Exploring nuclear collectivity within the IMSRG

PAINT2025

Workshop on Progress in Ab Initio Nuclear Theory

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Outline

Introduction

- Physics case
- Quantities of interest

IMSRG multipole moments

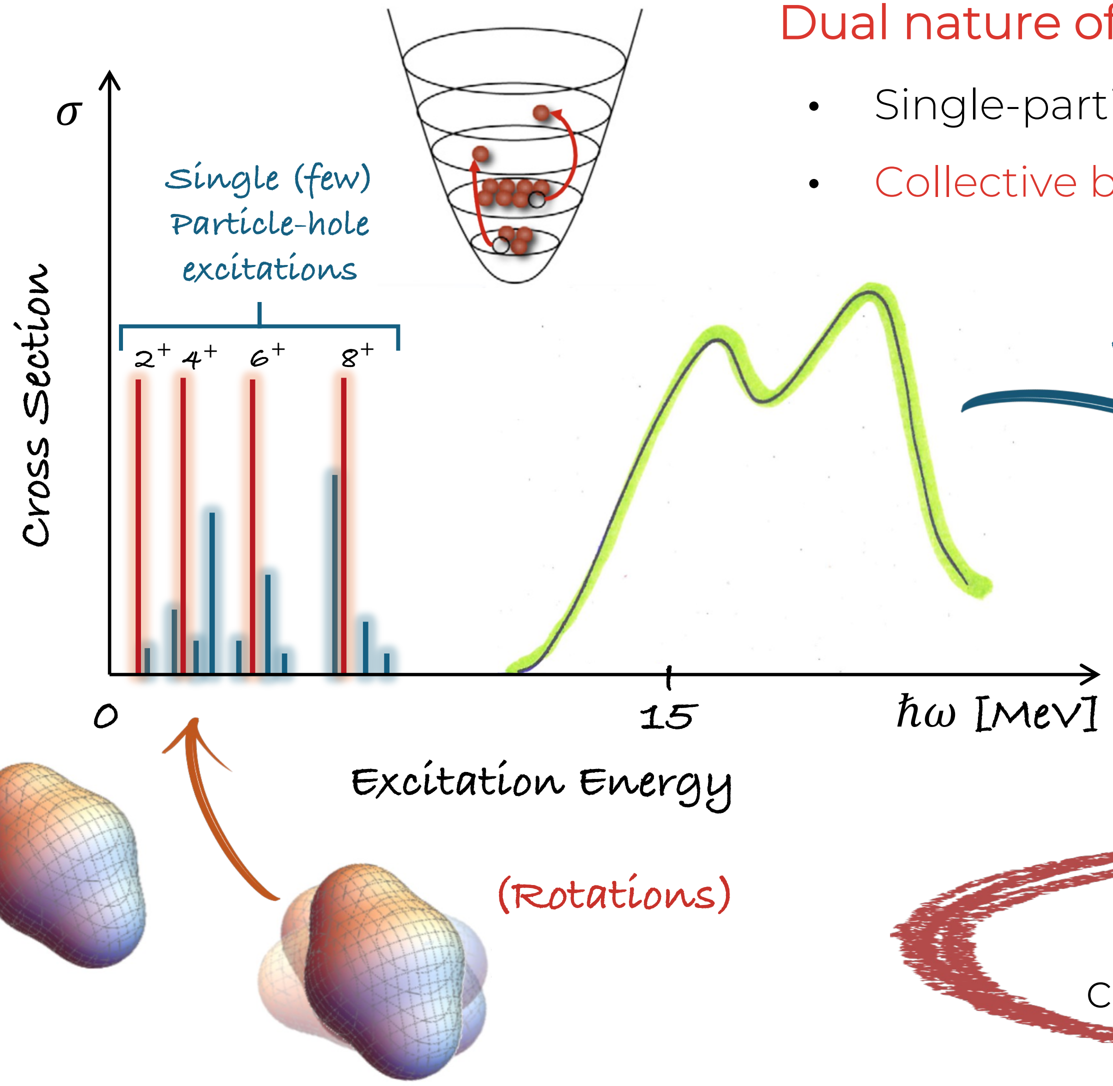
- Sum rule exhaustion
- Strategies for moments evaluation
- Numerical results

An IMSRG response ?

- Theoretical foundations
- Collective resonances in ^{40}Ca

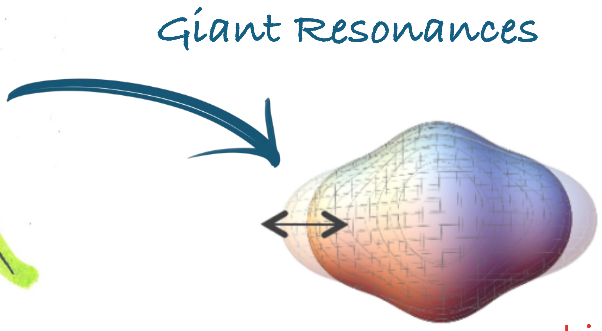
Conclusions

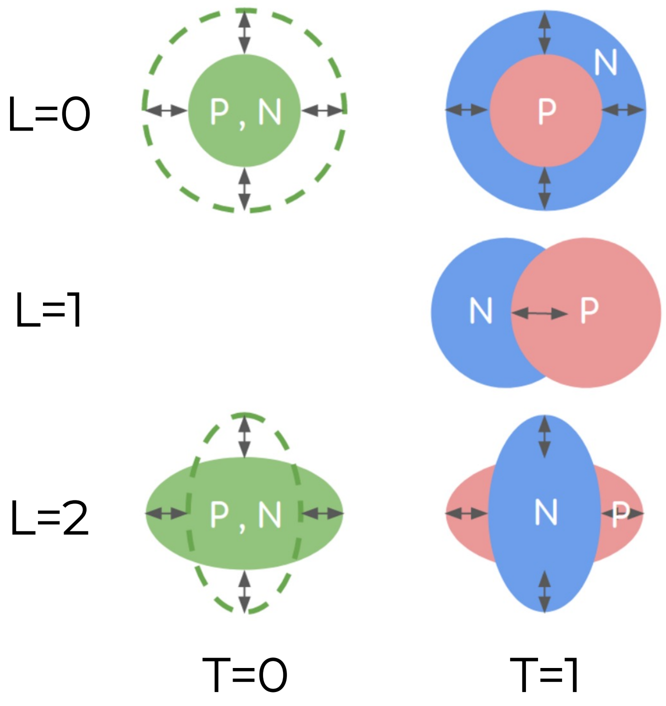
Giant Resonances



Dual nature of nucleus

- Single-particle features
- Collective behaviour





Liquid drop picture
vibrations, oscillations

Giant Resonances (GRs)

