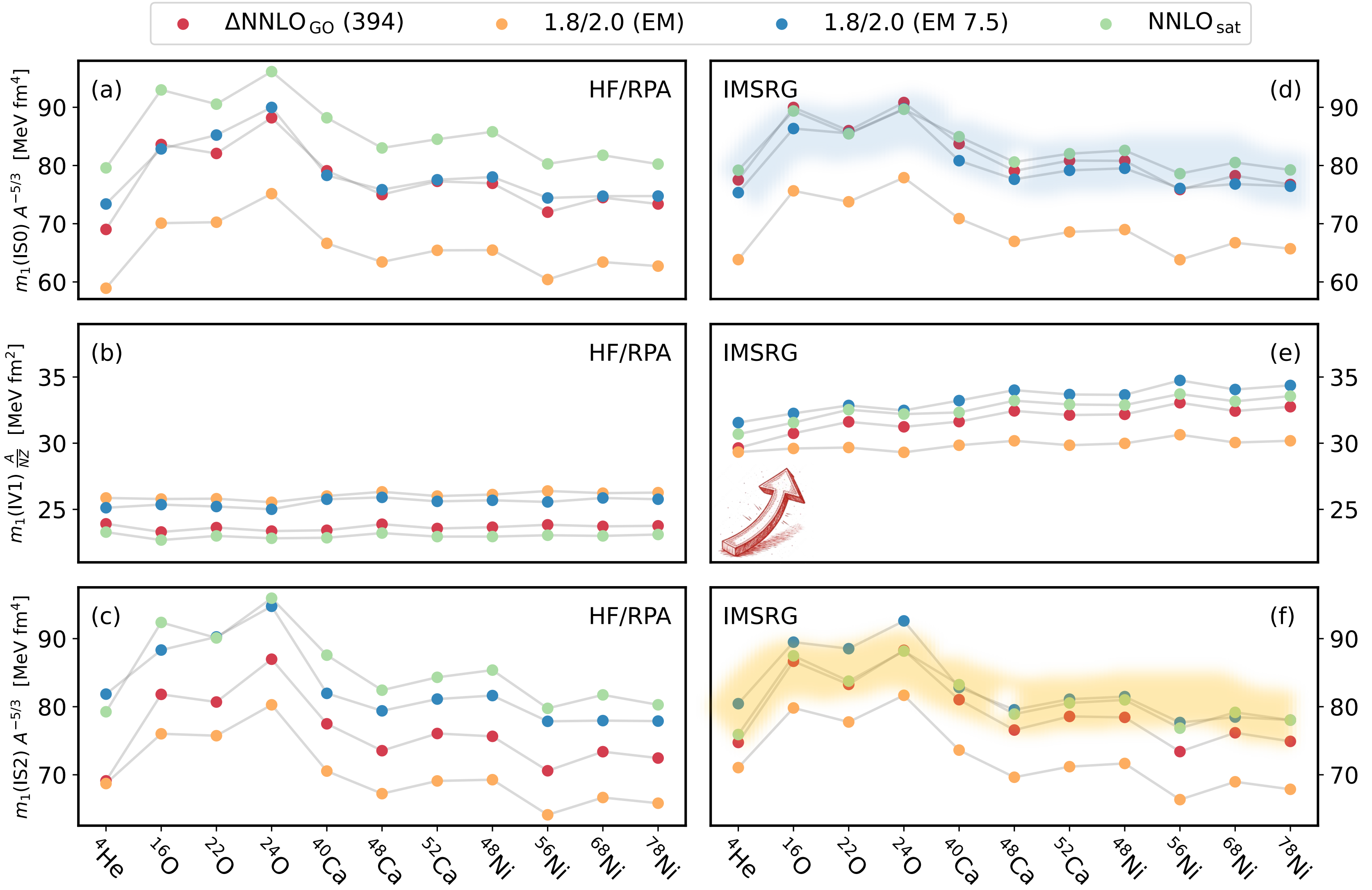
$$\beta_2 \equiv \frac{4\pi}{3r_0^2} \frac{\langle Q_2 \cdot Q_2 \rangle^{1/2}}{A^{5/3}}$$

