Ab initio description of monopole resonances

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DFG

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EMMI

Outline

Introduction

- Physics case
- The ab initio philosophy

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PGCM – open-shell systems

- Theoretical insights
- Numerical results
- Comparison to experiment

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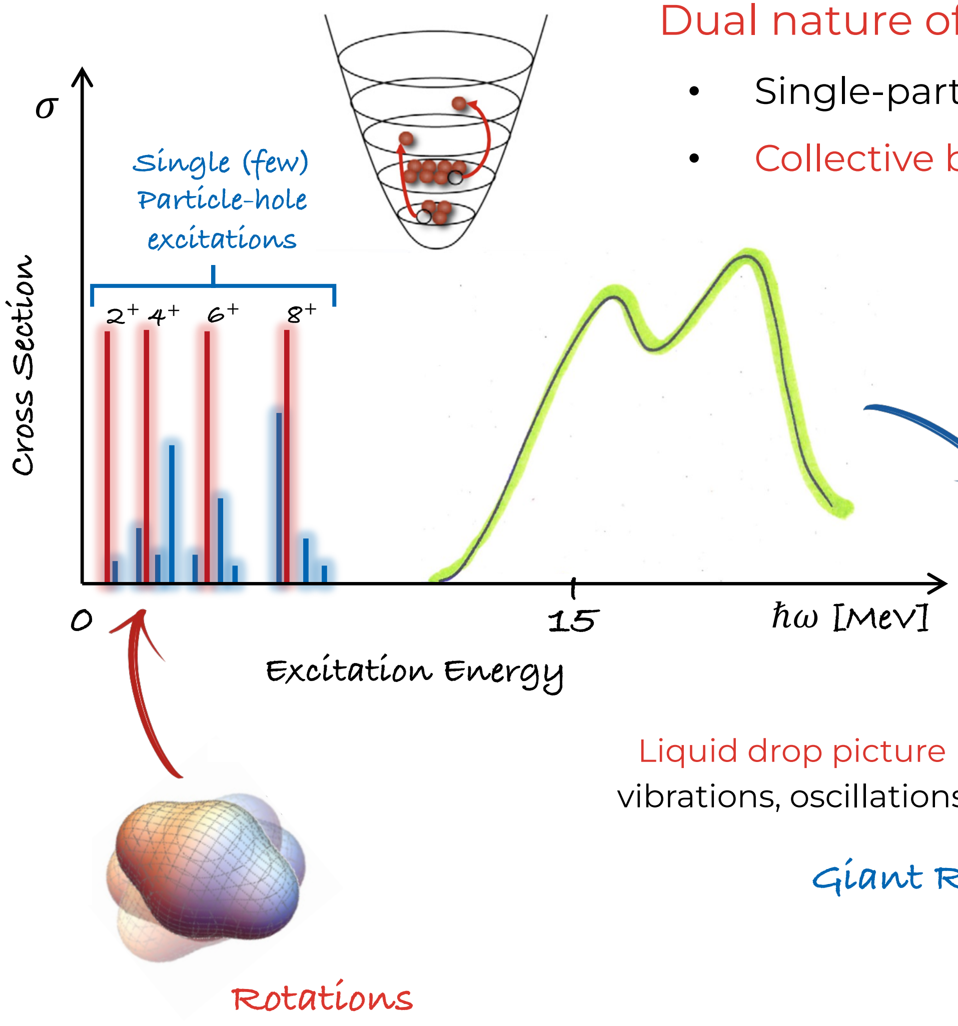
Challenges and opportunities