clearest manifestation of collective motion

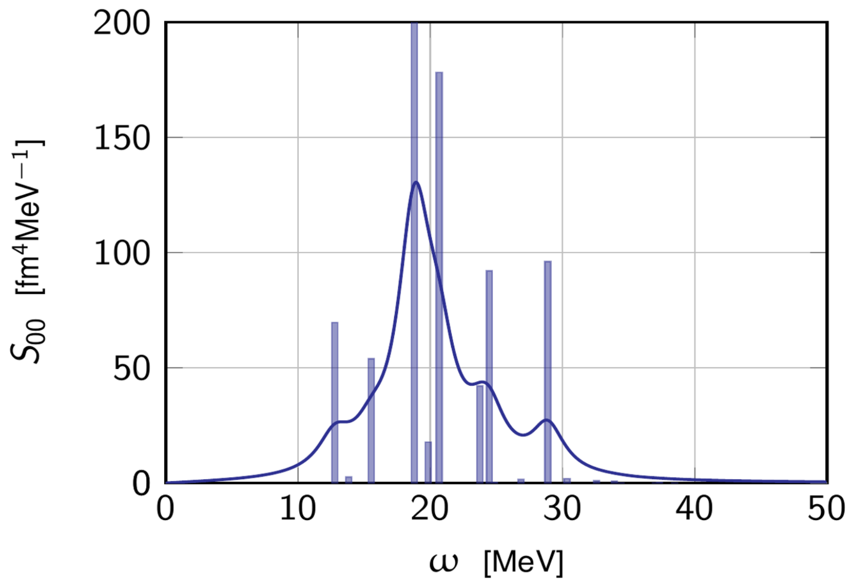
[Pictures from Dytrych et al., PRL, 2020]

Average properties – strength moments

Studied quantity: multipole strength

- Transition amplitudes: height of peaks
- Energy difference: position of peaks

$$S_Q(\omega) \equiv \sum_\nu | \langle \Psi_\nu | Q | \Psi_0 \rangle |^2 \delta(E_\nu - E_0 - \omega)$$



Related moments

$$m_k(Q) \equiv \int_0^\infty S_Q(\omega)\, \omega^k \, d\omega$$
$$= \sum_\nu (E_\nu - E_0)^k | \langle \Psi_\nu | Q | \Psi_0 \rangle |^2$$

Quantify the most relevant features of the strength

$$\bar{E}(Q) \equiv \frac{m_1(Q)}{m_0(Q)} \qquad E_k(Q) \equiv \sqrt{\frac{m_k(Q)}{m_{k-2}(Q)}}$$

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Moment operators

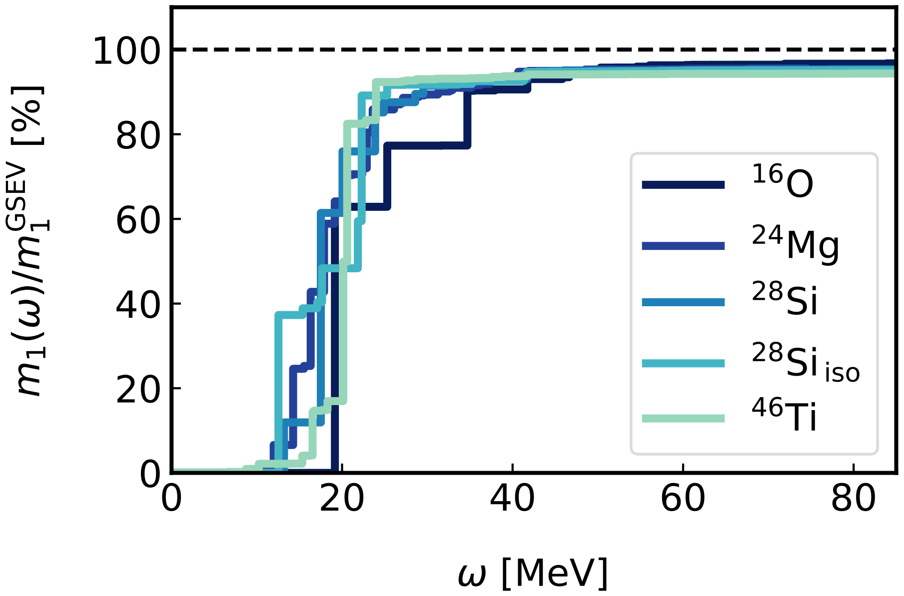
Different evaluation streategies for the moments

$$S_Q(\omega) \equiv \sum_\nu |\langle \Psi_\nu | Q | \Psi_0 \rangle|^2 \delta(E_\nu - E_0 - \omega)$$

$$m_k(Q) \equiv \int_0^\infty S_Q(\omega)\, \omega^k \, d\omega$$

$$= \sum_\nu (E_\nu - E_0)^k |\langle \Psi_\nu | Q | \Psi_0 \rangle|^2$$ → Must know excited states — 6-7 % difference in PGCM

$$\equiv \langle \Psi_0 | M_k(Q) | \Psi_0 \rangle$$ → Ground state only



[EPJA (2024) 60, 155]

Complexity is shifted to the operator structure

$$M_k(Q) \equiv (-1)^i C_i C j \qquad \forall \;\; k \geq 0$$

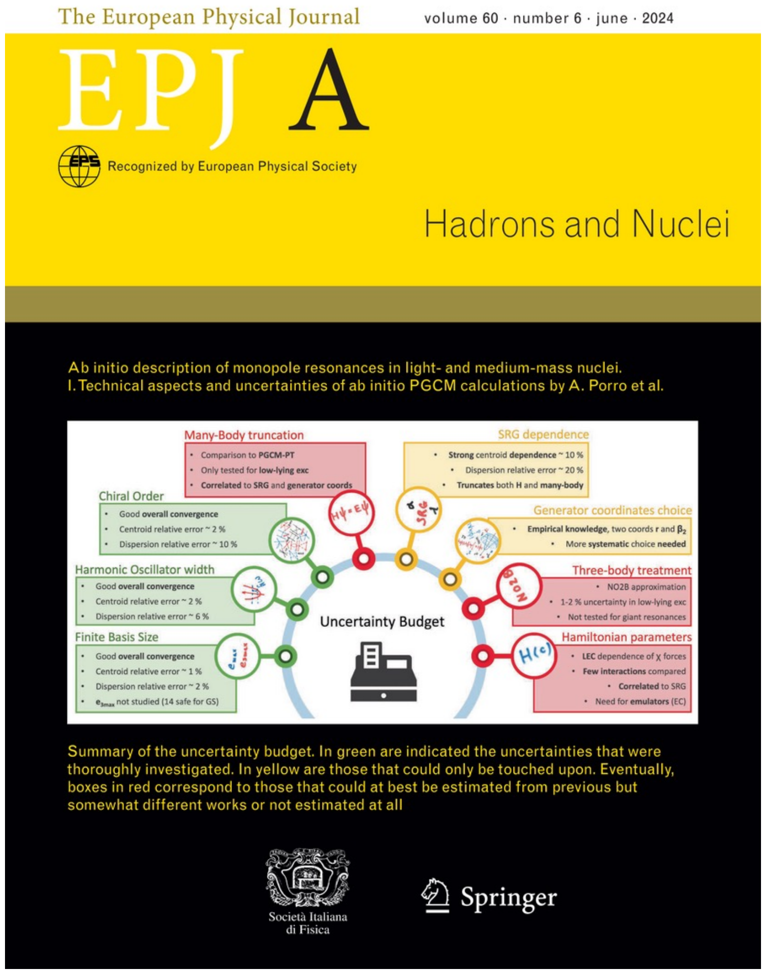
$$M_k(Q) \equiv \frac{1}{2}(-1)^i [C_i, C_j] \qquad \forall \;\; \text{odd} \;\; k > 0$$

$$C_j \equiv \underbrace{[H, [H, ...[H, [H}_{j \text{ times}}, Q]]...]]$$

Many-body operators

- Exact up to m_1 $\quad H = H^{[1]} + H^{[2]}$

Previous PGCM study



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Regular Article - Theoretical Physics