Higher invariants also fundamental

[Poves et al., PRC 101 (2020) 054307]



Interaction sensitivity



Monopole

- Reduced spread
- ~5% correlations effect

Dipole

- Increase up to 40%
- 2% spread (w/o 1.8/2.0(EM))

Quadrupole

- Reduced spread
- ~5% correlations effect

Photoabsorption cross section

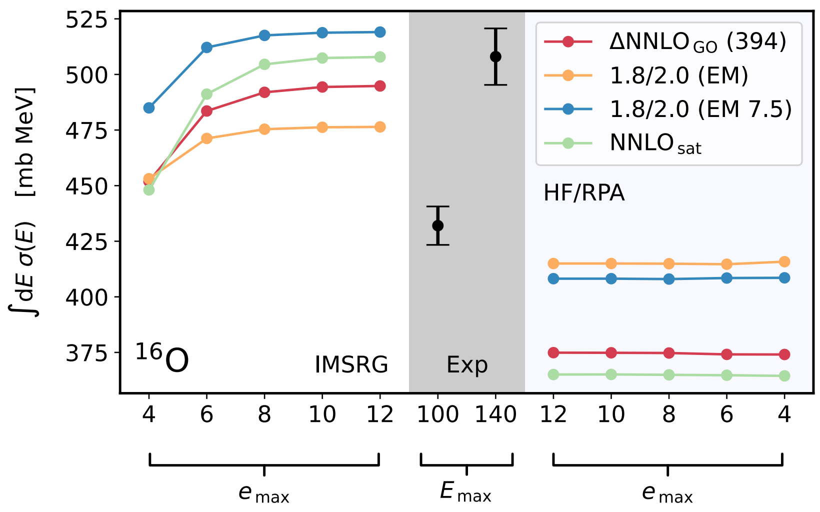
Comparison to exp only makes sense for integrated quantities

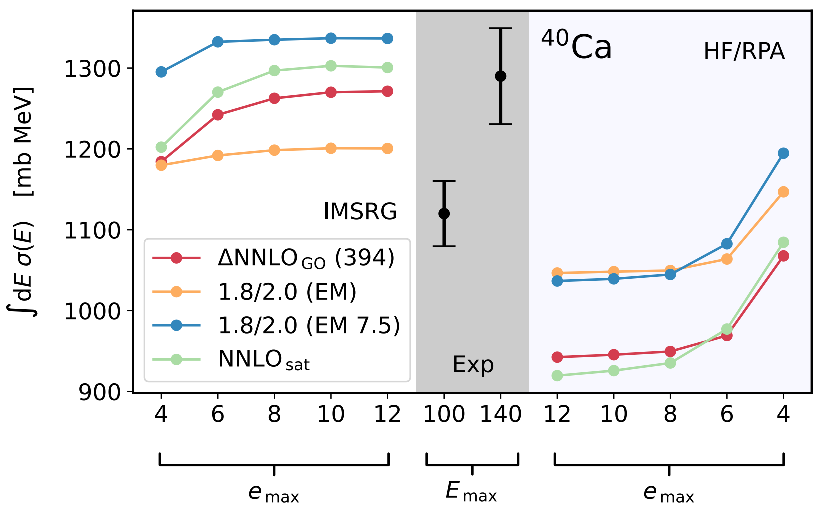
Pion-production threshold

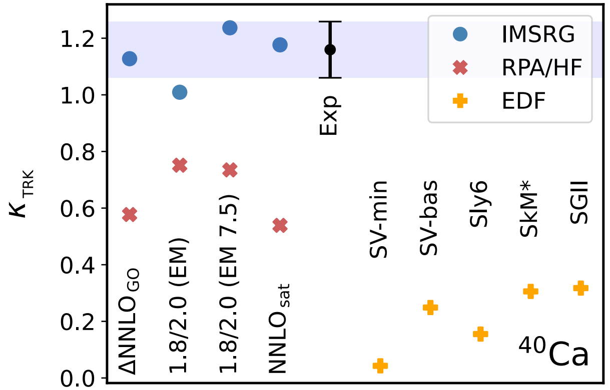
$$\int_0^\infty \sigma(E)\mathrm{d}E = \frac{2\pi^2}{\hbar c}\langle\Psi_0|[D,[H,D]]|\Psi_0\rangle = \frac{16\pi^3}{9}\alpha\, m_1(\mathrm{IV1}) \qquad \int_0^{E_{\max}}\sigma(E)\mathrm{d}E$$

