Impact of ground-state correlations on the nuclear response

ECT* workshop
Next generation *ab initio* nuclear theory

Trento, July 16th, 2025

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TECHNISCHE UNIVERSITÄT DARMSTADT

DFG

SFB 1245

EMMI

Outline

Introduction

- Physics case
- Existing ab initio methods

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IMSRG multipole moments

- Moments of the strength
- IMSRG implementation
- Model-space convergence

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- Comparison to experiment
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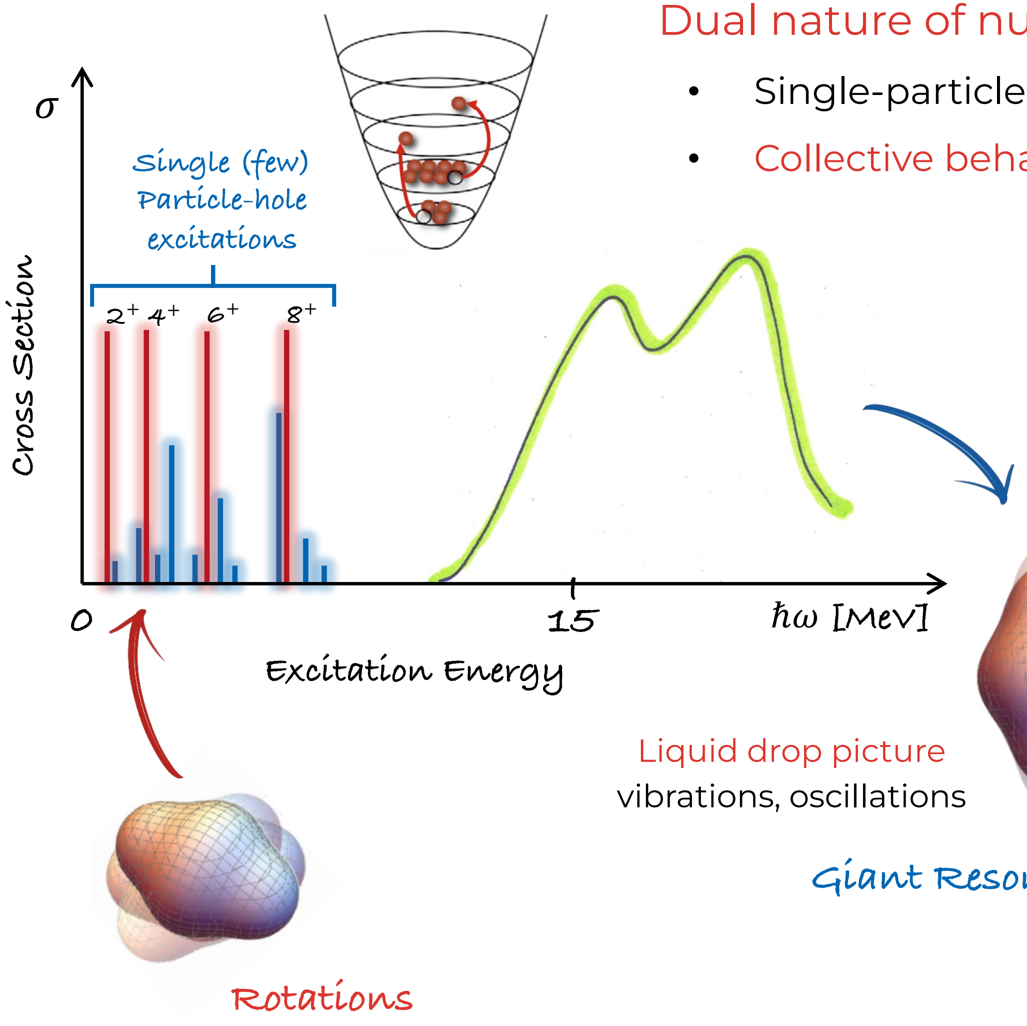
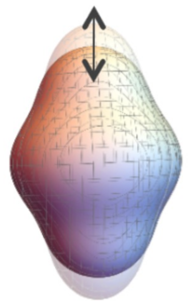
Nuclear spectroscopy



Dual nature of nucleus

- Single-particle features
- Collective behaviour



Liquid drop picture
vibrations, oscillations

Giant Resonances

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

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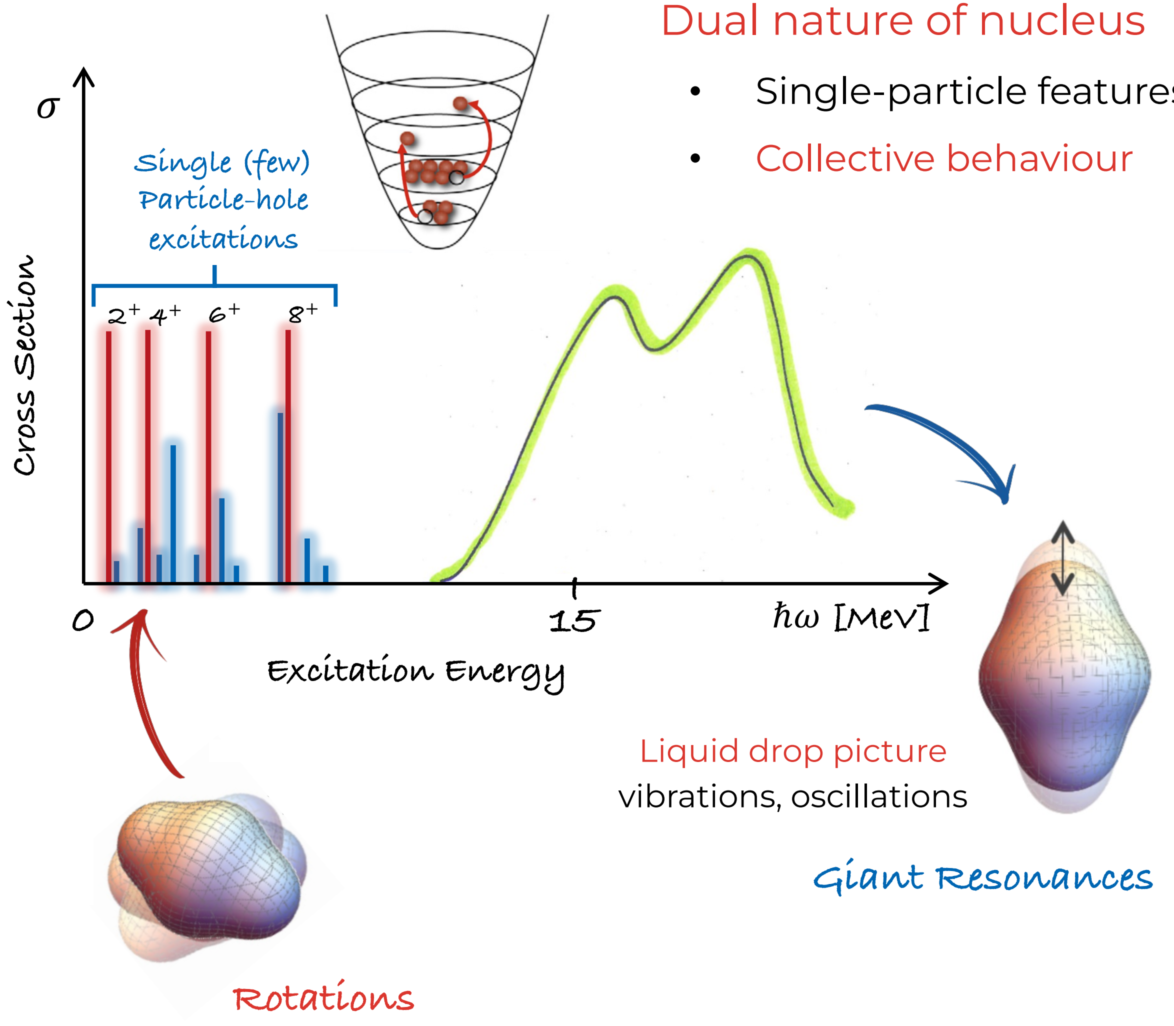

Response function

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

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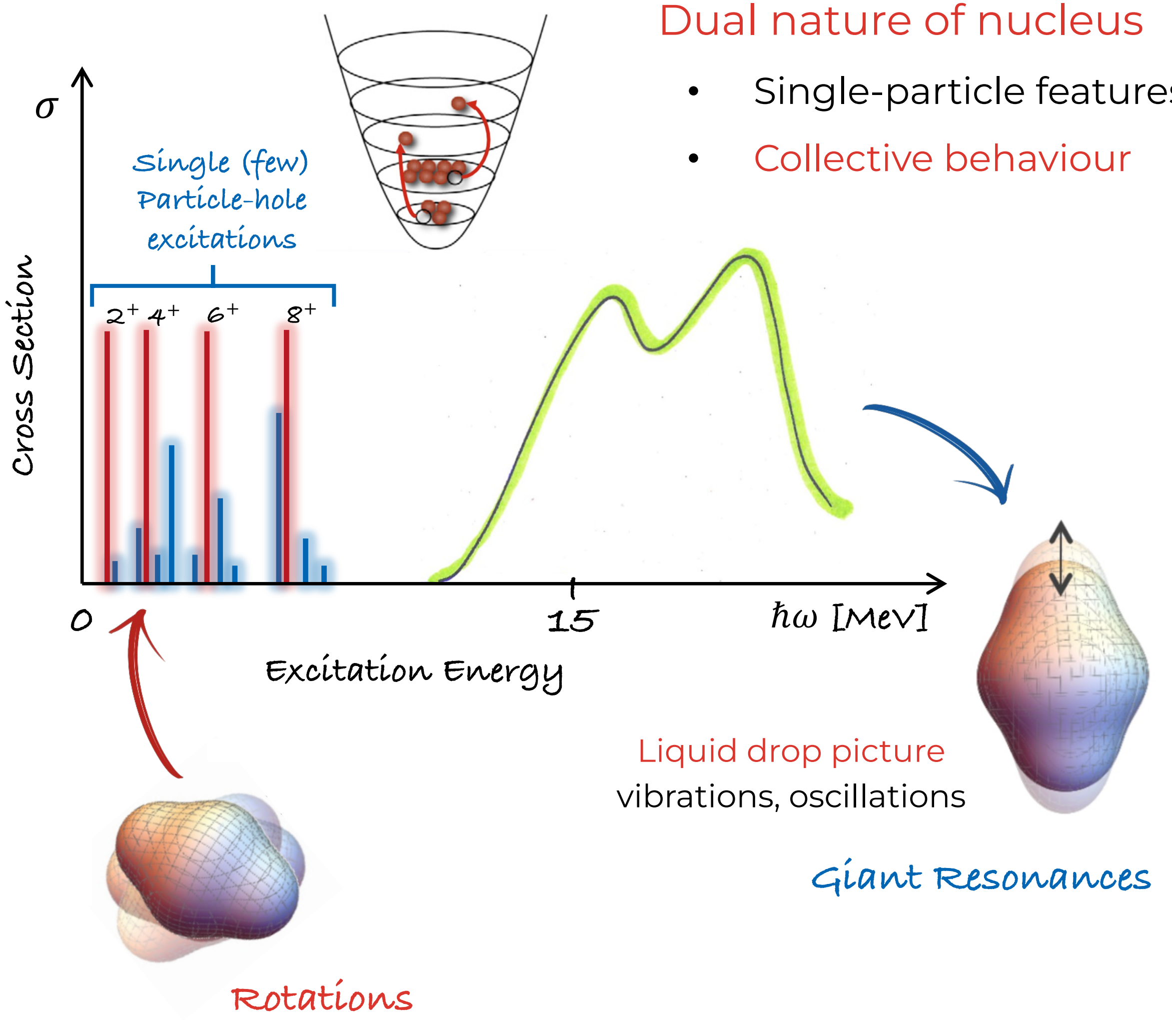

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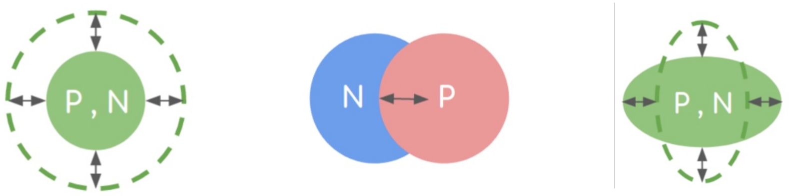