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

III. Moments evaluation in ab initio PGCM calculations

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

Strategy in the IMSRG framework

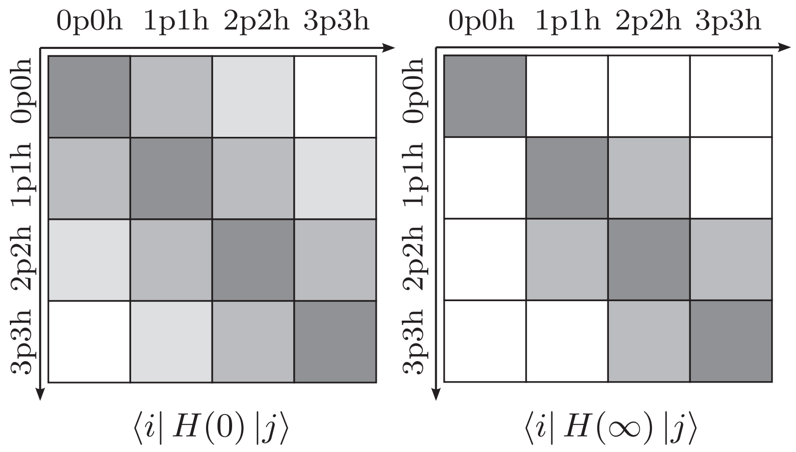
Unitary transformation

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

Diagonal Off-diagonal

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

Slater determinant



$$\lim_{s\to\infty}$$

Steps

- Start from the moment operator in the HO basis $M_1(Q) = \frac{1}{2}[Q^\dagger, [H, Q]]$ $M_0(Q) = Q^\dagger Q$
- Perform an IMSRG(2) calculation
- Consistently evolve the moment operators using Magnus $U(s) \equiv e^{\Omega(s)}$

Quadrupole focus I: Kumar invariants

0th quadrupole moment

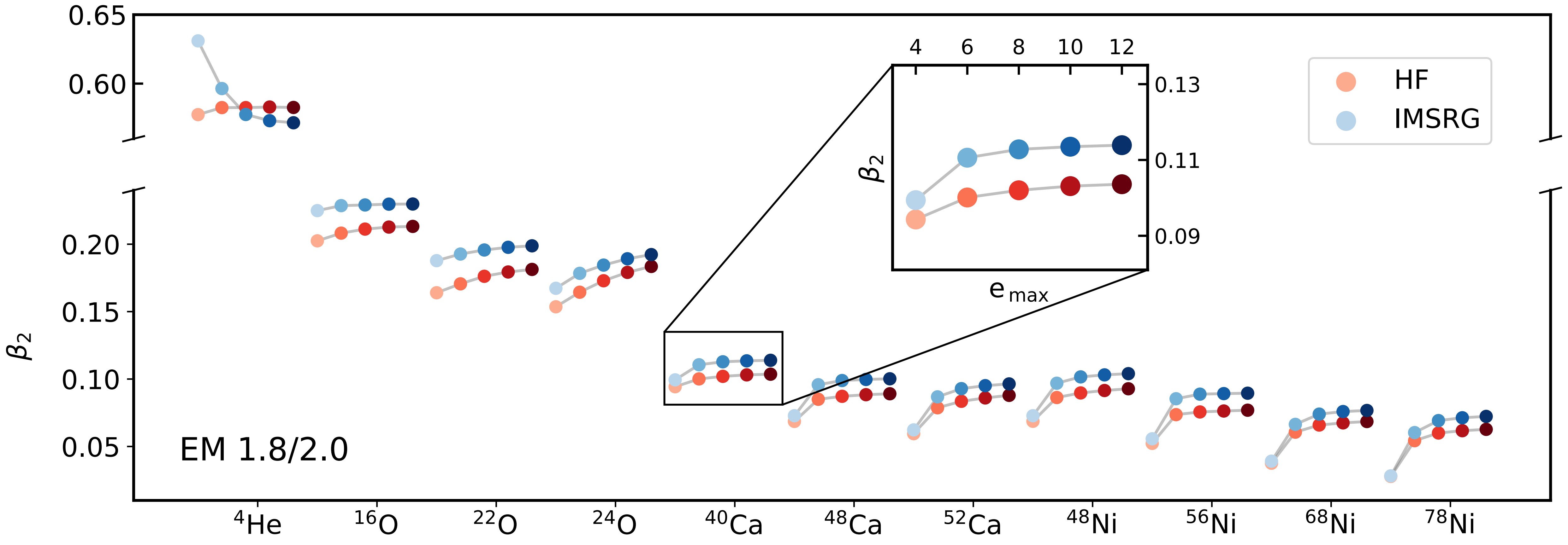
$$m_0(Q_2) = \langle Q_2 \cdot Q_2 \rangle$$

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]