$$\approx 60\,\frac{NZ}{A}(1+\kappa)\quad \mathrm{mb}\cdot\mathrm{MeV}$$

TRK sum rule [Ahrens et al., NPA, 1975]







Comparison to EDF calculations

[Courtesy of P.-G. Reinhard]

Both needed for consistent description

- Ground-state correlations
- Commutator expression generates 2-body currents

Photoabsorption cross section

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$$\int_0^\infty \sigma(E)\mathrm{d}E = \frac{2\pi^2}{\hbar c}\langle\Psi_0|[D,[H,D]]|\Psi_0\rangle = \frac{16\pi^3}{9}\alpha\, m_1(\mathrm{IV1})$$

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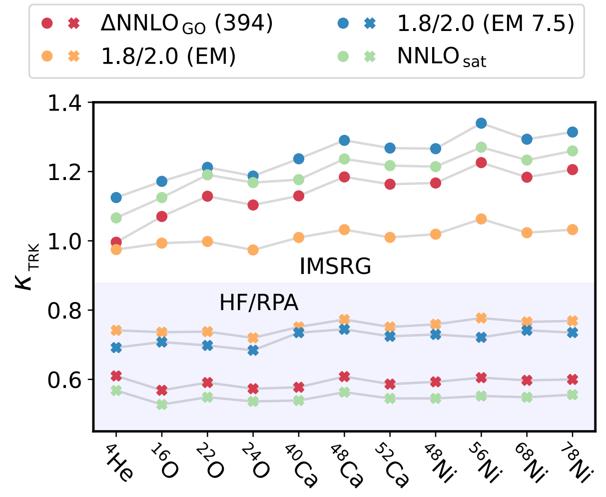
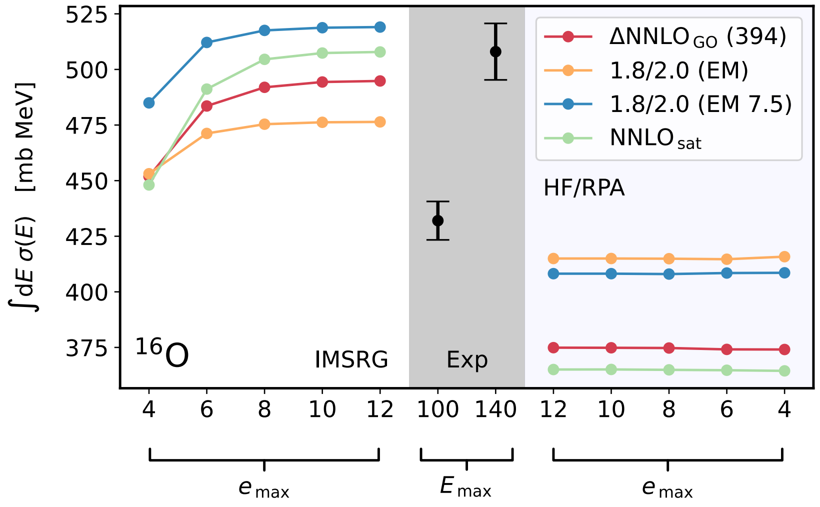
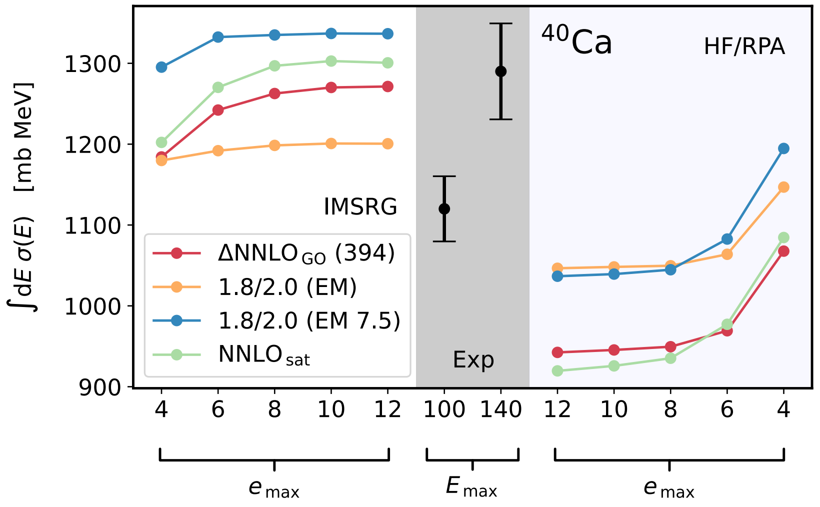
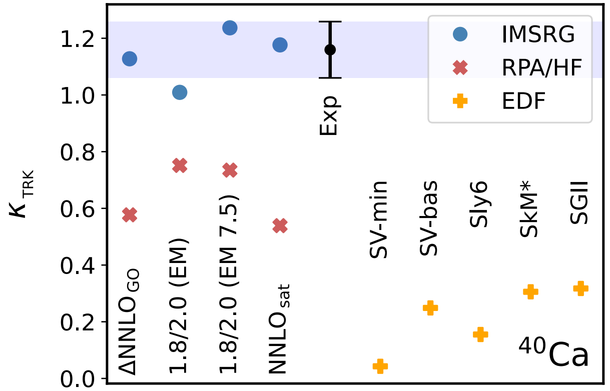
TRK sum rule