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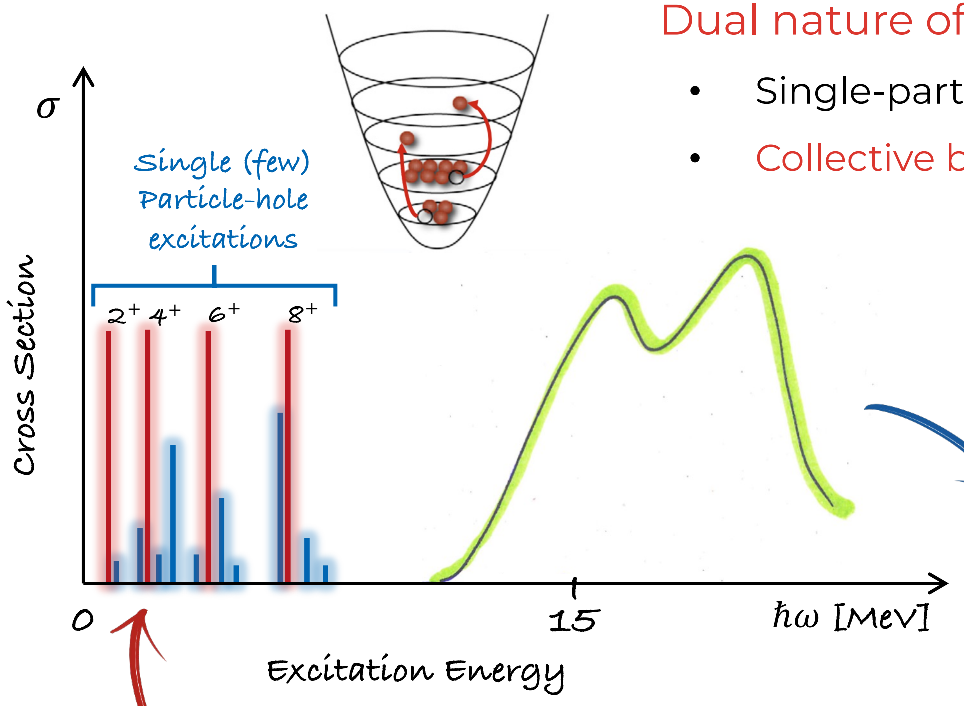

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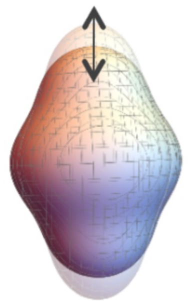

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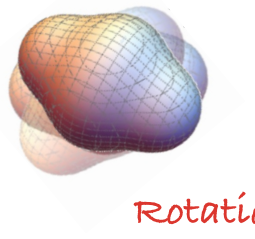

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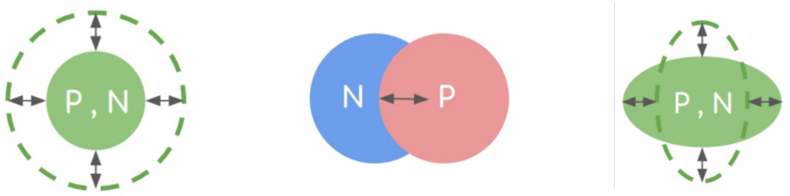

Different excitations

Different methods

Established techniques*

*Excluding virtually exact methods

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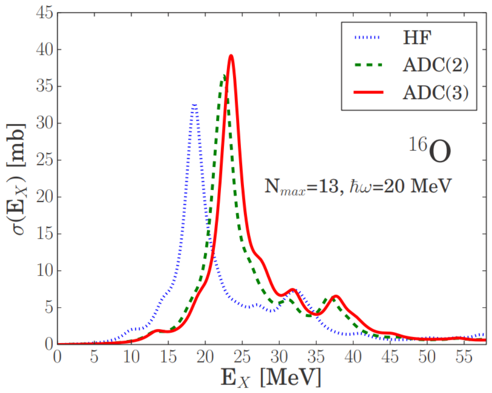
SC(G)GF

- Polarisation
- Low-lying states (neighbouring)



[Barbieri, Raimondi, PRC, 2019]

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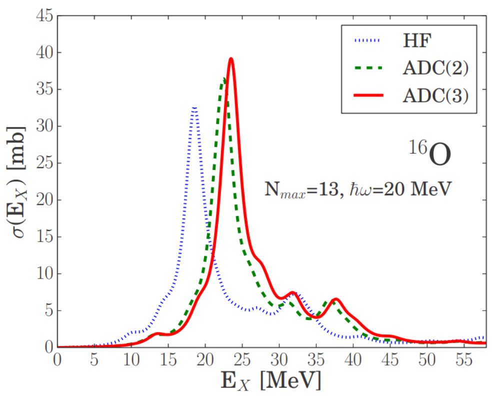

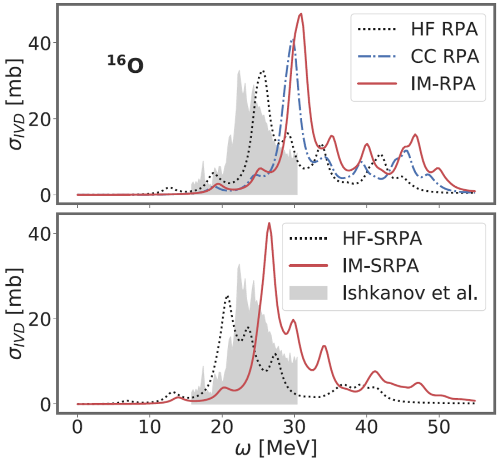

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- Continuum
- 2p2h complete

EOM-IMSRG

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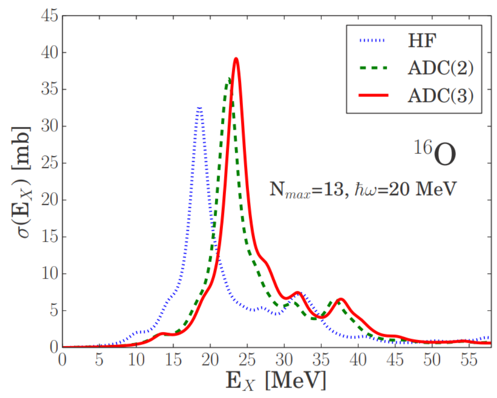

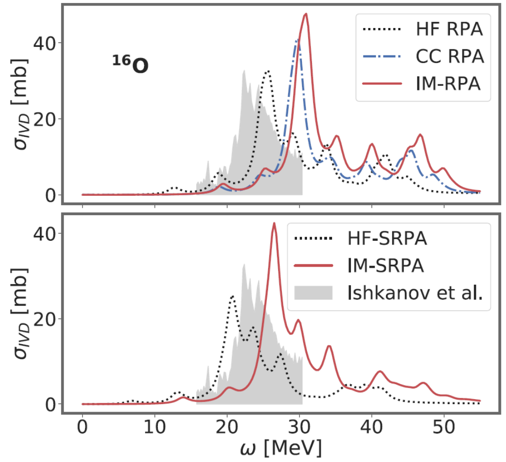

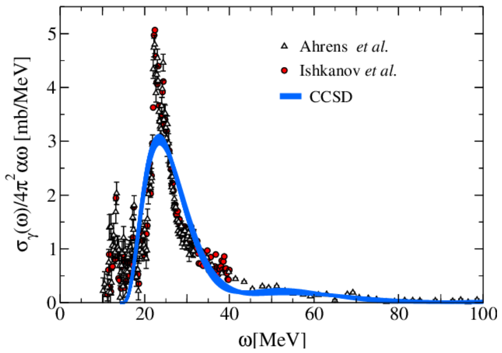

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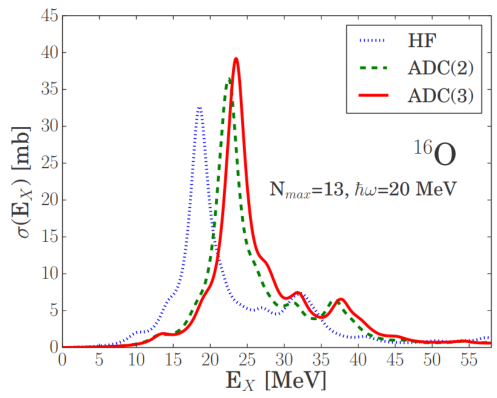
- Low-lying states



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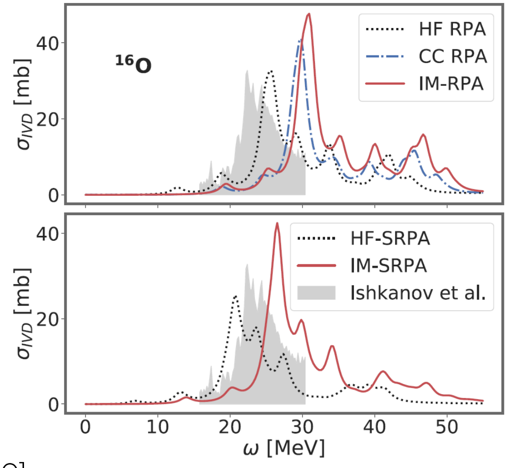

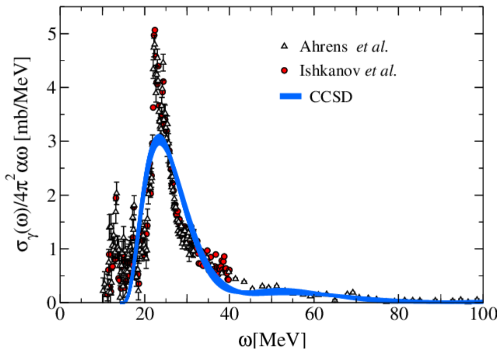

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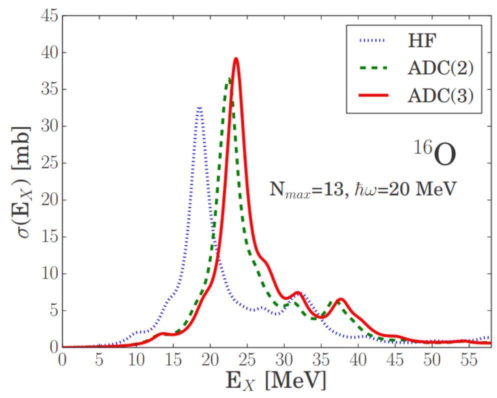

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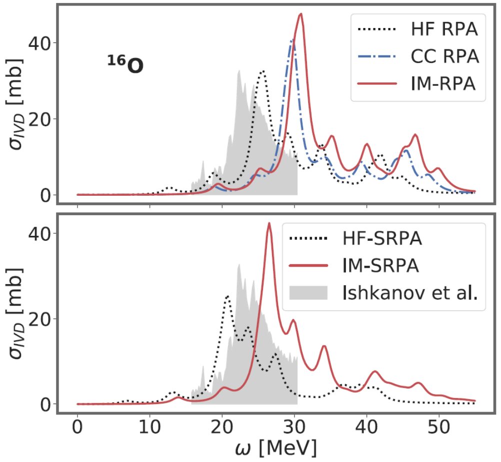

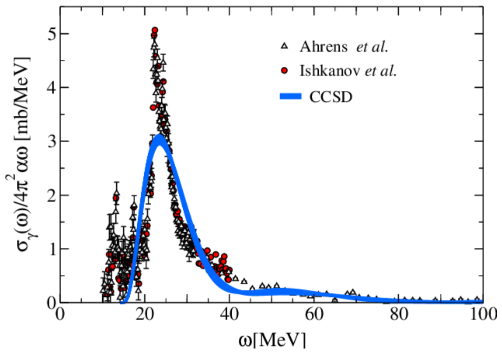

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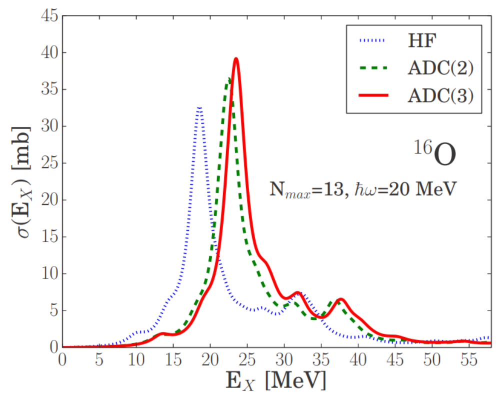

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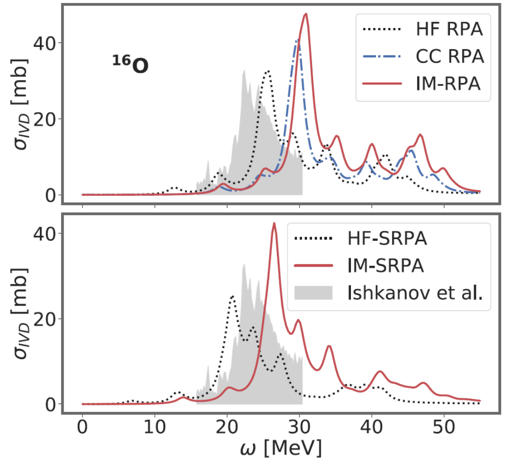

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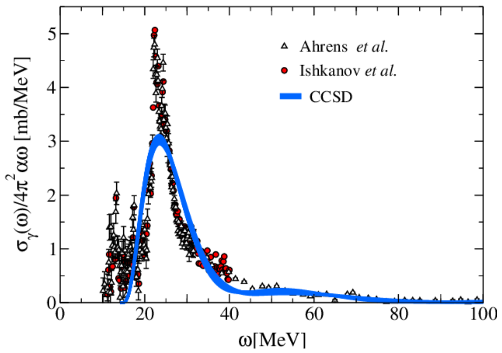

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How complete is the excited states description ?