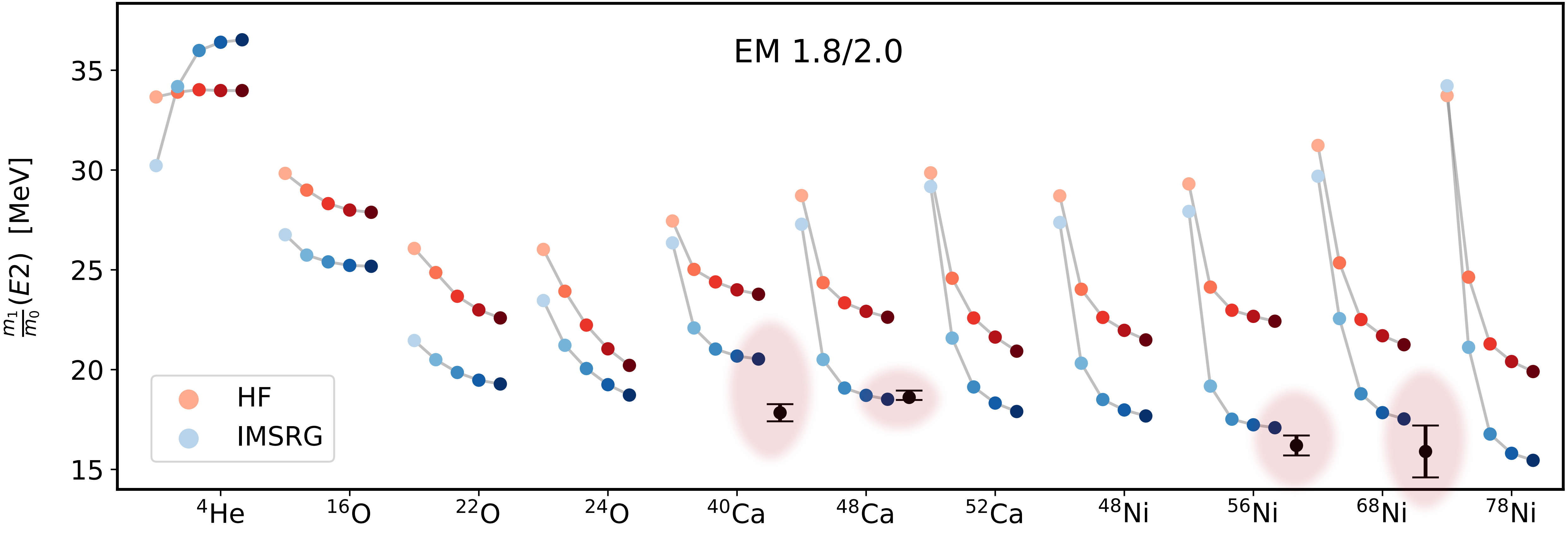


Quadrupole focus II: GQR centroid

Centroid of the quadrupole strength

$$\bar{E}(Q_2) \equiv \frac{m_1(Q_2)}{m_0(Q_2)}$$

IMSRG(2) GQR study across the nuclear chart



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Fragmenting the strength

Generalisation of the moment operators

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

Improving the previous description coupling several modes

Physical interpretation

Perturbation Q_α Response → Response Q_β Perturbation

Family of centroids

$$\bar{E}(Q) \equiv \frac{m_1(Q)}{m_0(Q)}$$

$$E_k(Q) \equiv \sqrt{\frac{m_k(Q)}{m_{k-2}(Q)}}$$

Family of equations

$$[\mathcal{M}_{1,\,\alpha\beta} - \omega_\nu \mathcal{M}_{0,\,\alpha\beta}] f_\nu^\beta = 0$$

$$[\mathcal{M}_{k,\,\alpha\beta} - \omega_\nu^2 \mathcal{M}_{k-2,\,\alpha\beta}] f_\nu^\beta = 0$$

Variation in the subspace

$$\delta Q \in \{Q_\alpha,\ \alpha = 1, \ldots, N\}$$

Optimal superposition

$$Q_\nu = f_\nu^\alpha Q_\alpha$$

Generalised eigenvalue problem

(GCM-like equation but in an operator space)

The sum rules used as input are satisfied by construction

i.e.: if IMSRG(2) is used, then m_0 and m_1 are IMSRG(2) exact

K=3 returns the RPA equations (local RPA)

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

Implementation details

- Moment operators implemented within the imsrg++ code [github.com/ragnarstroberg/imsrg]
- J-scheme expressions of moments 0 and 1 from [Lu and Johnson, PRC 97 (2018) 3, 034330]
- Benchmarked vs QFAM code [Beaujeault-Taudière, Frosini et al., PRC 107 (2023), L021302]
- Operator space explored in present calculations

$$Q_\alpha \in \{r^{\lambda+\ell}Y_{\lambda\mu},\ \ell = 0, 2, 4, 6, 8, 10;\ j_\lambda(qr)Y_{\lambda\mu}, q \in [q_{\min}, q_{\max}]\,\}$$

Long-wavelength limit $r^\lambda Y_{\lambda\mu}$ describes pure surface vibrations

$\ell \neq 0$ Introduces local compressions (volume)

Spherical Bessel functions: higher volume modes

K=0 equation implemented

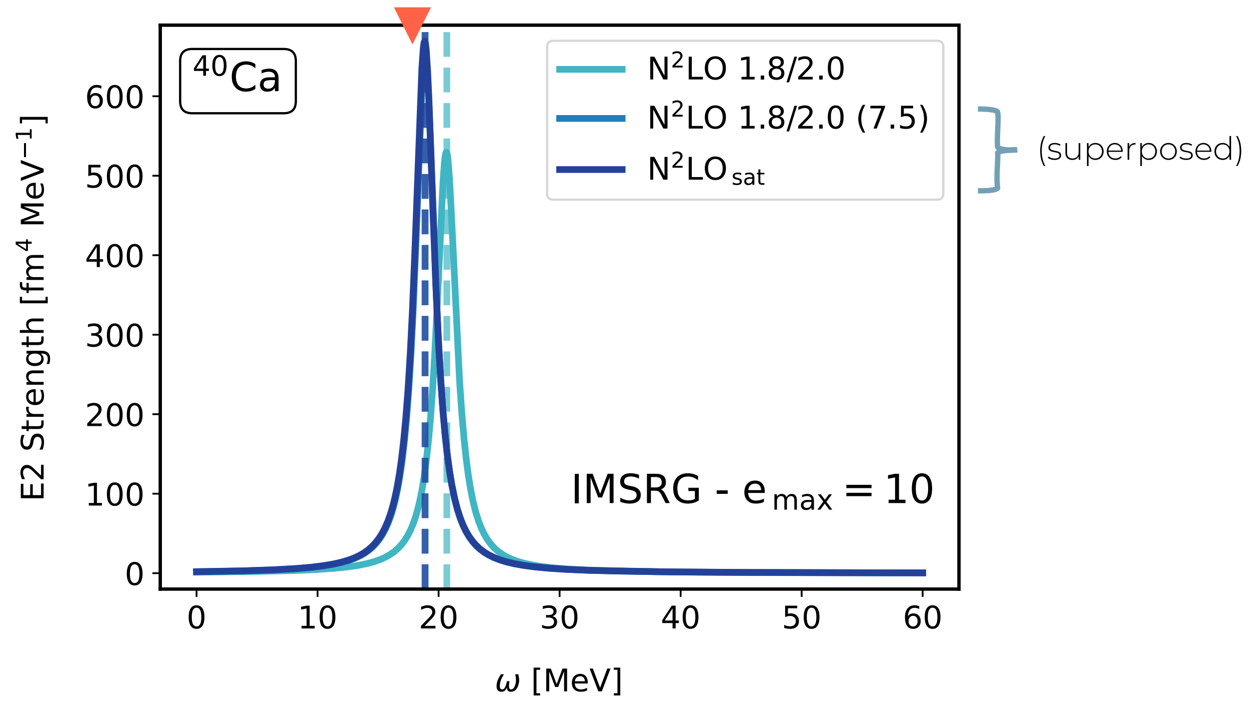
$$[\mathcal{M}_{1,\,\alpha\beta} - \omega_\nu \mathcal{M}_{0,\,\alpha\beta}]f_\nu^\beta = 0$$