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From moments to response

Family of average energies

$$\bar{E}_k(Q) \equiv \frac{m_k(Q)}{m_{k-1}(Q)}$$

$$\tilde{E}_k(Q) \equiv \sqrt{\frac{m_k(Q)}{m_{k-2}(Q)}}$$

Series of inequalities

$$\cdots \leq \sqrt{\frac{m_{k+1}}{m_{k-1}}} \leq \frac{m_{k+1}}{m_k} \leq \sqrt{\frac{m_{k+2}}{m_k}} \leq \frac{m_{k+2}}{m_{k+1}} \leq \cdots$$

How to go from average to exact energies ?

Excitation operator approach

$$Q_\nu^\dagger \left|\Psi_0\right\rangle = \left|\Psi_\nu\right\rangle$$

Exact case: inequalities beocme equalities

$$\tilde{E}_k(Q_\nu^\dagger) = \bar{E}_k(Q_\nu^\dagger) = (E_\nu - E_0) = \omega_\nu \quad \forall k$$

Use this property to determine $Q_\nu^\dagger$

Expand in a basis

$$Q_\nu^\dagger = \sum_\alpha X_\nu^\alpha \, q_\alpha^\dagger$$

$$\{q_\alpha^\dagger, \, \alpha = 1, \ldots, N\}$$

Differentiate

$$\delta\tilde{E}_k(Q_\nu^\dagger) = 0$$

$$\delta\bar{E}_k(Q_\nu^\dagger) = 0$$

Family of variational equations

$$\delta m_k(Q_\nu^\dagger) - \tilde{E}_k^2(Q_\nu^\dagger)\delta m_{k-2}(Q_\nu^\dagger) = 0$$

$$\delta m_k(Q_\nu^\dagger) - \bar{E}_k(Q_\nu^\dagger)\delta m_{k-1}(Q_\nu^\dagger) = 0$$

Solutions converge in the full space

An Equation of Motion

Take k=1

$$\delta m_1(Q_\nu^\dagger) - \omega_\nu(Q_\nu^\dagger)\delta m_0(Q_\nu^\dagger) = 0$$

Where

$$\mathsf{M}_{k,\alpha\beta} \equiv m_k(q_\alpha, q_\beta^\dagger)$$

$$m_k(q_\alpha, q_\beta^\dagger) = \sum_\nu (E_\nu - E_0)^k \langle\Psi_0|q_\alpha|\Psi_\nu\rangle \langle\Psi_\nu|q_\beta^\dagger|\Psi_0\rangle$$