Uncertainty quantification / benchmark

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Challenges and opportunities

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Studied quantity: multipole response

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Related moments

$$\begin{aligned} m_k(Q_\lambda) &\equiv \int_0^\infty E^k S(Q_\lambda, E) dE \\ &= \sum_{\mu\nu} (E_\nu - E_0)^k |\langle \Psi_\nu | Q_{\lambda\mu} | \Psi_0 \rangle|^2 \end{aligned}$$

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

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- 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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Exact implementation up to m_1

Effective two-body Hamiltonian

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

Spherical tensor operators

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

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Previous PGCM study

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

THE EUROPEAN PHYSICAL JOURNAL A

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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

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]

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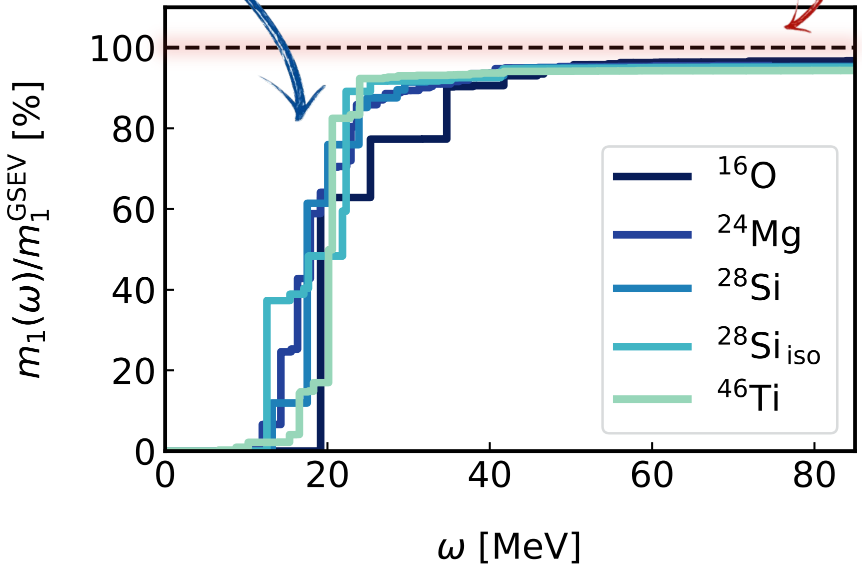

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6-7 % difference in PGCM

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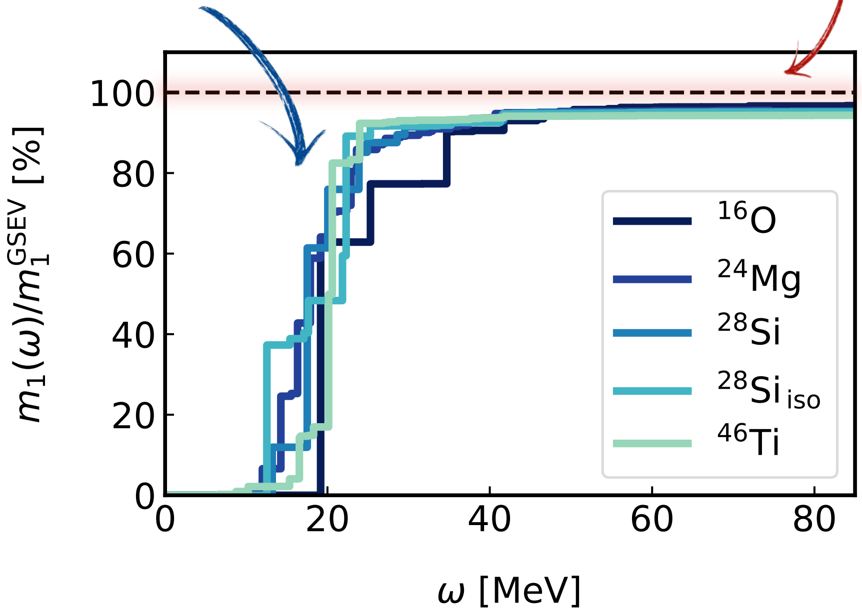

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Strategy in the IMSRG framework

Unitary transformation

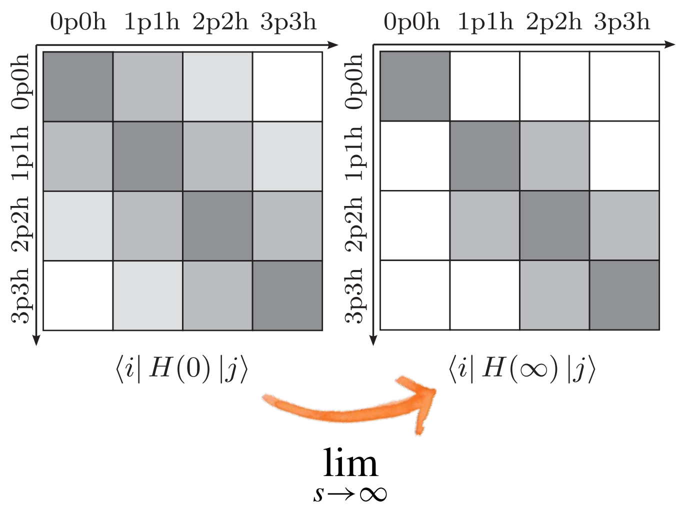
$$H(s) = U(s) H U^\dagger(s)$$
$$\equiv H^{\mathrm{d}}(s) + H^{\mathrm{od}} \rightarrow H^{\mathrm{d}}(\infty)$$

Diagonal

Off-diagonal

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

Slater determinant



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Strategy in the IMSRG framework

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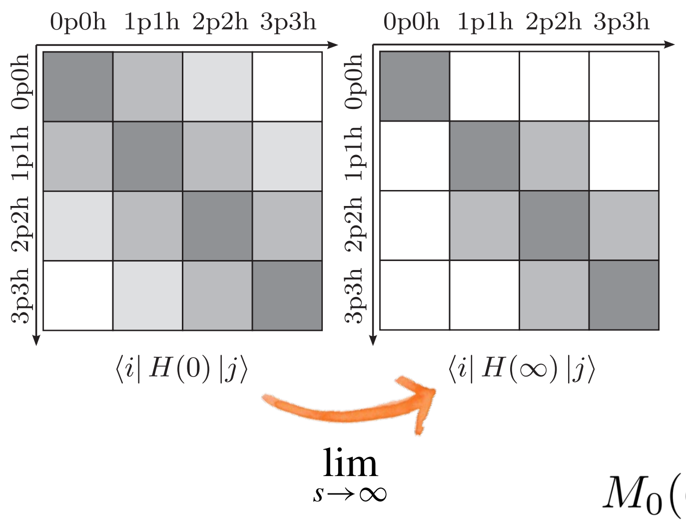

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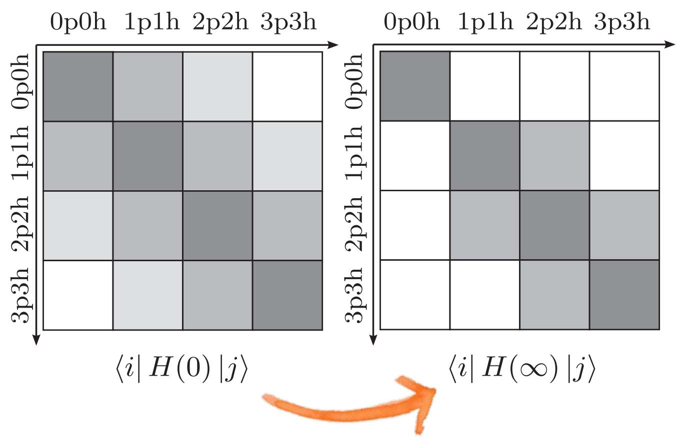

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J-scheme expressions of m_0 and m_1

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

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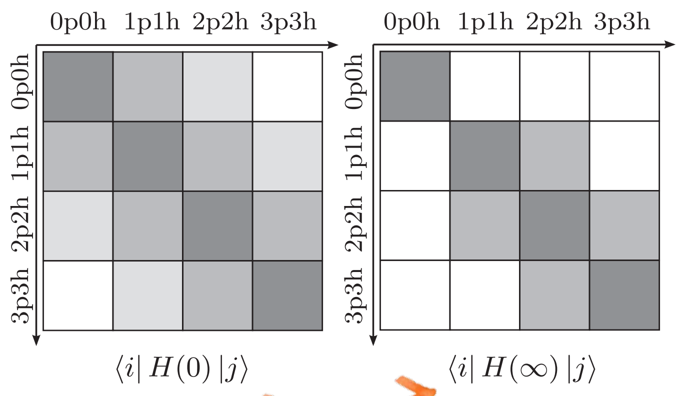

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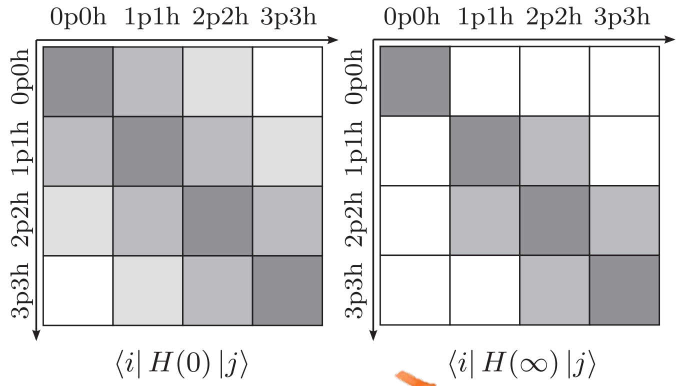

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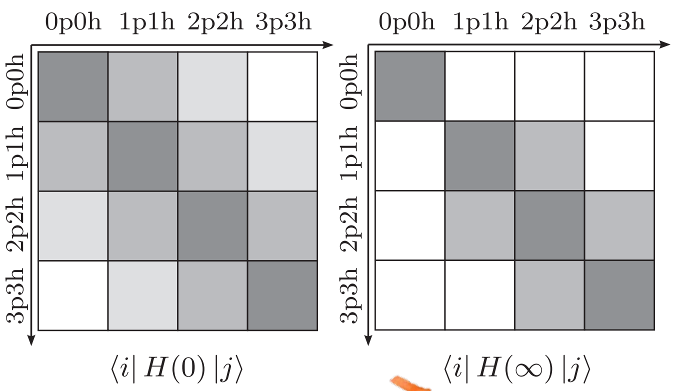

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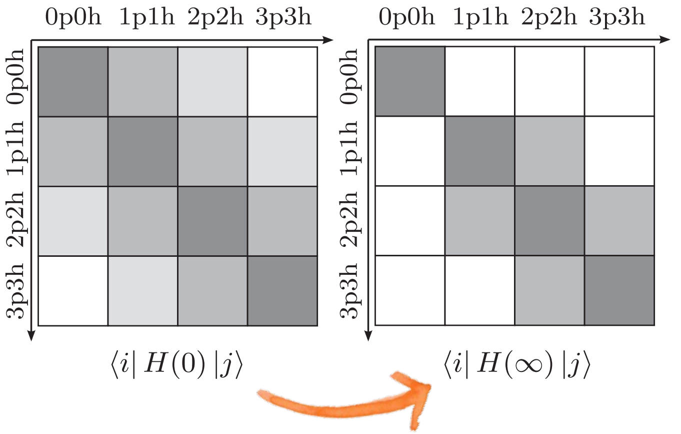

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Benchmarks

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

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[github.com/ragnarstroberg/imsrg]

Model-space convergence

Dipole response

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

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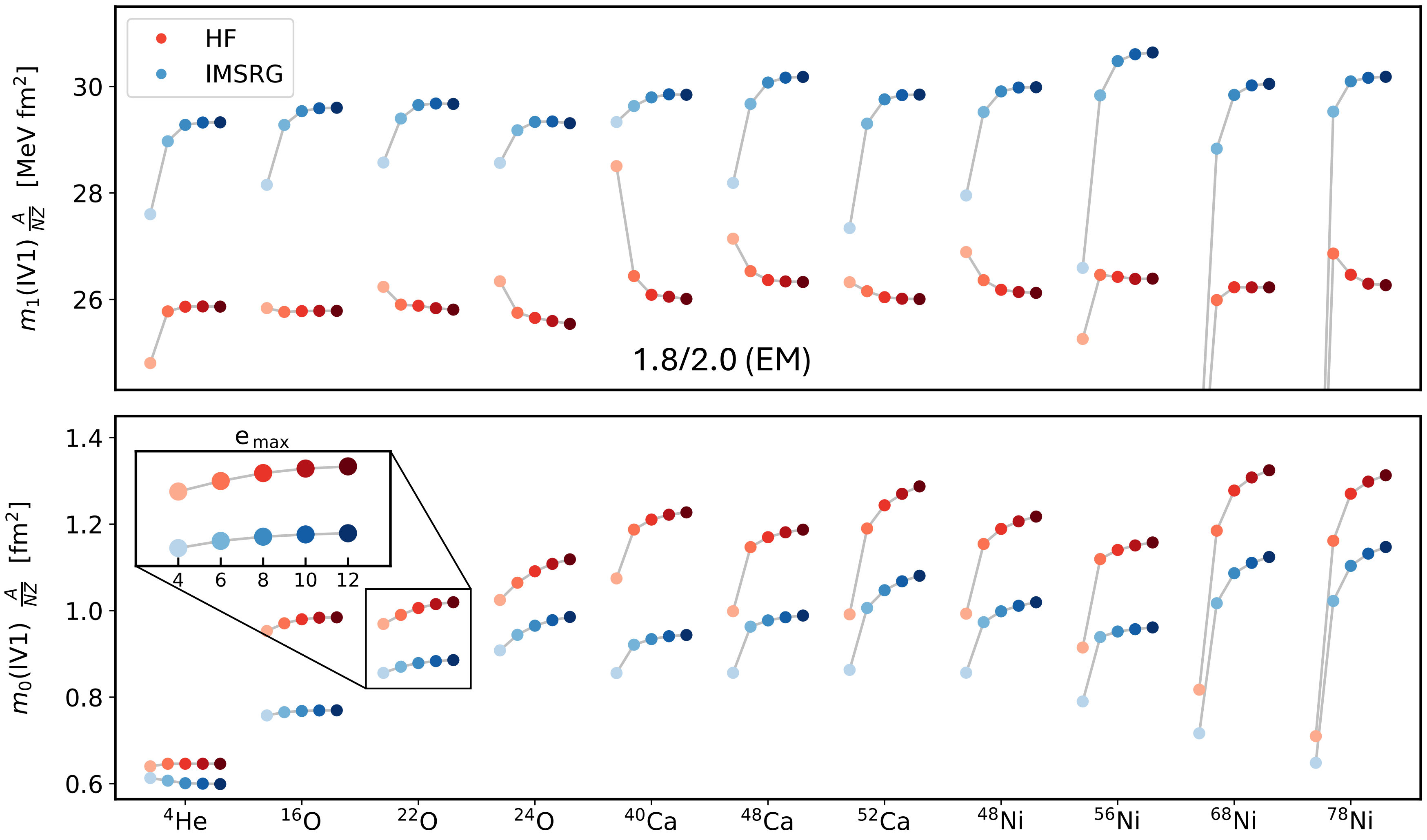