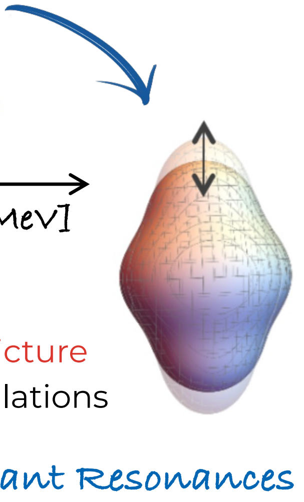
Nuclear spectroscopy

Dual nature of nucleus

- Single-particle features
- Collective behaviour



Liquid drop picture
vibrations, oscillations



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

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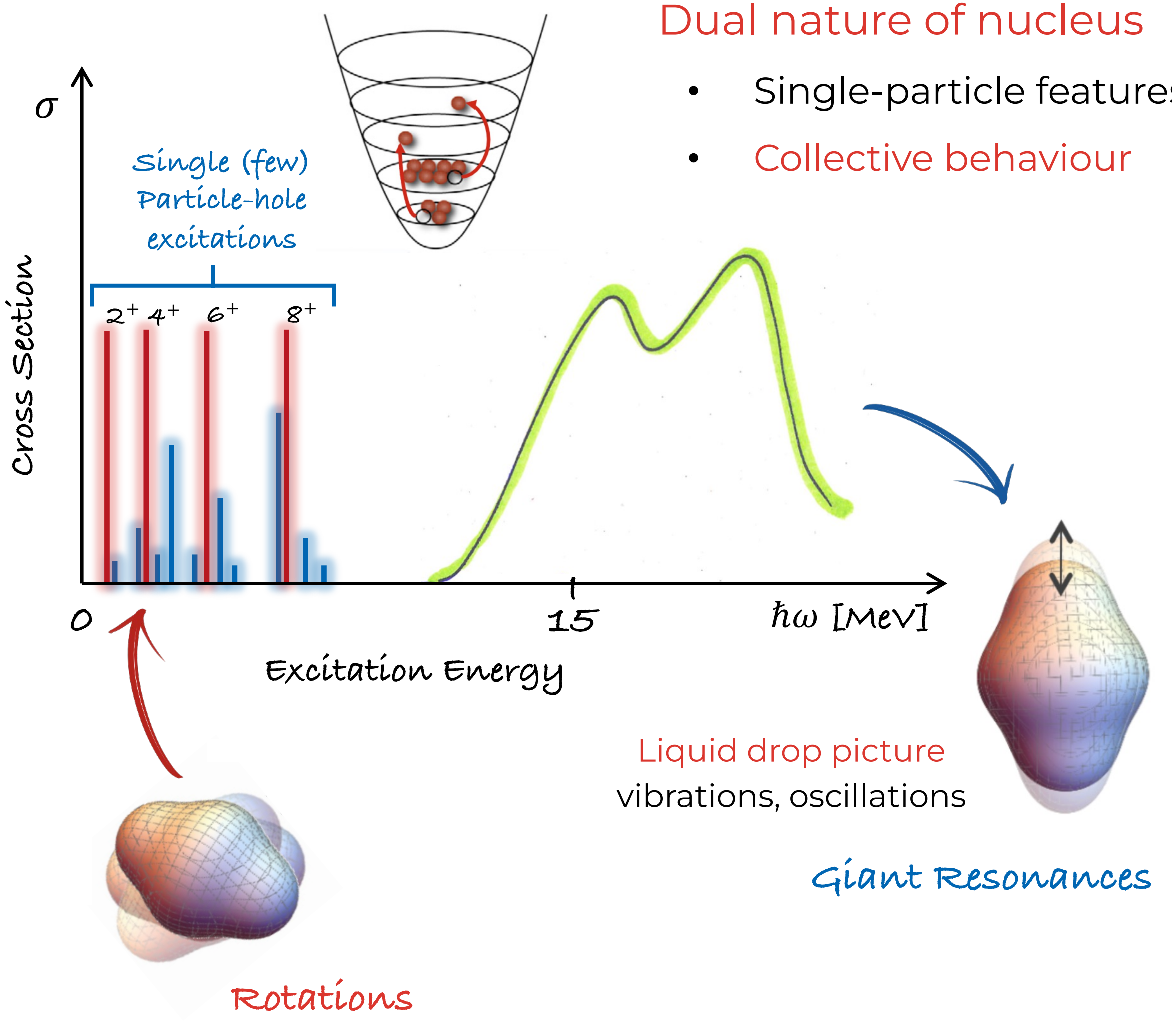