In this case

$$m_1(q_\alpha, q_\beta^\dagger) = \langle\Psi_0|q_\alpha\,[H, q_\beta^\dagger]|\Psi_0\rangle$$

$$m_0(q_\alpha, q_\beta^\dagger) = \langle\Psi_0|q_\alpha q_\beta^\dagger|\Psi_0\rangle$$

$$\sum_\beta [\mathsf{M}_{1,\,\alpha\beta} - \omega_\nu \mathsf{M}_{0,\,\alpha\beta}] X_\nu^\beta = 0$$

Generalised eigenvalue problem

(GCM-like equation but in an operator space)

Strictly equivalent to the EOM (Rowe)

K=3 returns the RPA equations

`[PG Reinhard et al., PRA 41 (1990) 10, 5568]`

Theoretical comparison

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

The method is exact in the full space

Approximations introduced here:

- IMSRG(2) ground state
- One-body operator space

Physical motivation

Excitations MUST be mostly 1B

(e.g. electromagnetic)

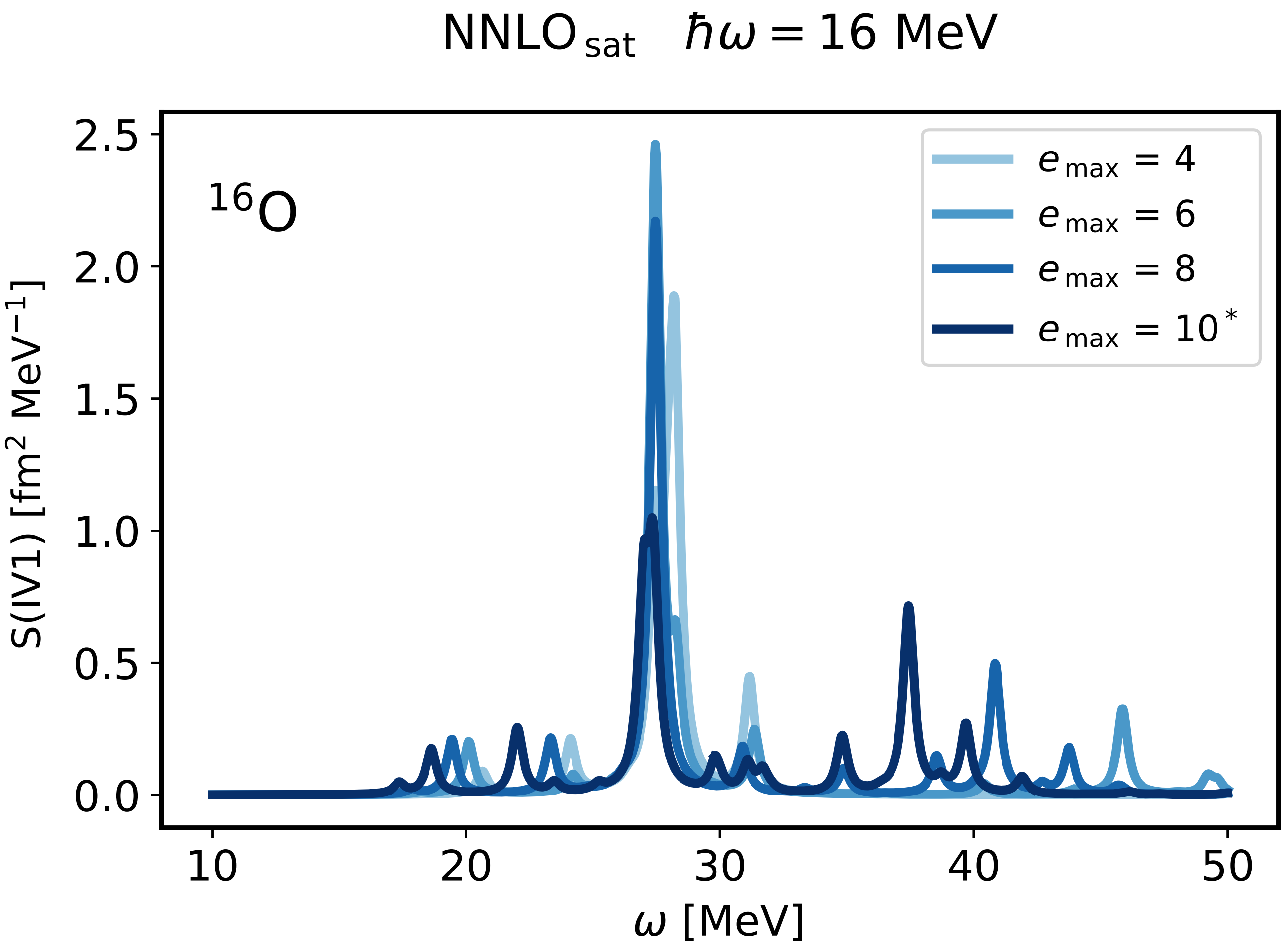
N.B.: 1B wrt correlated GS

Sum rules are exhausted by the 1B space

Independently on the chosen GS

Easier interpretation of approx. levels

Dipole response (preliminary)



Basis size for 1^- response

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

Good e_{max} convergence (GR)

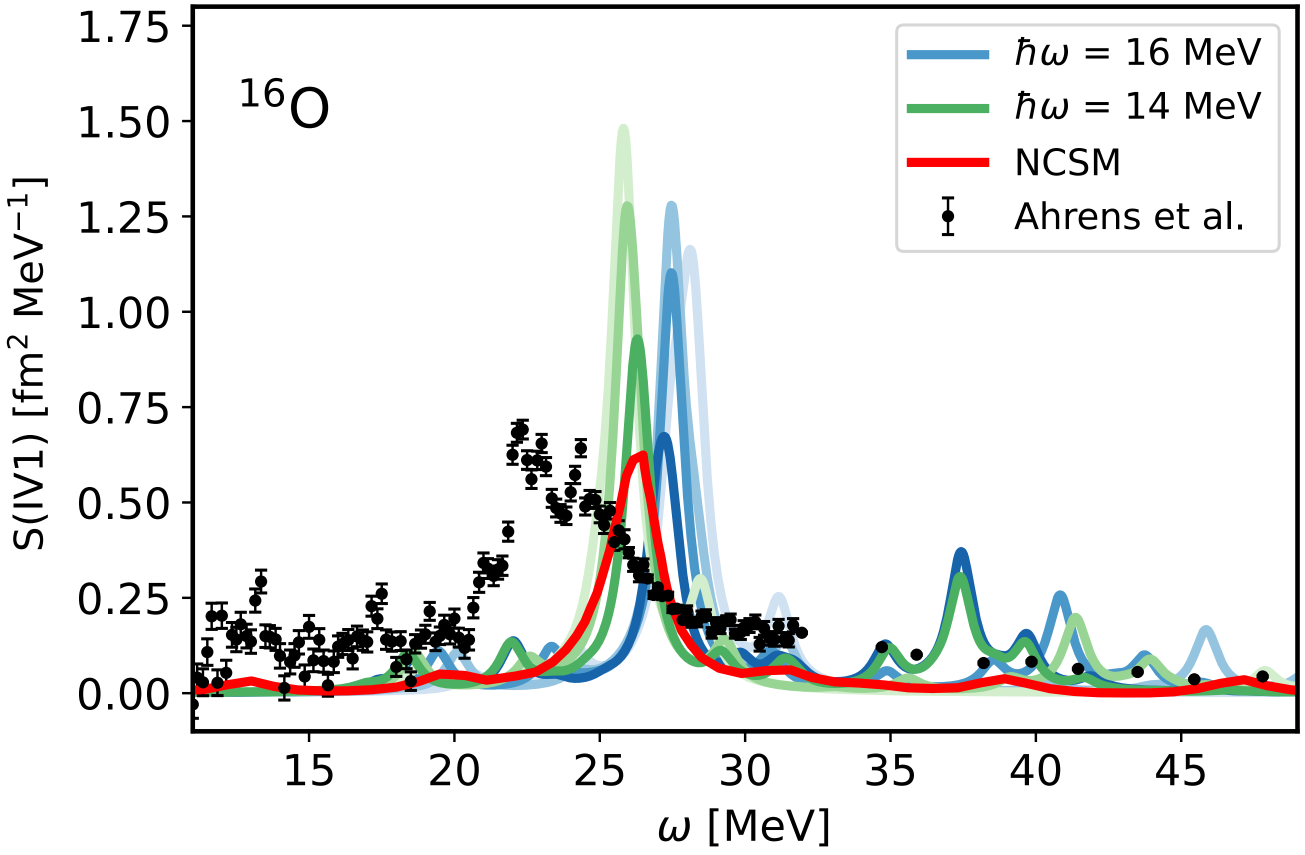
Energy-based truncation for large spaces