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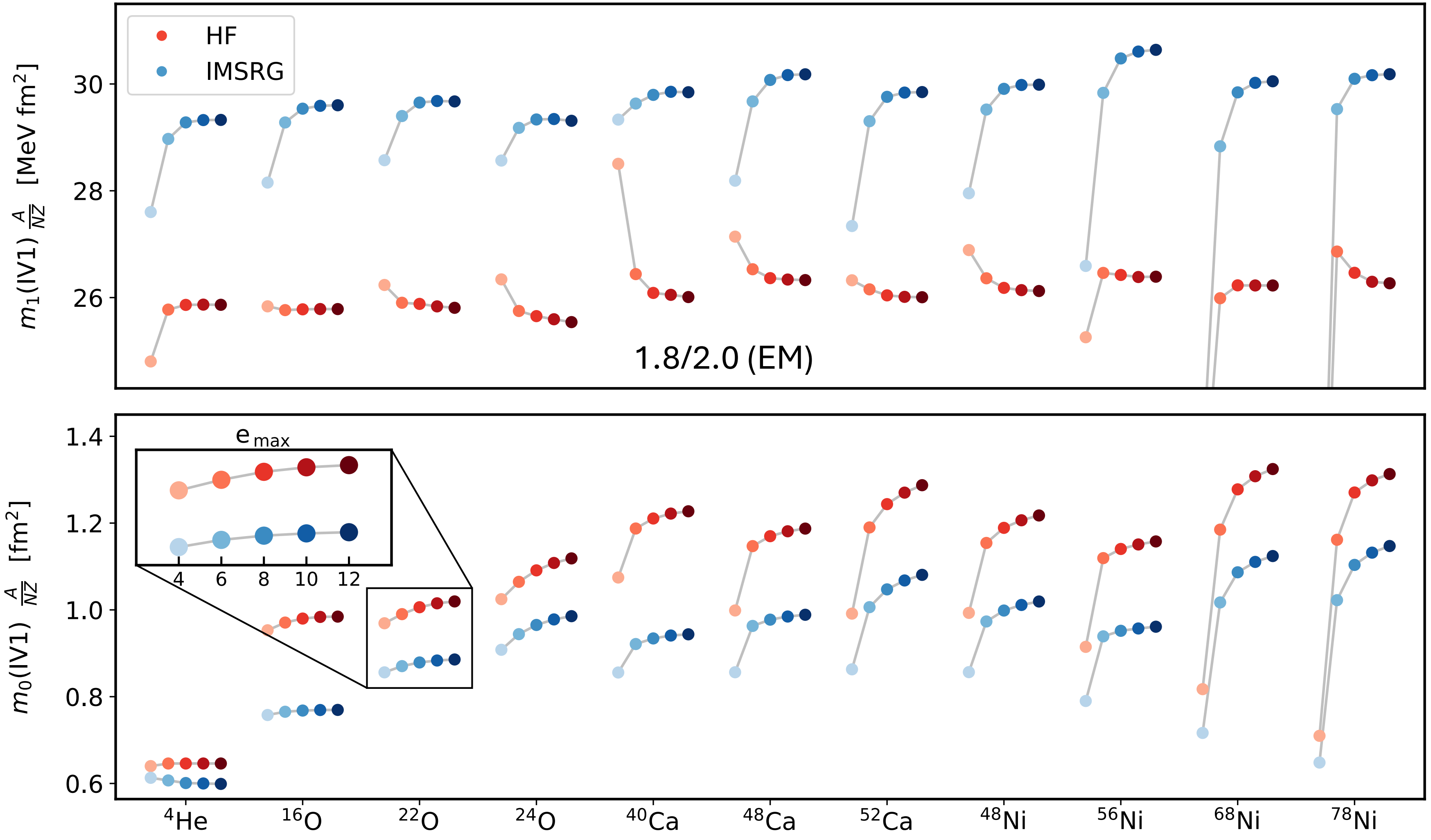
- Large correlation impact
- Relative difference ~0.2%
- Similar error for $\hbar\omega$ variations



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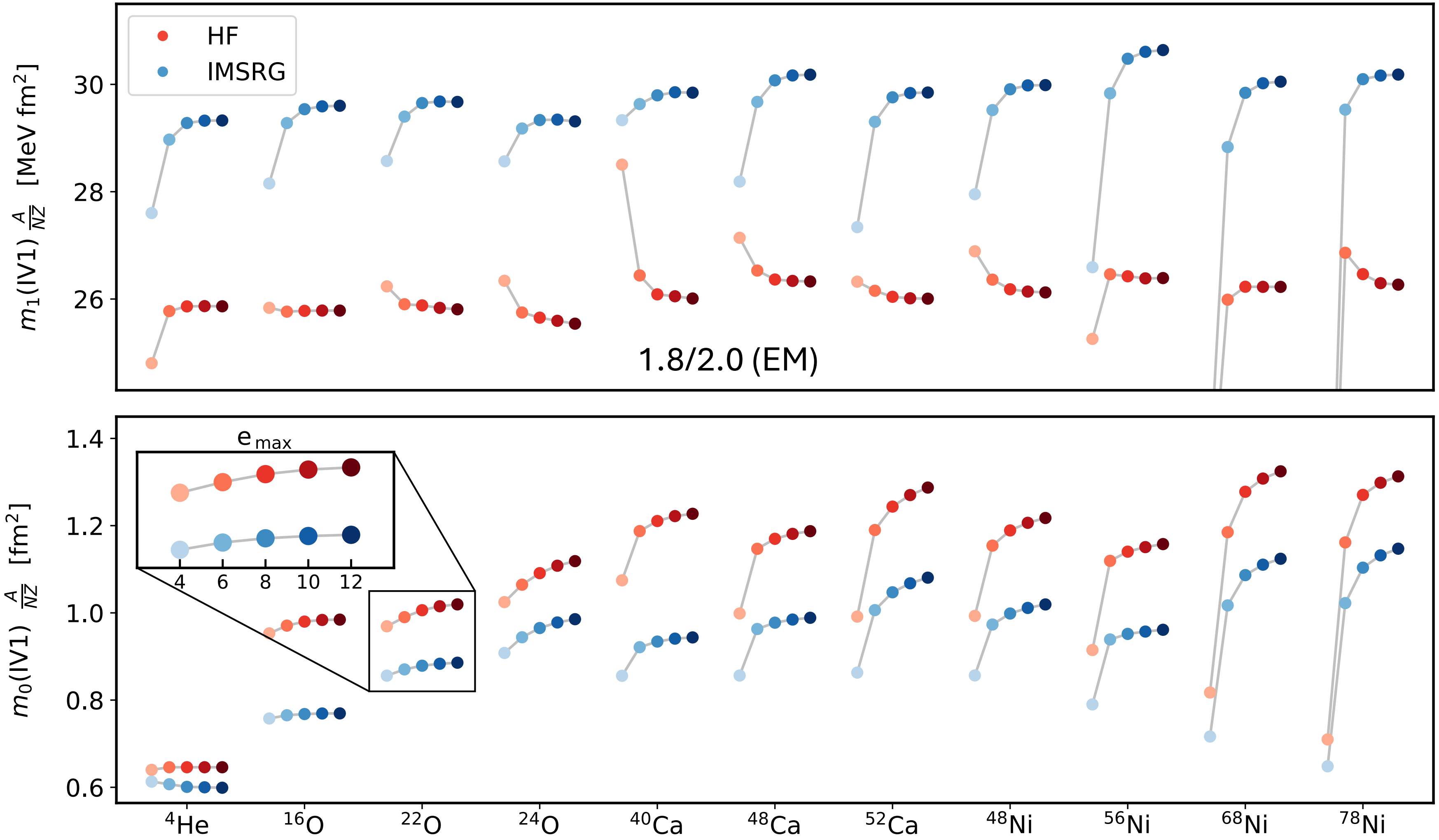
$$M_0(Q_\lambda) \equiv \sum_\mu (-1)^\mu Q_{\lambda,-\mu} Q_{\lambda\mu}$$

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



Introduction

- Physics case
- Existing ab initio methods

IMSRG multipole moments

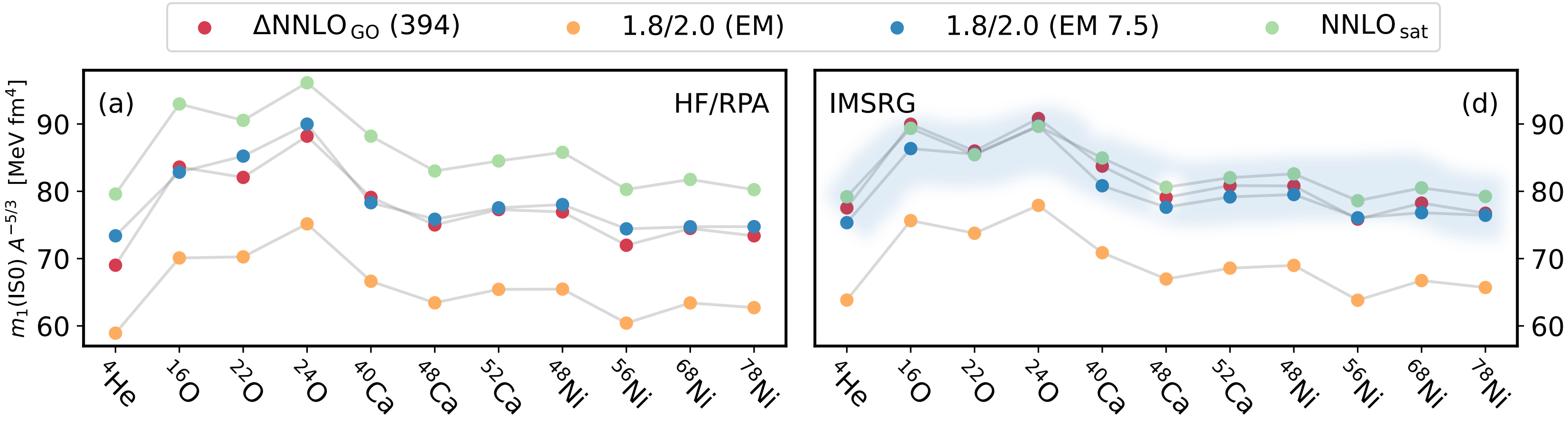
- Moments of the strength
- IMSRG implementation
- Model-space convergence