Response function

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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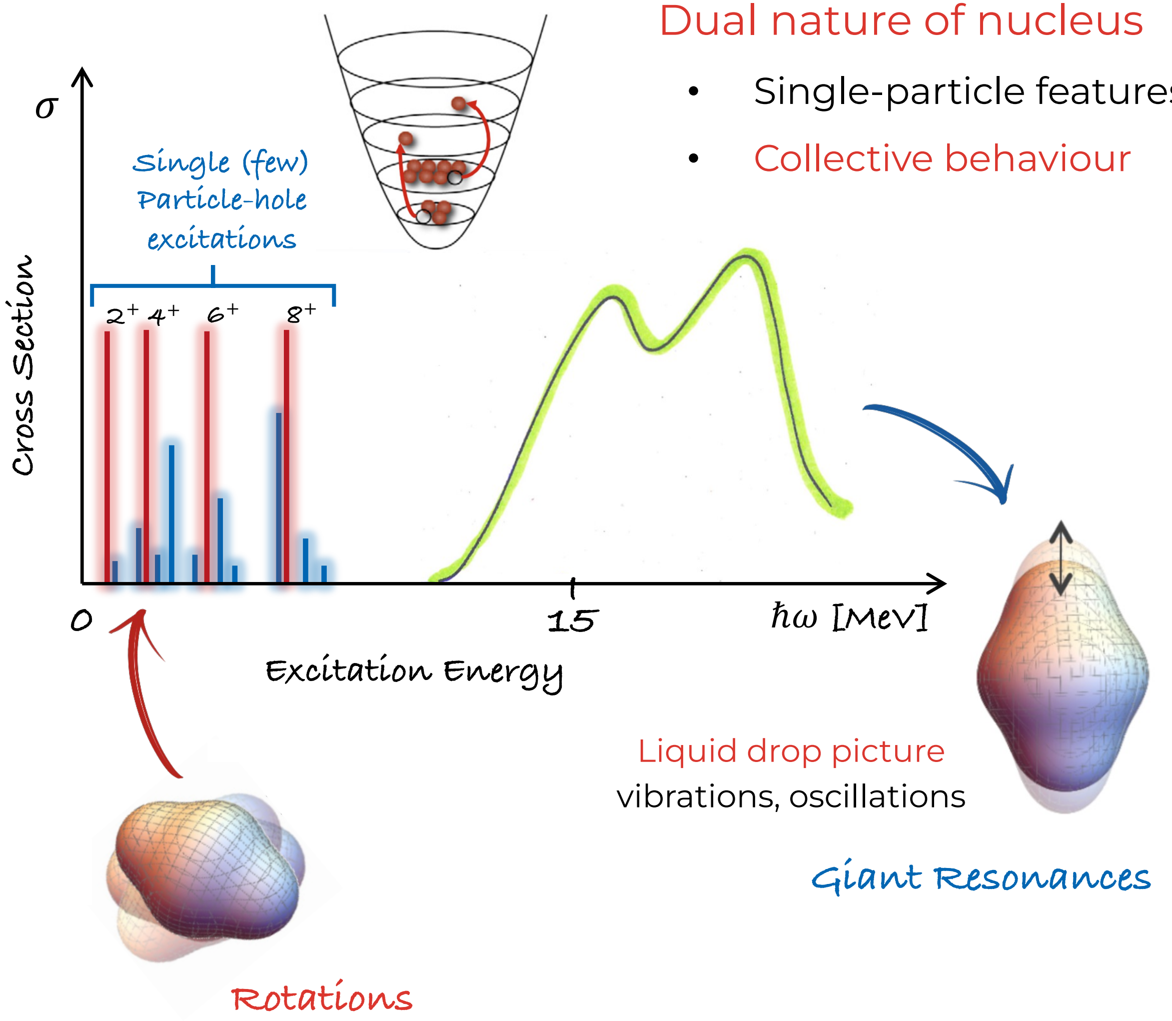