Larger spaces affordable with truncations

$NNLO_{sat}$ [Ekström et al, PRC 91(5), 051301, 2015]

Dipole response (preliminary)

NNLO$_{sat}$



Small residual frequency dependence

Constraints on converged value

Energy too high wrt experiment

Agreement with NCSM

[Stumpf, Wolfgruber and Roth, arXiv:1709.06840v1]

NNLO$_{sat}$ [Ekström et al, PRC 91(5), 051301, 2015]

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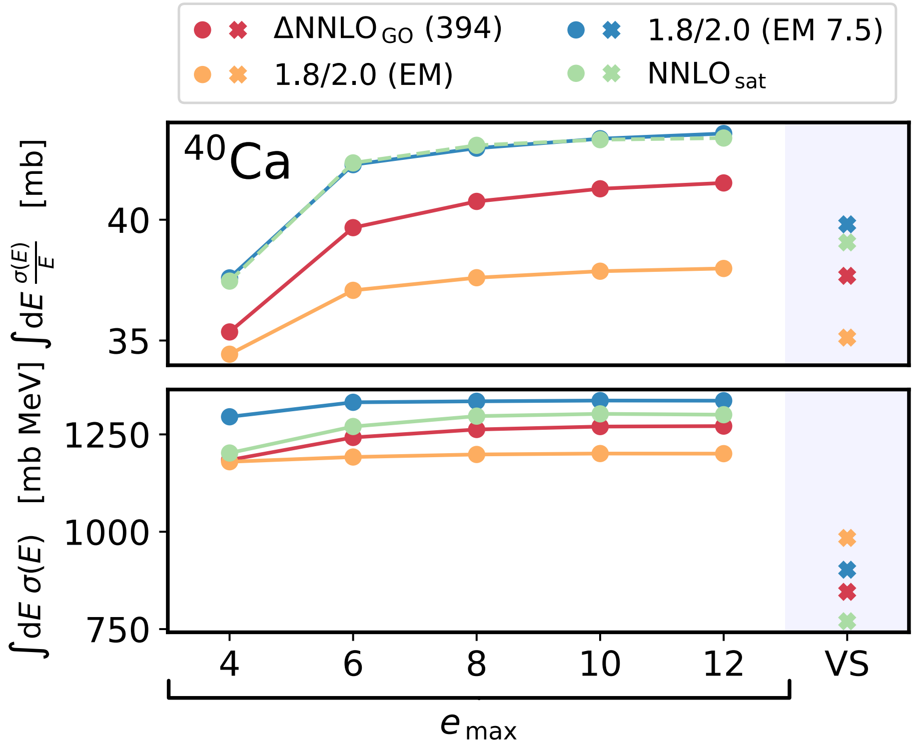
Going open-shell (moments)

Comparison to VS calculation for ^{40}Ca with ^{28}Si core

- Large uncertainties for m_1 and m_0
- Two-step decoupling
- Is the core well described ? (deformation)

Other possibilities within the IMSRG

- Multi-reference formulation
- Symmetry-breaking calculations



Response

- No limitation on the GS many-body method of choice
- Further efforts for model-space convergence
- Comparison to existing methods (EOM, LIT etc.)
- May be useful for a better understanding of H properties