Numerical results

- Interaction sensitivity
- Comparison to experiment
- Comparison to sum rules

Challenges and opportunities

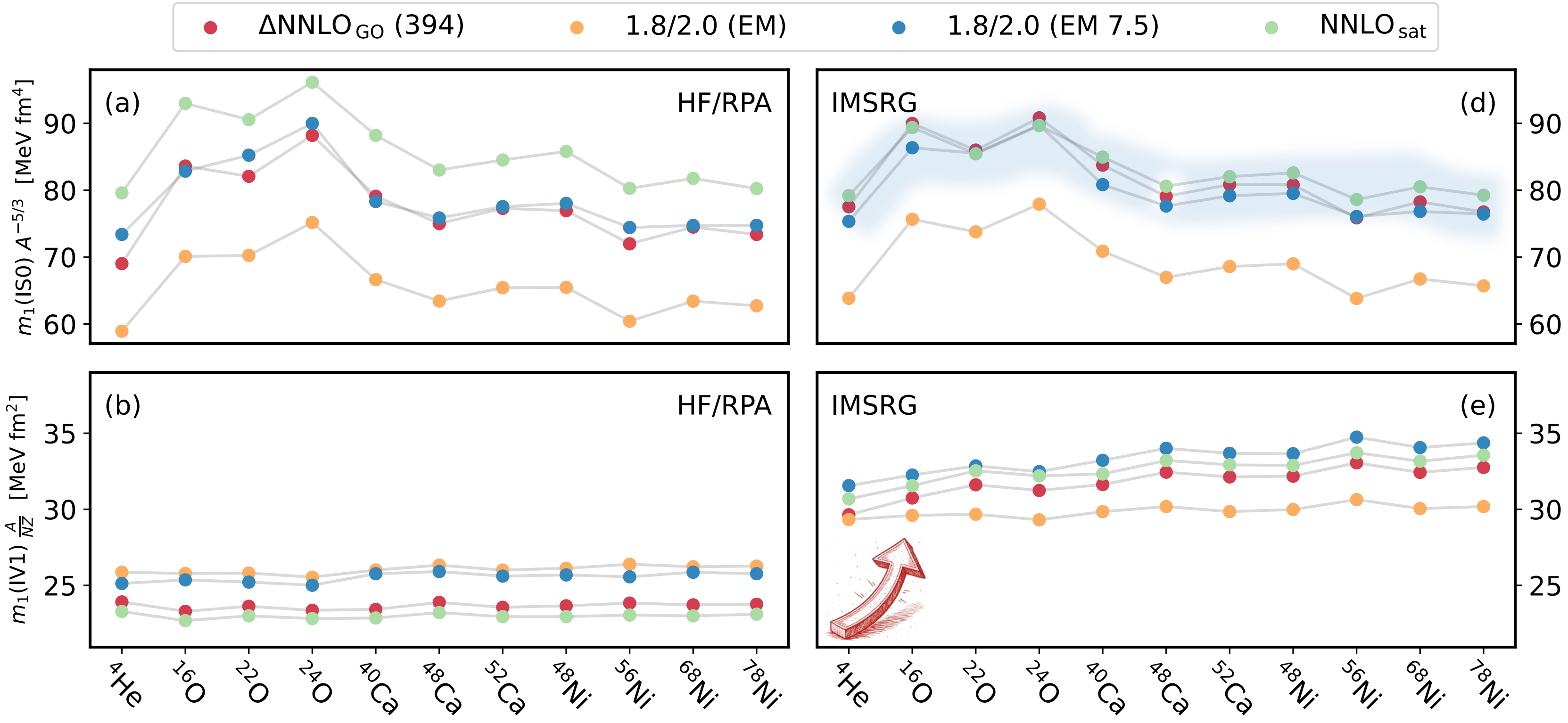
Interaction sensitivity



Monopole

- Reduced spread
- ~5% correlations effect

Interaction sensitivity



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Dipole

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

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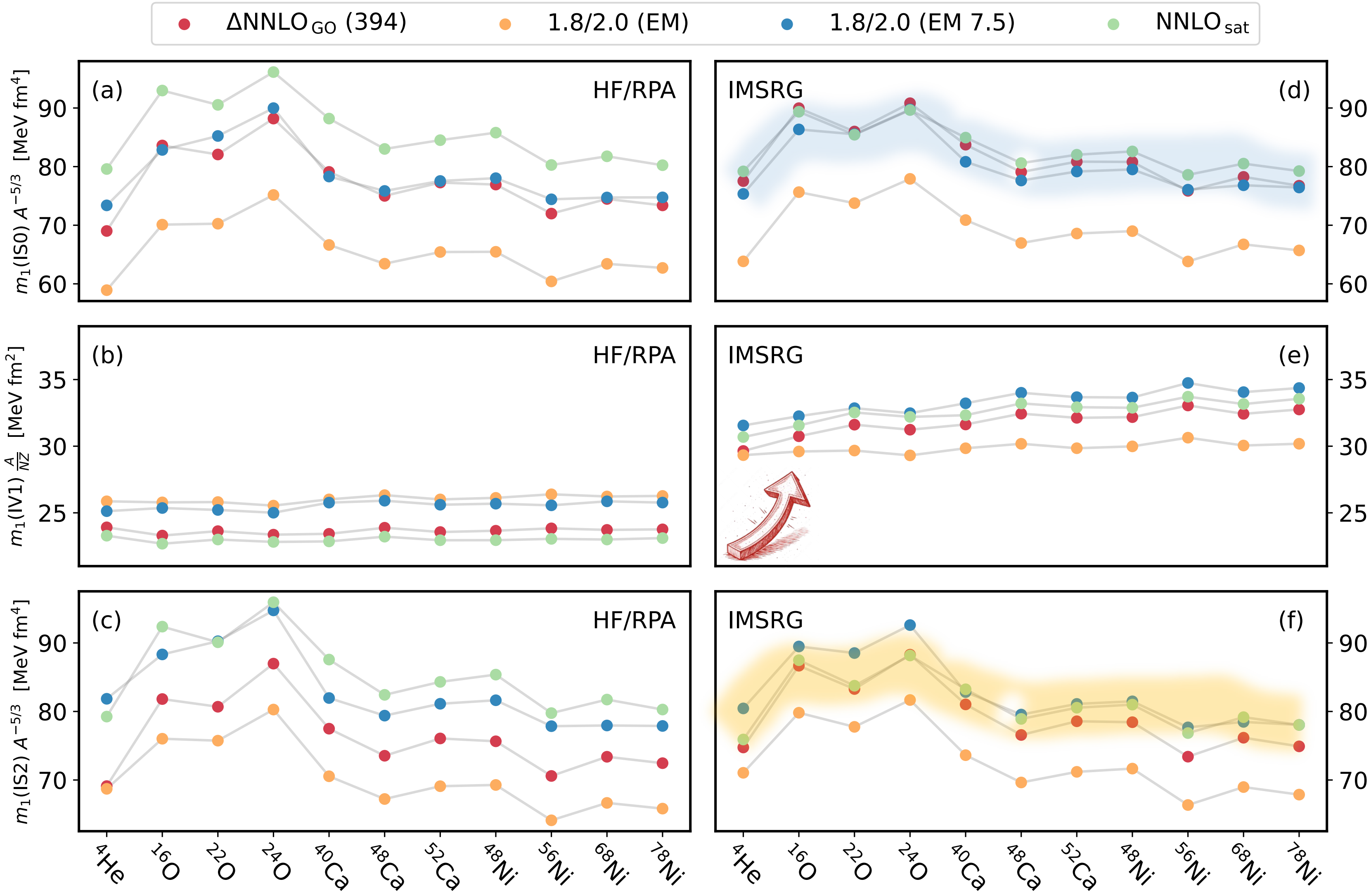

Monopole

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Dipole

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Quadrupole

- Reduced spread
- ~5% correlations effect

Photoabsorption cross section

Comparison to exp only makes sense for integrated quantities

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

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

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Pion-production threshold

$$\int_0^{E_{\max}} \sigma(E)\mathrm{d}E$$

[Ahrens et al., NPA, 1975]

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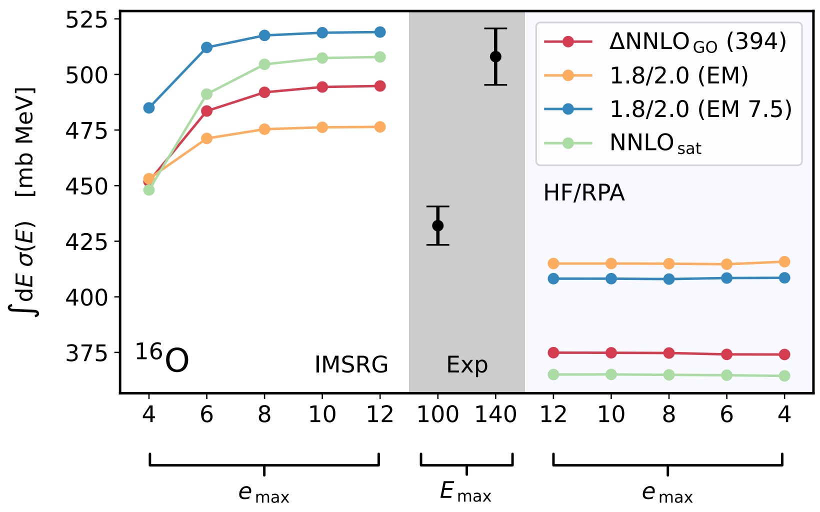

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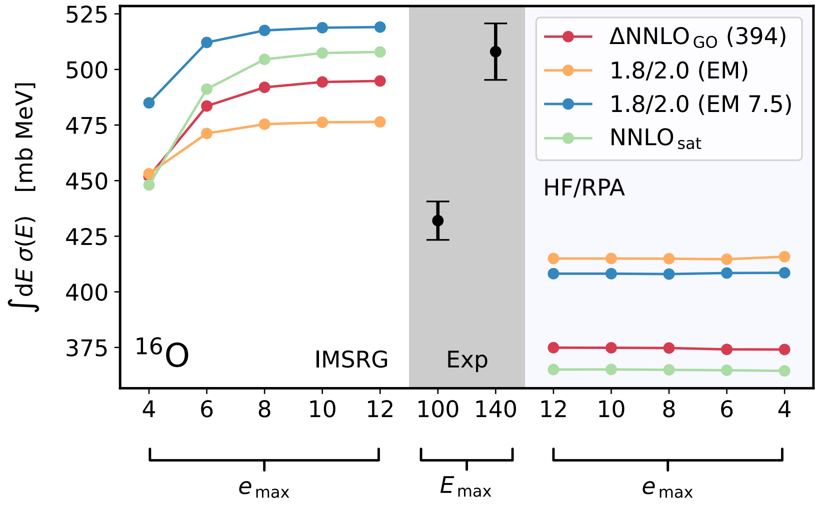

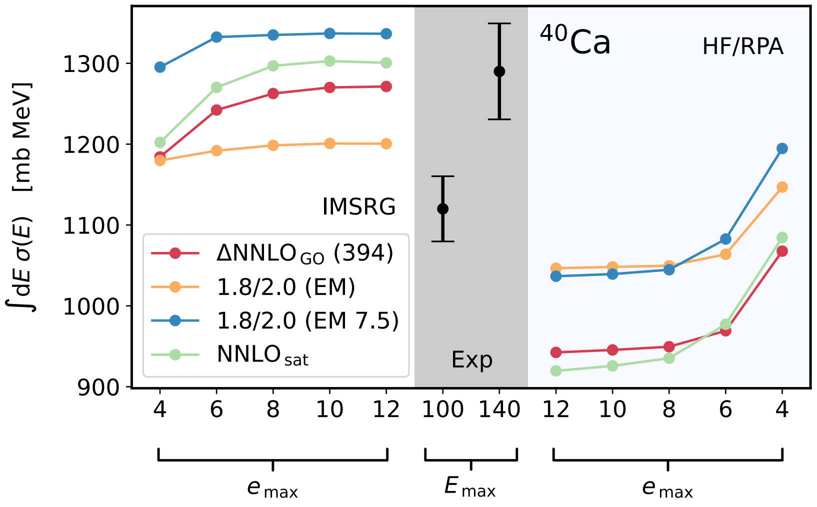

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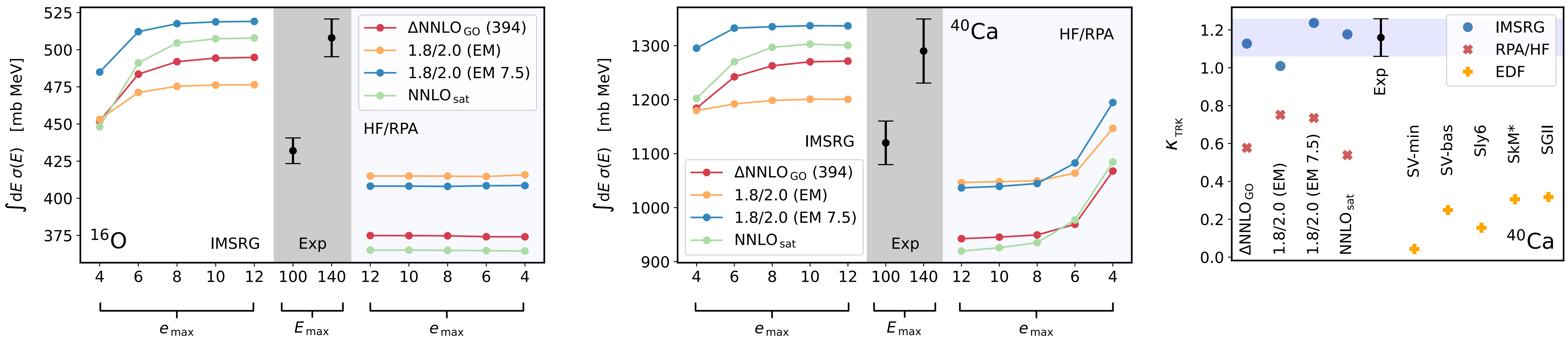

Comparison to EDF calculations

[Courtesy of P.-G. Reinhard]

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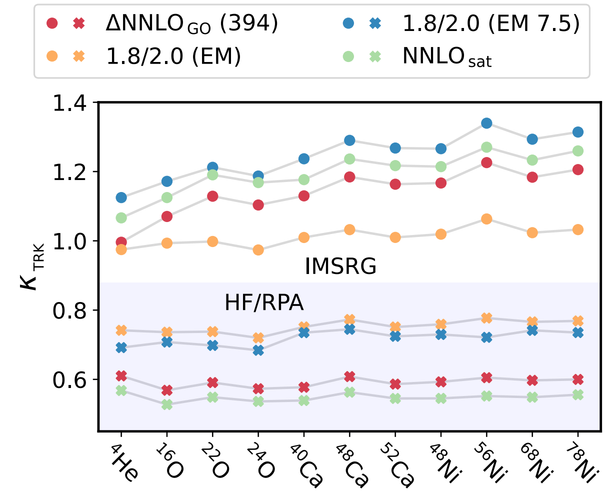