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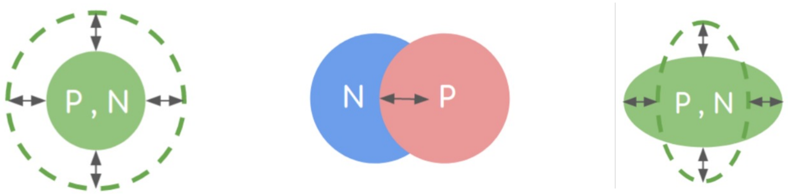

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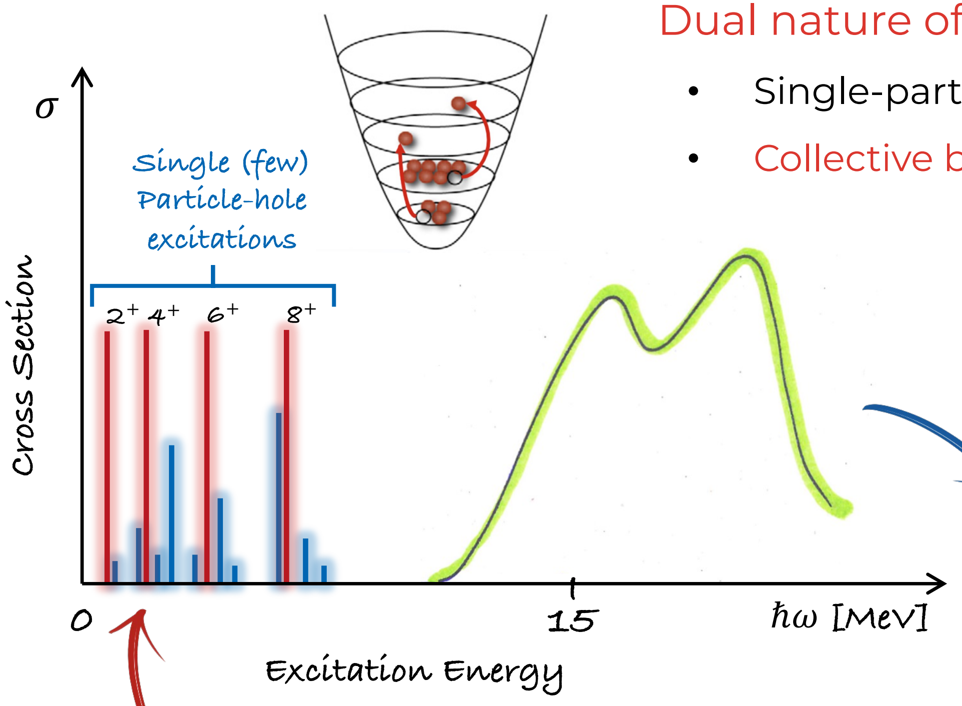

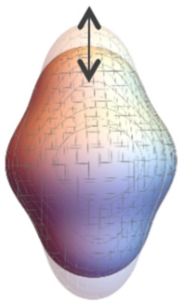

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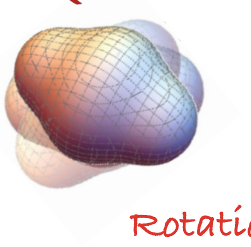
Giant Resonances