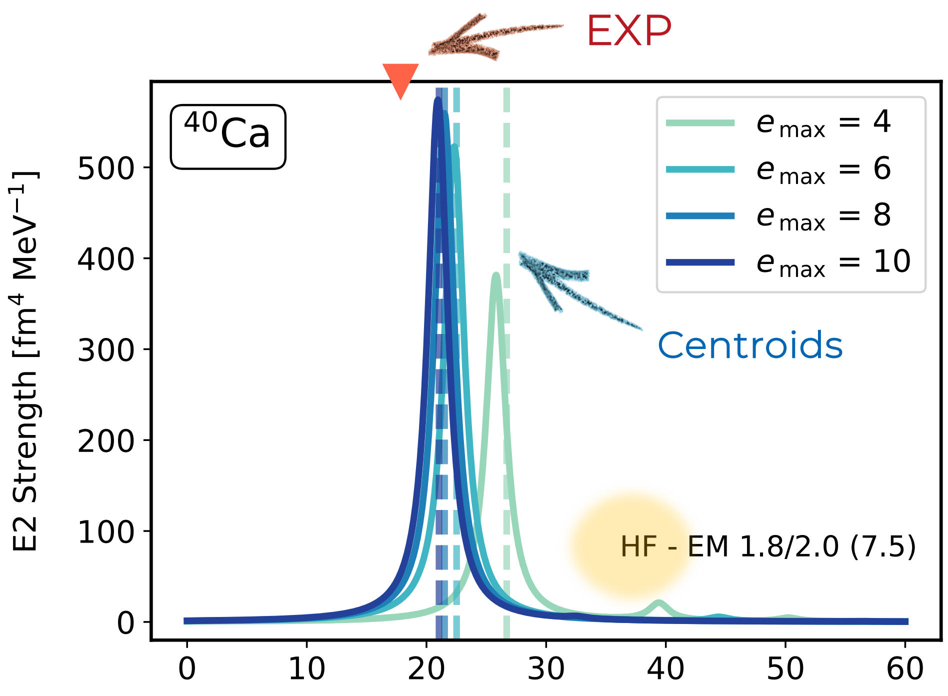
$$M_1(Q_\alpha, Q_\beta) = \frac{1}{2}[Q_\alpha^\dagger, [H, Q_\beta]]$$

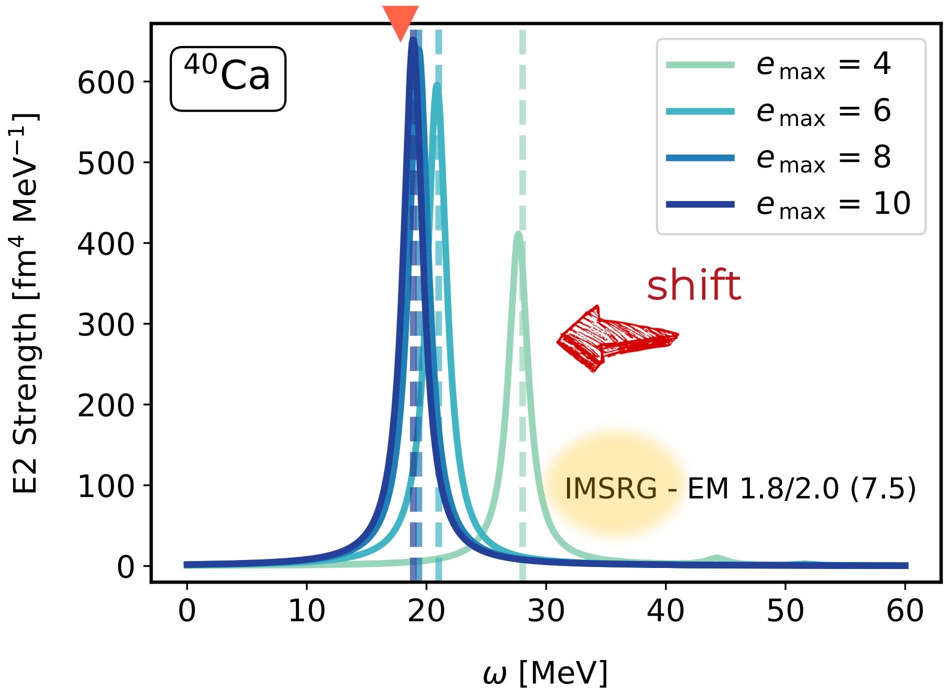
$$M_0(Q_\alpha, Q_\beta) = Q_\alpha^\dagger Q_\beta$$

Results - Quadrupole

- Important energy shift due to correlation
- Little fragmentation
- Negligible energy shift due to modes coupling
- Good e_{max} convergence $\hbar\omega = 16$ MeV $e_{3\,max} = 24$
- Interaction comparison