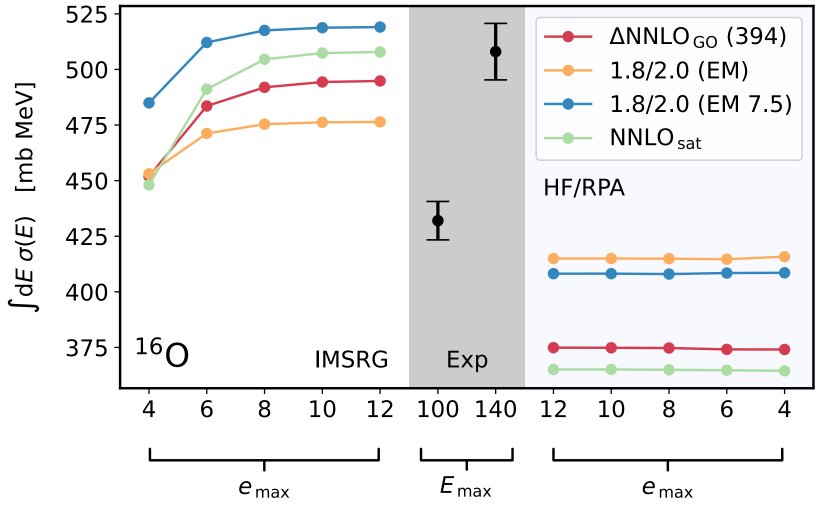

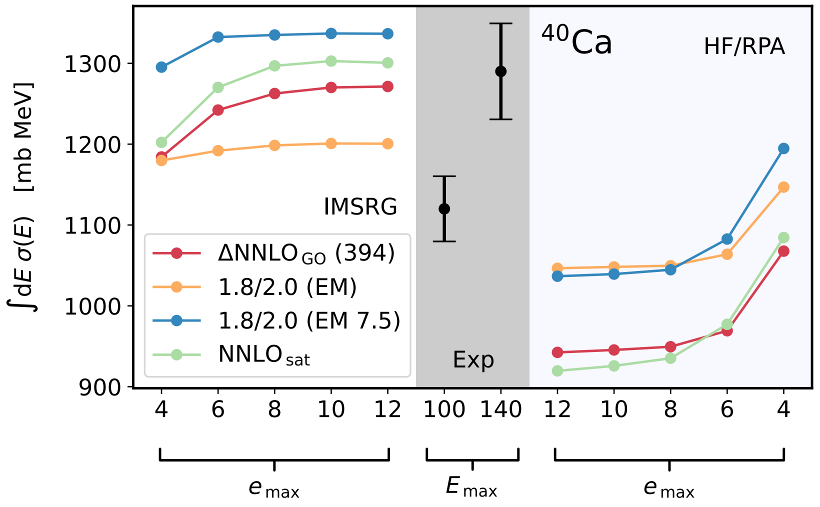

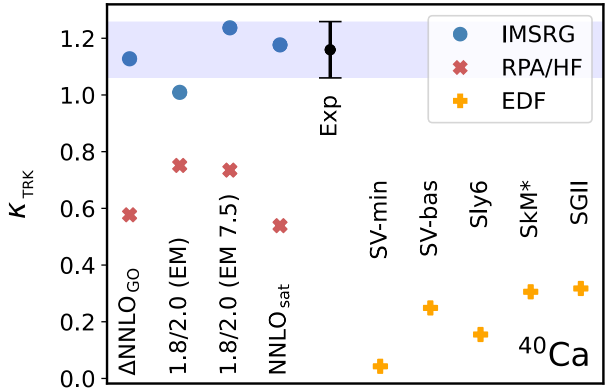

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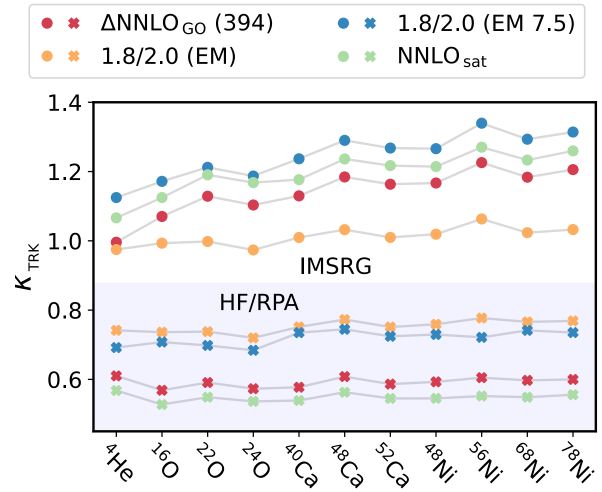

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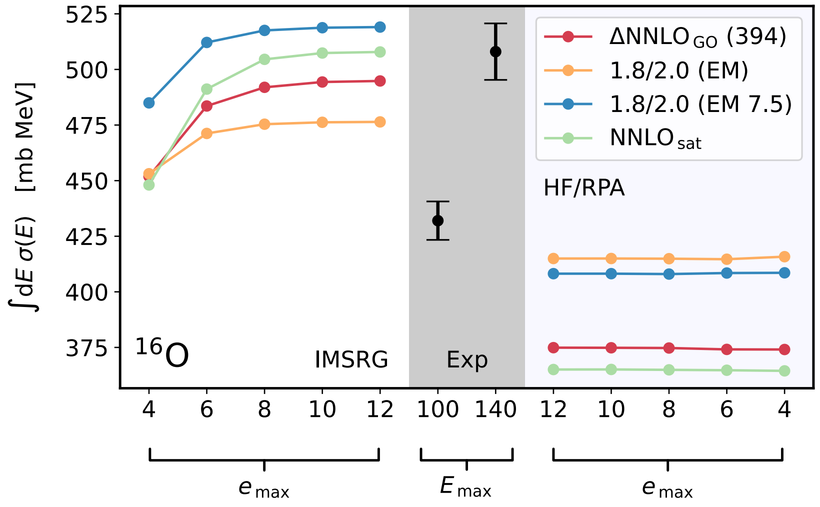

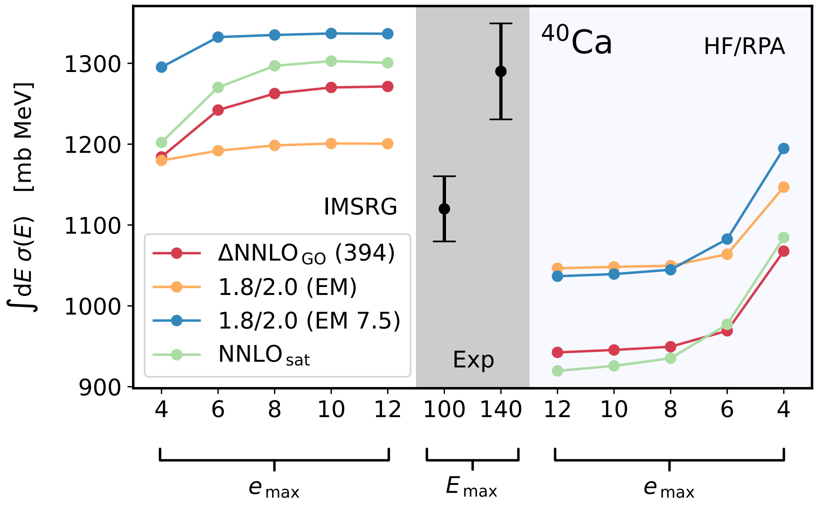

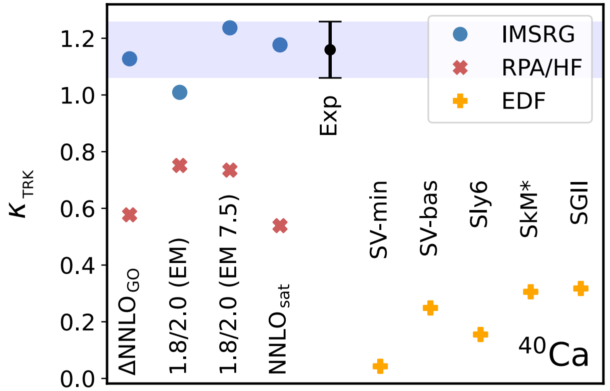

Both needed for consistent description

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

Comparison to EDF calculations

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Comparison to sum rules

Sum rules extensively studied in the past

$$\mathrm{EWSR}(Q_\lambda(\vec{r})) = \frac{1}{2}\langle\Psi_0|[Q_\lambda^\dagger(\vec{r}),[T+V(\vec{r}),Q_\lambda(\vec{r})]]|\Psi_0\rangle$$

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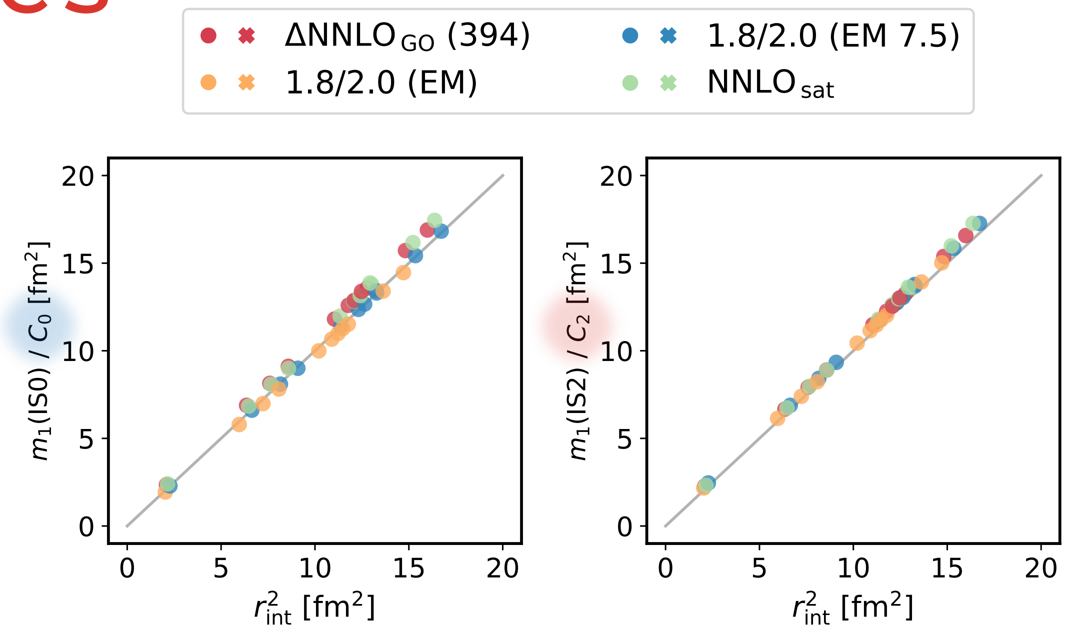

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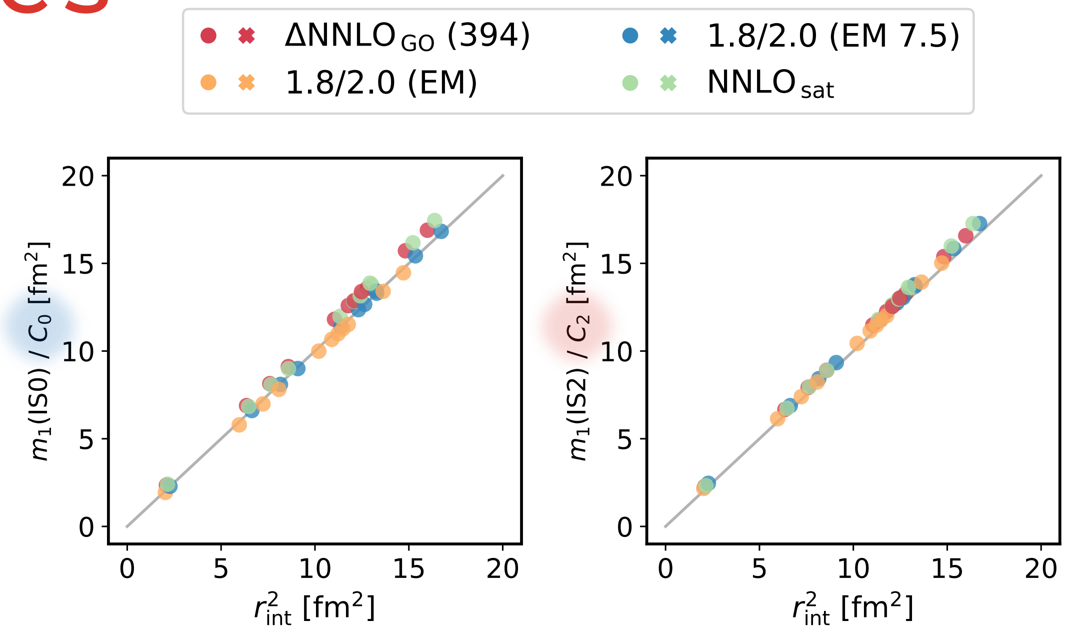
True if continuity Eq is only 1B

$$\vec{\nabla}\cdot\vec{j}(\vec{r}) + \frac{i}{\hbar}[H,\rho(\vec{r})] = 0$$

$$\vec{\nabla}\cdot\vec{j}_{[1]}(\vec{r}) + \frac{i}{\hbar}[T,\rho_{[1]}(\vec{r})] = 0$$

If V local



Comparison to sum rules

Sum rules extensively studied in the past

$$\mathrm{EWSR}(Q_\lambda(\vec{r})) = \frac{1}{2}\langle\Psi_0|[Q^\dagger_\lambda(\vec{r}),[T+V(\vec{r}),Q_\lambda(\vec{r})]]|\Psi_0\rangle$$
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$$\mathrm{EWSR}_{\mathrm{int}}(r^2) = \frac{2\hbar^2}{m}\langle\Psi_0|r^2_{\mathrm{int}}|\Psi_0\rangle$$