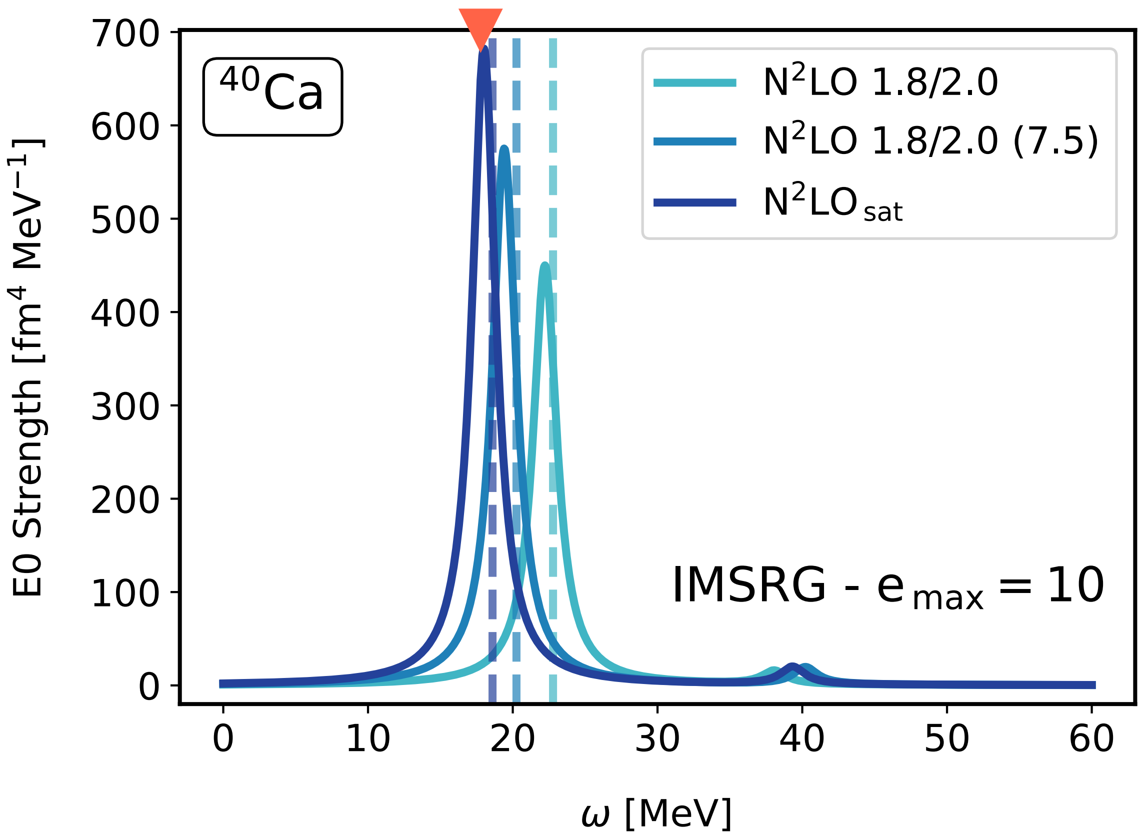






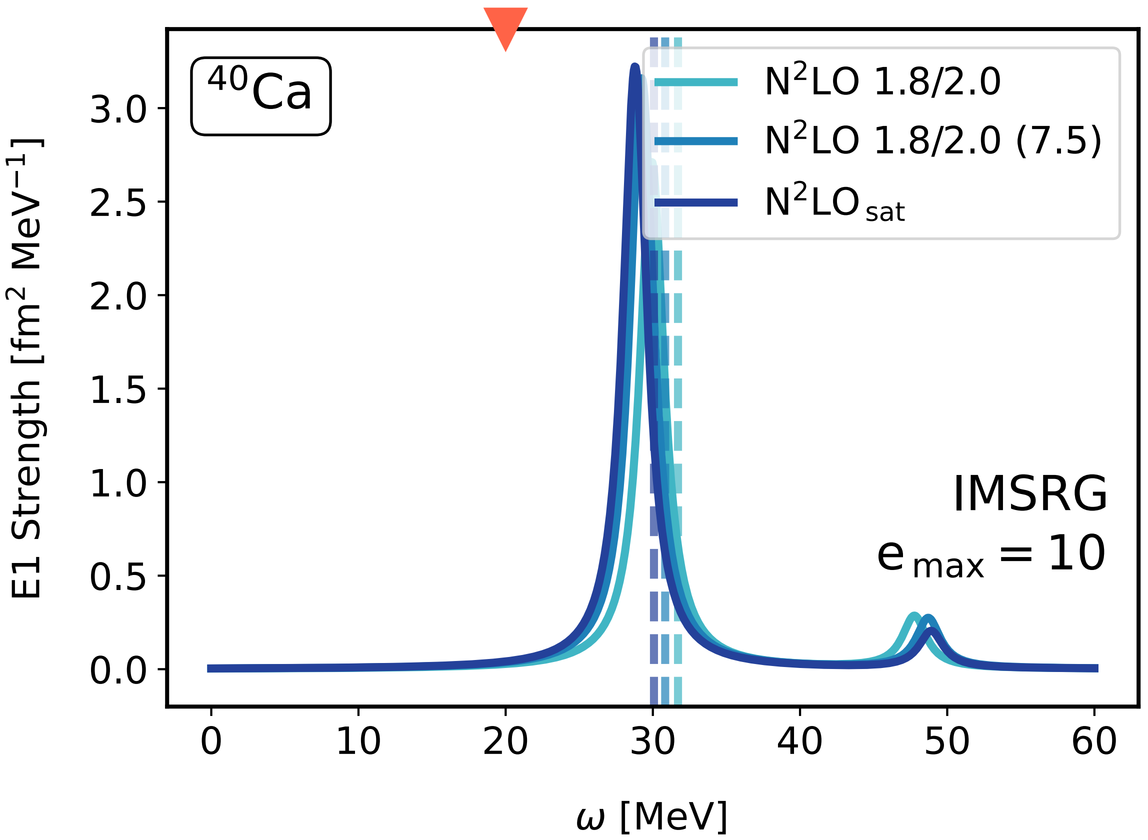
[Arthuis et al., arXiv:2401.06675v1]

Monopole



- Larger energy shift (~1 MeV) due to modes coupling
- Interaction dependence
- Nice agreement with experimental data

Dipole



- IMSRG shift towards too high energy
- Centre of Mass contaminants ?

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General considerations

- Useful to quantify the impact of dynamical correlation (many-body uncertainty)
- Little fragmentation in this frame
- The energy shift of the main resonance depends on the multipolarity

Open questions (among others)

- Where does this stand in a hierarchy of IMSRG-based approximations ? (TDA, 2ndTDA, EOM...)
- How to further enrich the operator space ?
- What's wrong with the dipole ? (also problematic in CC-LIT and IMSRG-...TDA)

Perspectives

- Focus on other systems and integration with VS-IMSRG for open-shell systems
- Enlarge the operator space
- Comparison to existing methods

Thank you for the attention

Robert Roth
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Jean-Paul Ebran
Mikael Frosini
Vittorio Somà

Francesca Bonaiti

Sonia Bacca

Backup slides

Dielectric theorem in the IMSRG

Add small perturbation to H

$$H(\lambda) = H + \lambda Q$$

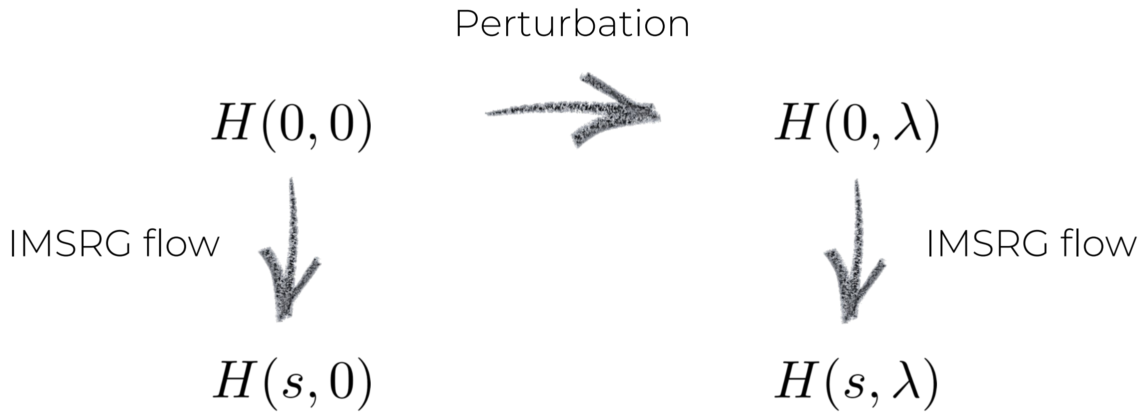
$$H(\lambda)\,|\Psi(\lambda)\rangle = E(\lambda)\,|\Psi(\lambda)\rangle$$

$$\begin{aligned} m_{-1}(Q) &= \sum_\nu \frac{|\langle \Psi_\nu | Q | \Psi_0 \rangle|^2}{E_\nu - E_0} \\ &= -\frac{1}{2}\left[\frac{\partial \langle \Psi(\lambda)|Q|\Psi(\lambda)\rangle}{\partial \lambda}\right]_{\lambda=0} \\ &= \frac{1}{2}\left[\frac{\partial^2 \langle \Psi(\lambda)|H|\Psi(\lambda)\rangle}{\partial \lambda^2}\right]_{\lambda=0} \end{aligned}$$

Numerically easier

Steps

- Solve the perutbed problem for HF
- Then evolve with the IMSRG
- Repeat for several lambdas and take the derivative

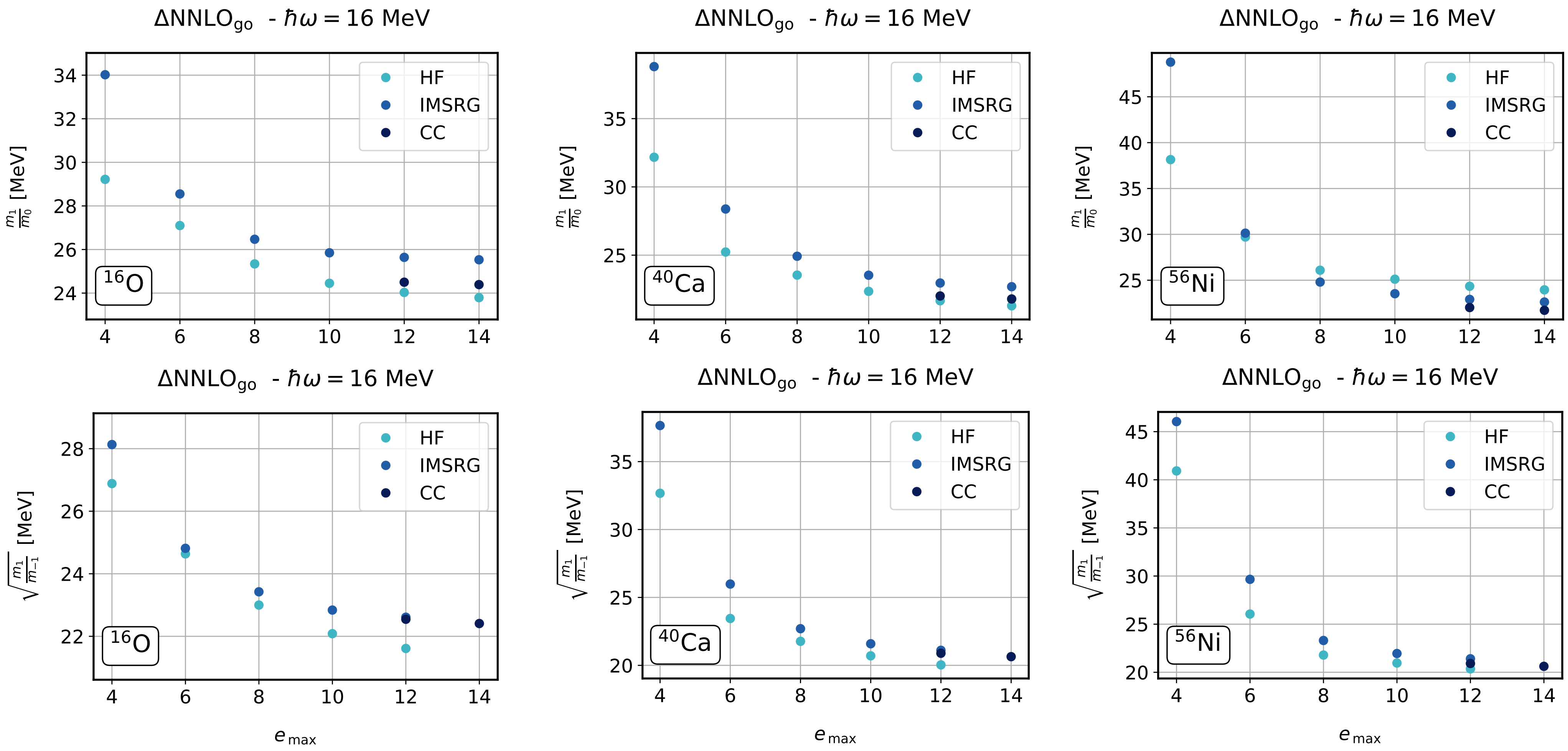


Disclaimer: only scalar perturbations

Results – Monopole resonance

Objective: characterise systematically impact of dynamical correlations

Comparison to CC-LIT



Comments

- Better agreement (CC – IMSRG) for low energy part of the spectrum
- CC sum rules are. Given by the sum over the excited states, more difficult to converge
- Too small 3-body basis here (needed for CC comparison)
- Experimental values are anyway smaller
- No interactions comparison performed

Different approaches

I. Centroid method

$$[\mathcal{M}_{1,\,\alpha\beta} - \omega_\nu \mathcal{M}_{0,\,\alpha\beta}] f_\nu^\beta = 0$$

The sum rules used as input are satisfied by construction

i.e.: if IMSRG(2) is used, then m_0 and m_1 are IMSRG(2) exact

$$M_1(Q_\alpha, Q_\beta) = \frac{1}{2}[Q_\alpha^\dagger, [H, Q_\beta]]$$

$$M_0(Q_\alpha, Q_\beta) = Q_\alpha^\dagger Q_\beta$$

Exact up to two-body

Fragmentation due to coupling

II. Scaling method

$$[\tilde{\mathcal{M}}_{3,\,\alpha\beta} - \omega_\nu^2 \tilde{\mathcal{M}}_{1,\,\alpha\beta}] f_\nu^\beta = 0$$

$$\tilde{M}_{3,\,\alpha\beta} \propto \frac{1}{2}[P_\alpha^\dagger, [H, P_\beta]]$$

$$\tilde{M}_{1,\,\alpha\beta} \propto \frac{1}{2}[Q_\alpha^\dagger, [T, Q_\beta]]$$

The exact implementation is a **four-body** operator !