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$$m_1(Q_\lambda) \stackrel{?}{=} \mathrm{EWSR}(Q_\lambda)$$

True if continuity Eq is only 1B

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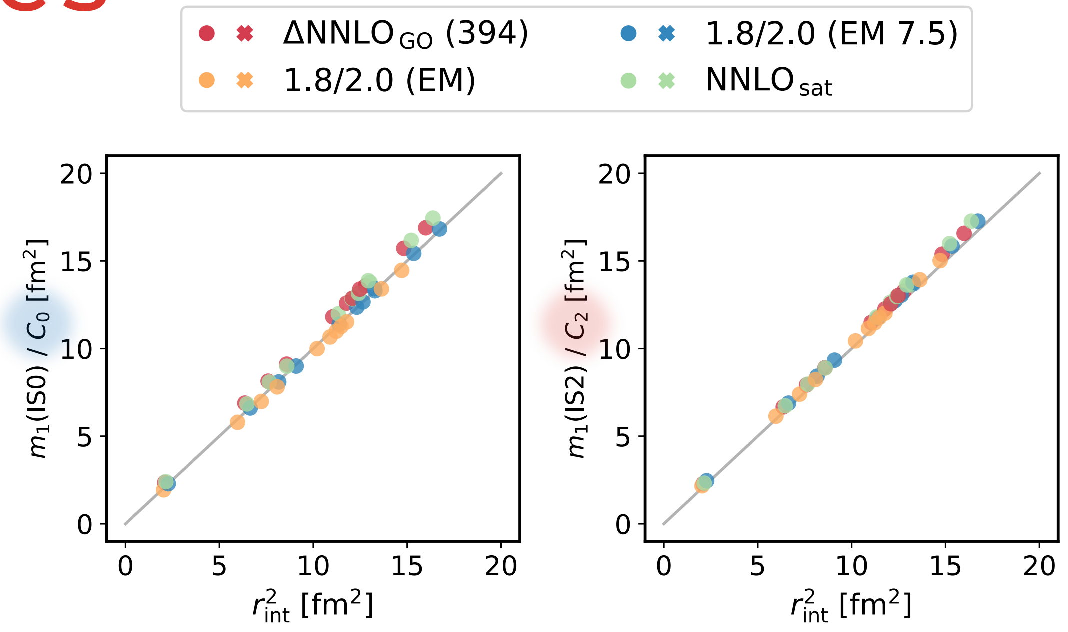

But many-body currents can be there !

$$\vec{\nabla}\cdot\vec{j}_{[\nu]}(\vec{r}) + \frac{i}{\hbar}\sum_{\mu=1}^{\nu}[H_{[\nu+1-\mu]},\rho_{[\mu]}(\vec{r})]_{[\nu]} = 0$$

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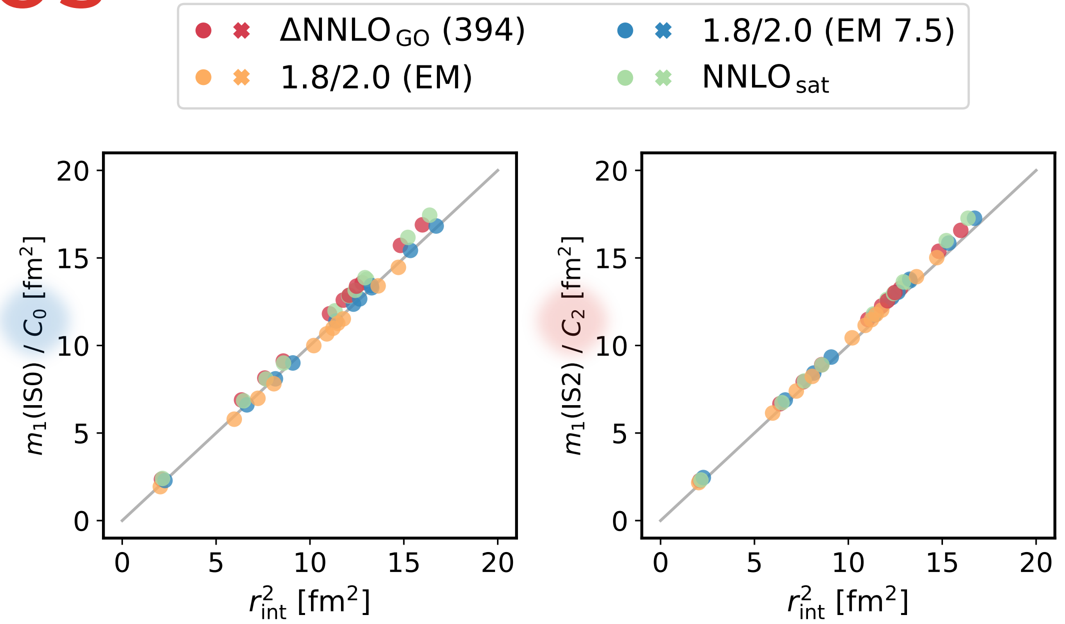

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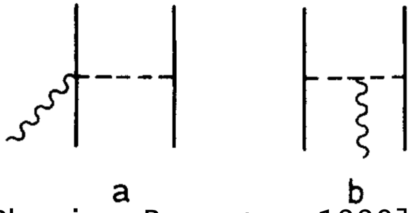
E.g. leading order exchange currents (Siegert's limit)

$$e\vec{J} = i[V_\pi(q),\vec{D}] \propto$$



[Christillin, Physics Reports, 1990]

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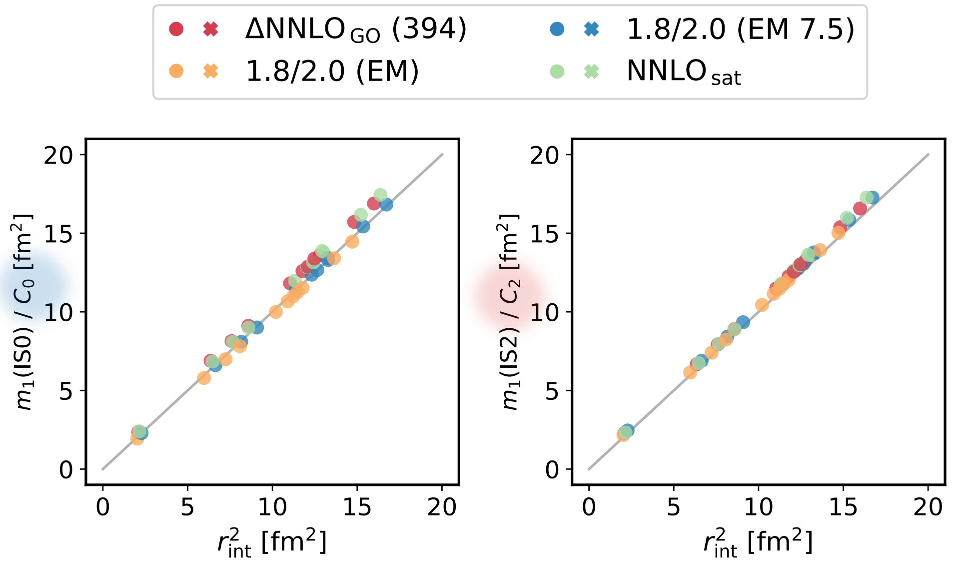

Let’s look more closely

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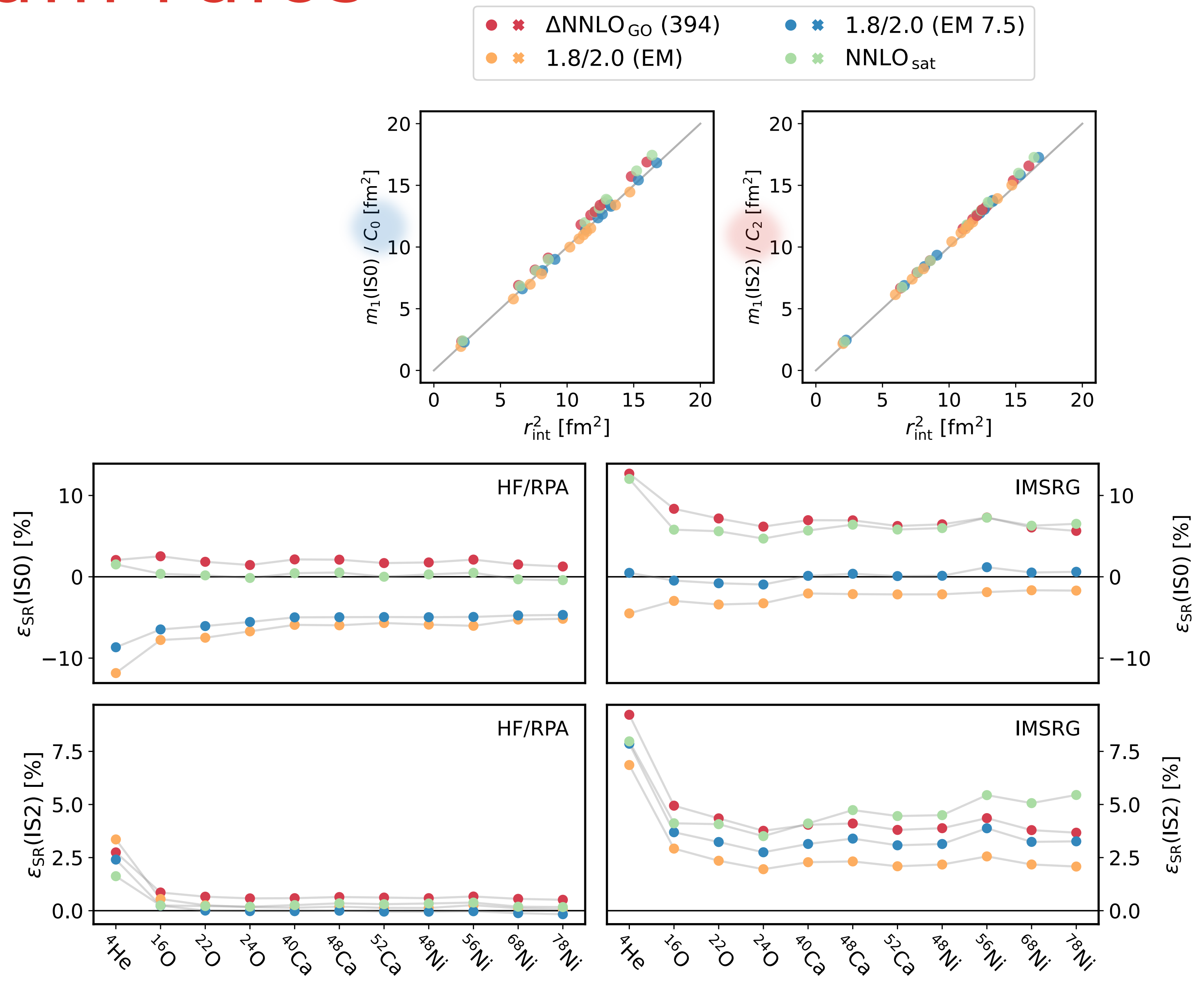

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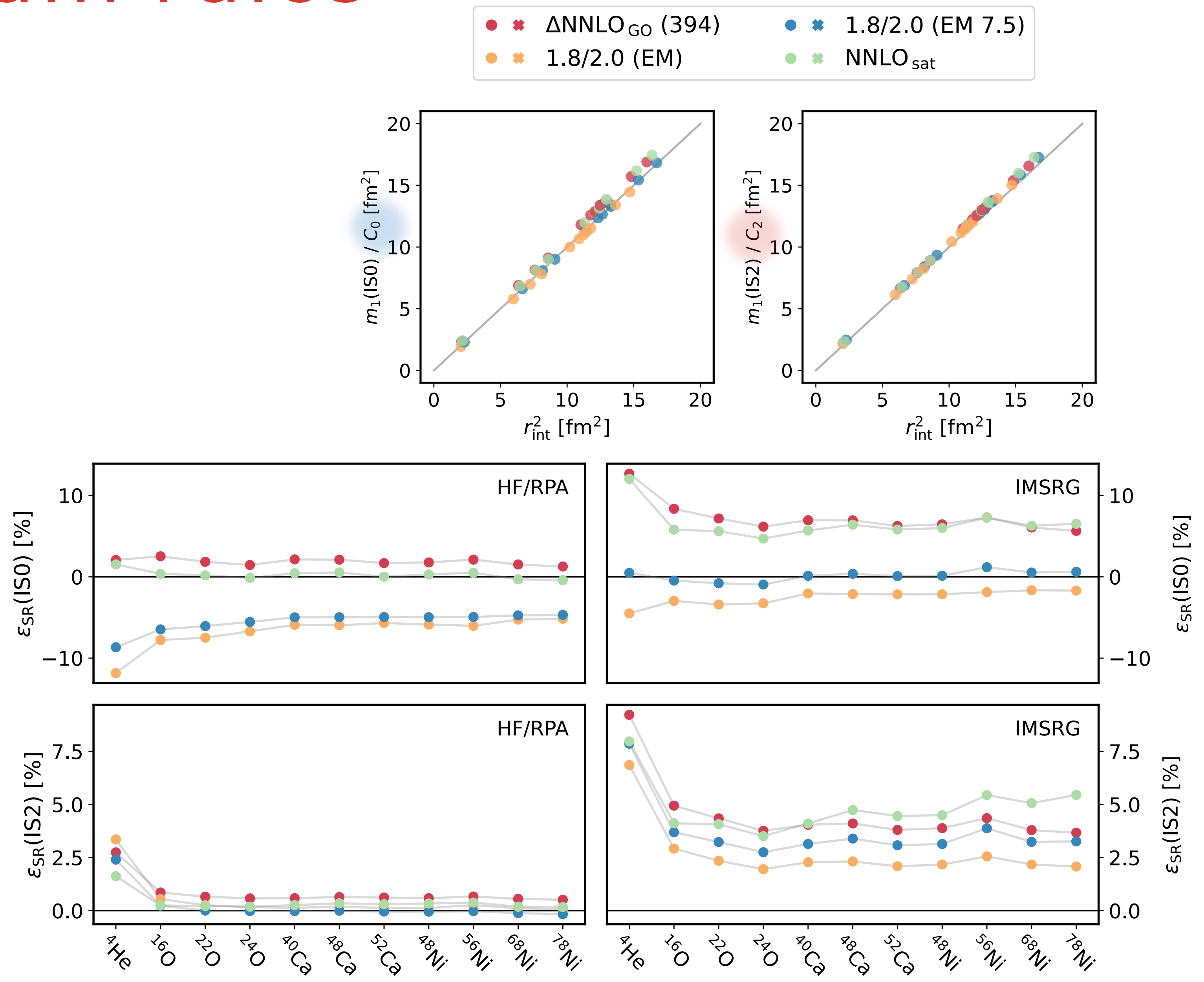
Differences from EWSR