Assume instead (true for most EDF, not for chiral interactions)

$$[H, Q(\vec{r})] = [T, Q(\vec{r})]$$

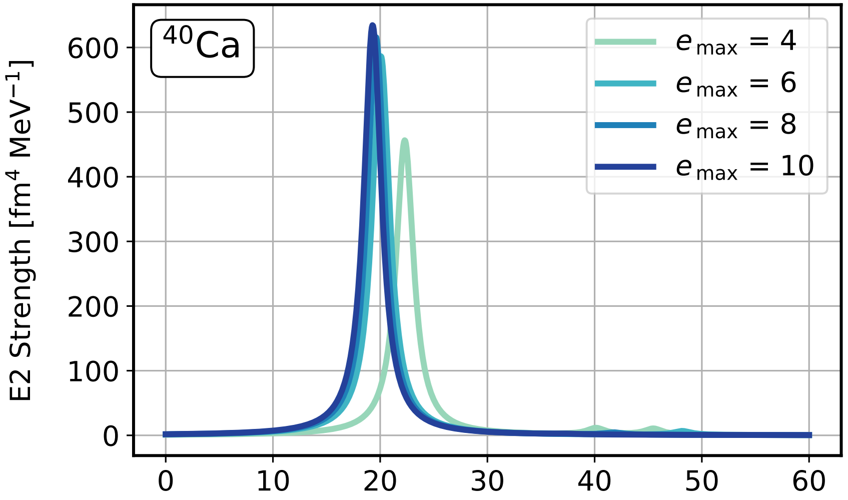
$$P_\alpha = \frac{i}{\hbar} M_\alpha [T, Q_\alpha]$$ generates a collective path

$$|\Phi(\eta)\rangle = e^{-\frac{i}{\hbar}\eta P_\alpha} |\Phi(0)\rangle$$

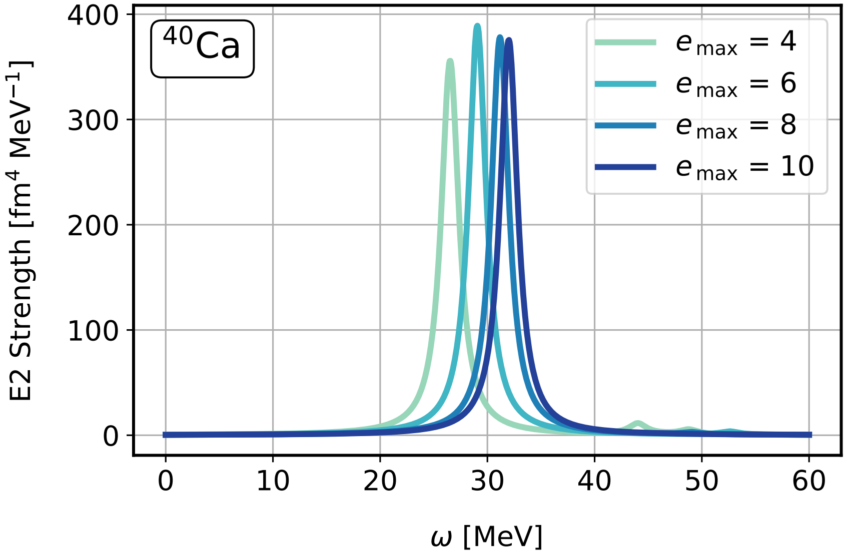
[Tanimura, Lacroix, Scamps, PRC 92 (2015), 034601]

Results – Scaling method

Scaling method HF - EM 1.8/2.0 (7.5)



Scaling method IMSRG - EM 1.8/2.0 (7.5)

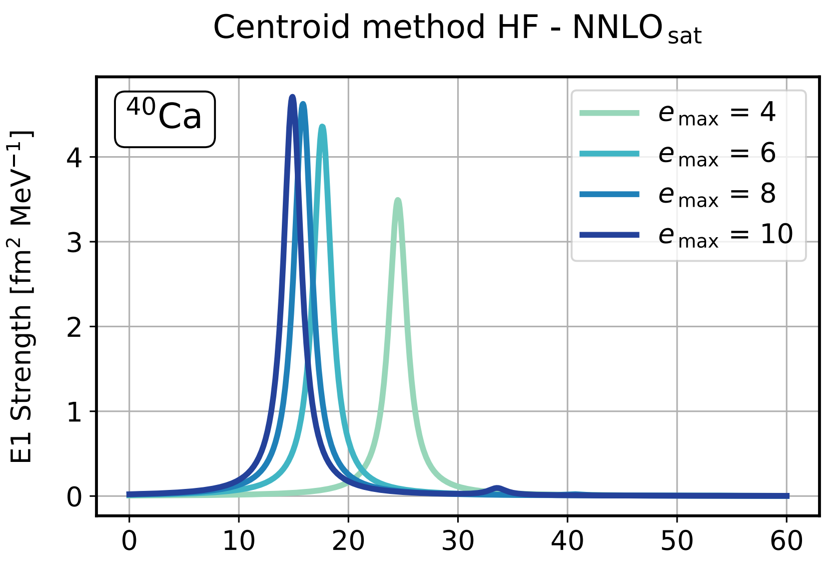


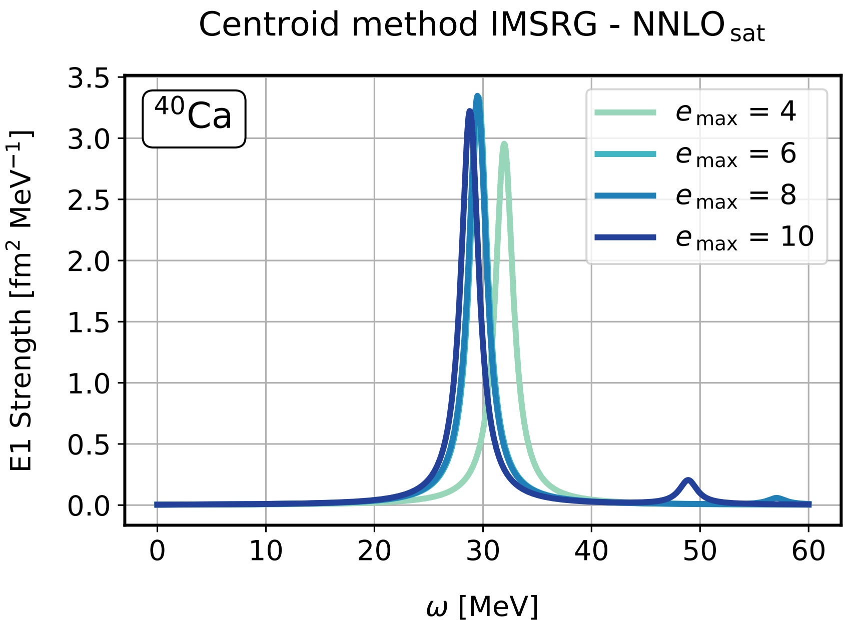
Comparison to RPA needed (soon)

BUT

The “deformation” picture doesn’t work well with the IMSRG

Results – Broken dipole





- For some reason, the dipole behaves differently
- Shift towards too high energy
- Also problematic in other methods (IMSRG-...TDA, CC-LIT)
- On the other hand, simple RPA seems to do great

What are we missing ?

- Limited operator space ?
- Interaction ?
- IMSRG flow ?
- Centre of Mass contaminants ?