- Nonlocalities
- Two-body currents



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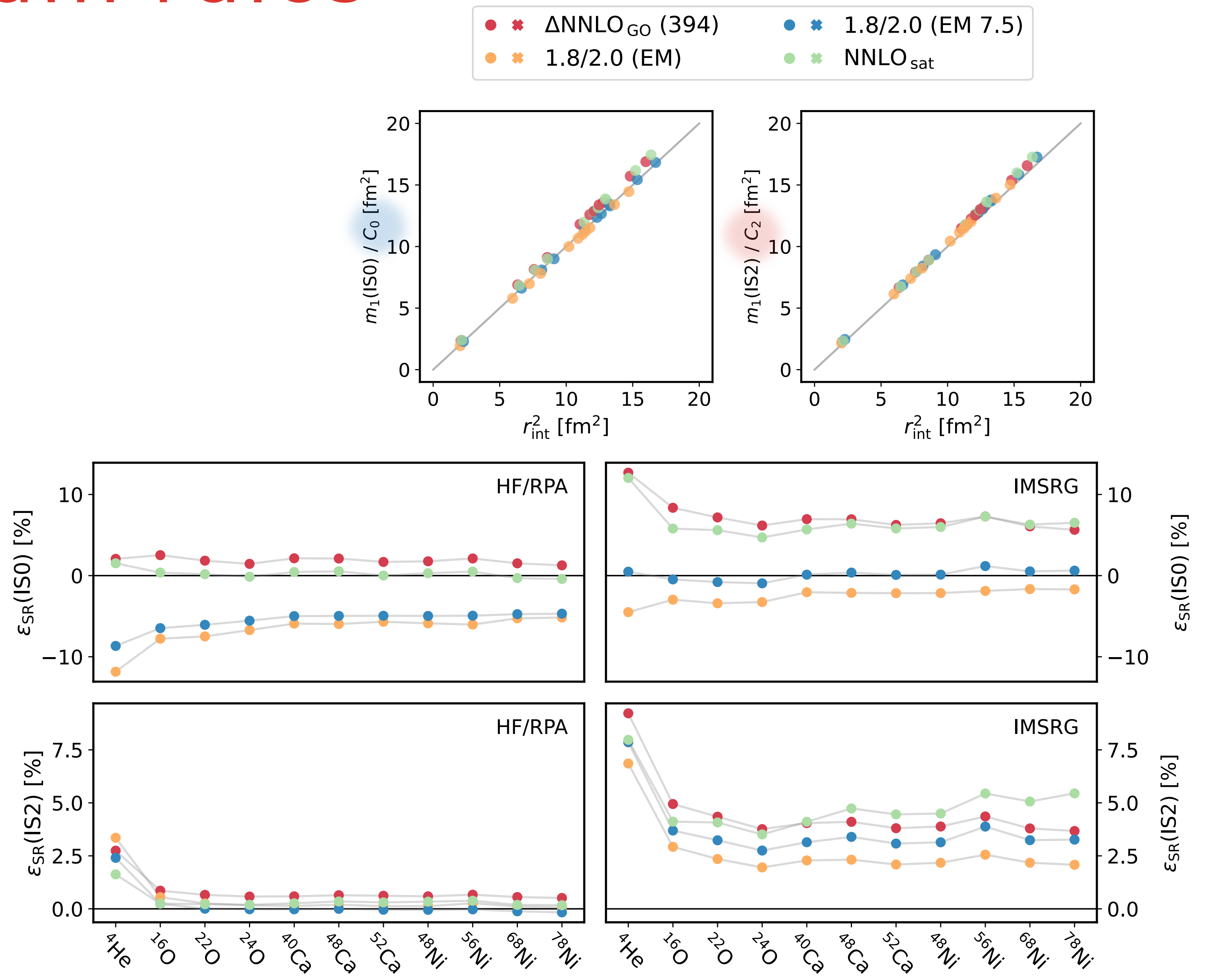

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m1 from moments is better !

Introduction

- Physics case
- Existing ab initio methods

IMSRG multipole moments

- Moments of the strength
- IMSRG implementation
- Model-space convergence

Numerical results

- Interaction sensitivity
- Comparison to experiment
- Comparison to sum rules

Challenges and opportunities

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Going open-shell

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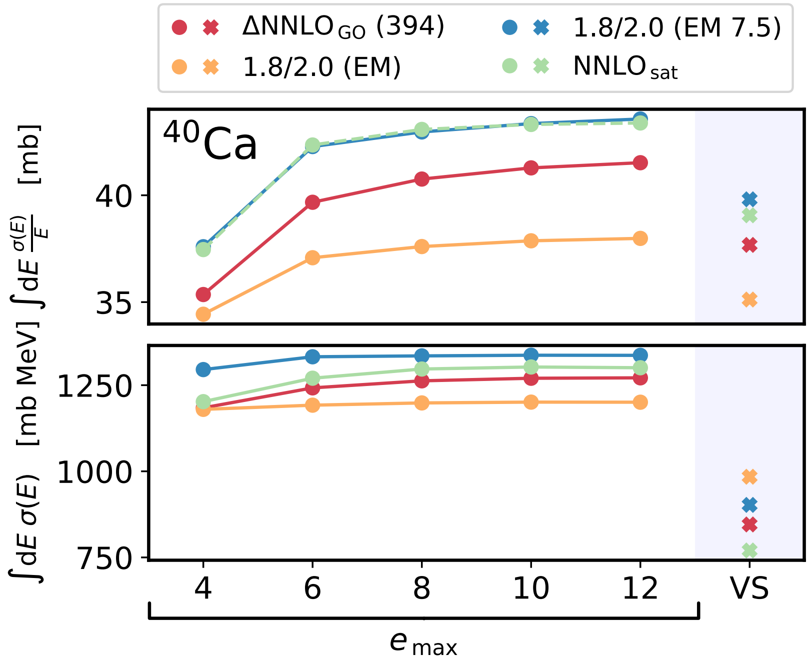
Comparison to VS calculation for ^{40}Ca with ^{28}Si core

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



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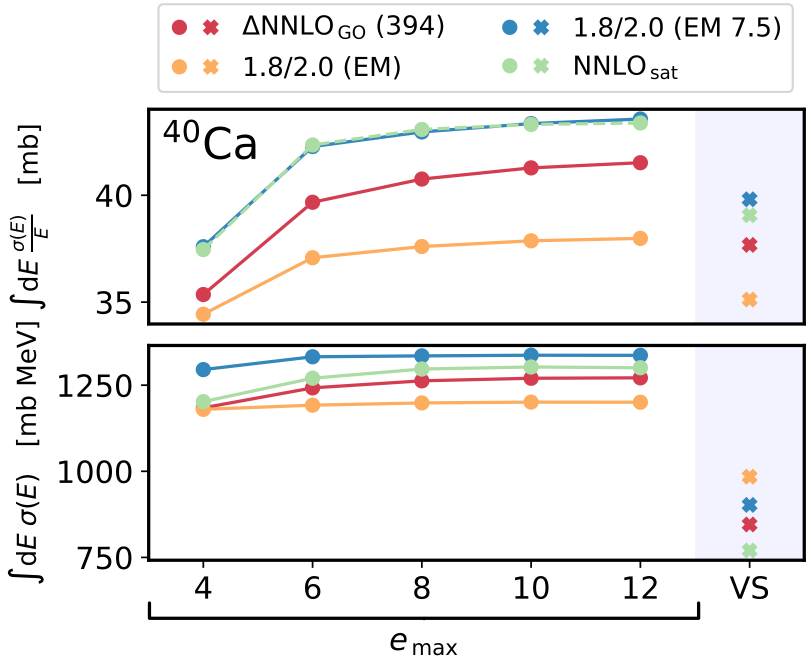
Other possibilities within the IMSRG

- Multi-reference formulation
- Symmetry-breaking calculations



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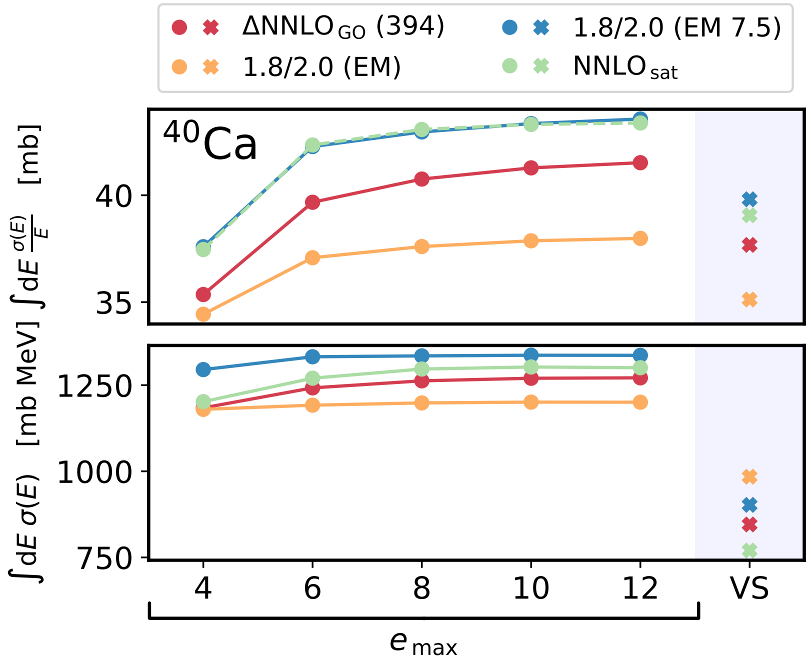

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Benchmarks and uncertainty quantification

No limitation on the many-body method (and operators) of choice

- Exact treatment of excited states
- Can benchmark response calculations going through exc states EOM, LIT etc. (can send matrix elements)

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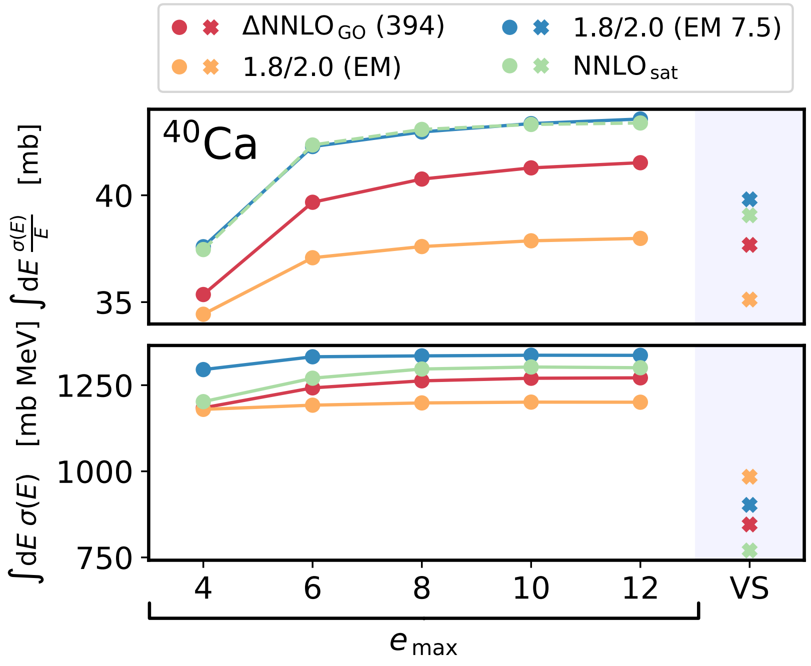

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Systematic studies of H properties

Thank you for the attention

Robert Roth
Achim Schwenk
Alexander Tichai

Thomas Duguet
Jean-Paul Ebran
Mikael Frosini
Vittorio Somà

Francesca Bonaiti

Sonia Bacca

Summary

- Moment method useful for uncertainty quantification /benchmark of exc states
- Can be used for systematic studies of H properties
- Small finite-basis uncertainty
- Correlation effect ~5% in monopole and quadrupole
- Qualitative change (~40%) for dipole
- Better agreement with data and smaller interaction spread
- Comparison to EWSR diagnostic of non-localities and two-body currents