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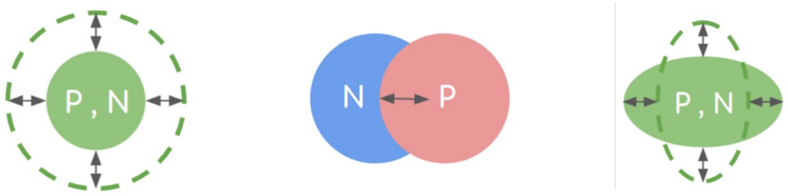

Compression properties

→ **Equation of State**

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

Ab initio Nuclear Structure

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

Ab initio Nuclear Structure

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INPUT HAMILTONIAN

Ab initio Nuclear Structure

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MANY-BODY SOLUTION

Ab initio Nuclear Structure

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

Systematic expansion of H

$$H = T + V_{\mathrm{LO}} + V_{\mathrm{NLO}} + V_{\mathrm{N^2LO}} + \dots$$

- Chiral expansion
- LEC fitted on data
- Up to A-body forces

Systematic many-body expansion

$$|\Psi_k^{\mathrm{A}}\rangle = \Omega|\Theta_k^{(0)}\rangle = |\Theta_k^{(0)}\rangle + |\Theta_k^{(1)}\rangle + |\Theta_k^{(2)}\rangle + \dots$$

- Wave operator on ref state
- Many possible methods

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Global philosophy

The approximate solution must be systematically improvable and approach the exact solution in a well-defined limit

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Uncertainties evaluation, quantify what is missing

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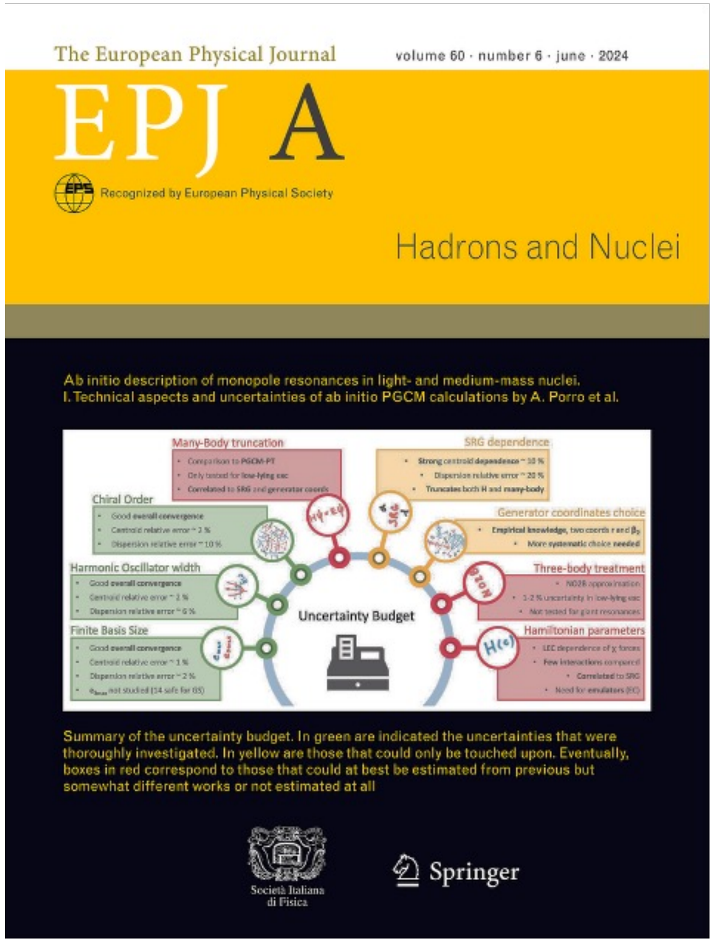
PGCM Results based on



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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

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

Projected Generator Coordinate Method

Schrödinger equation $H\left|\Psi_n\right\rangle = E_n\left|\Psi_n\right\rangle$

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Strong static correlations

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Open-shell systems → Strong static correlations → Symmetry-breaking reference states

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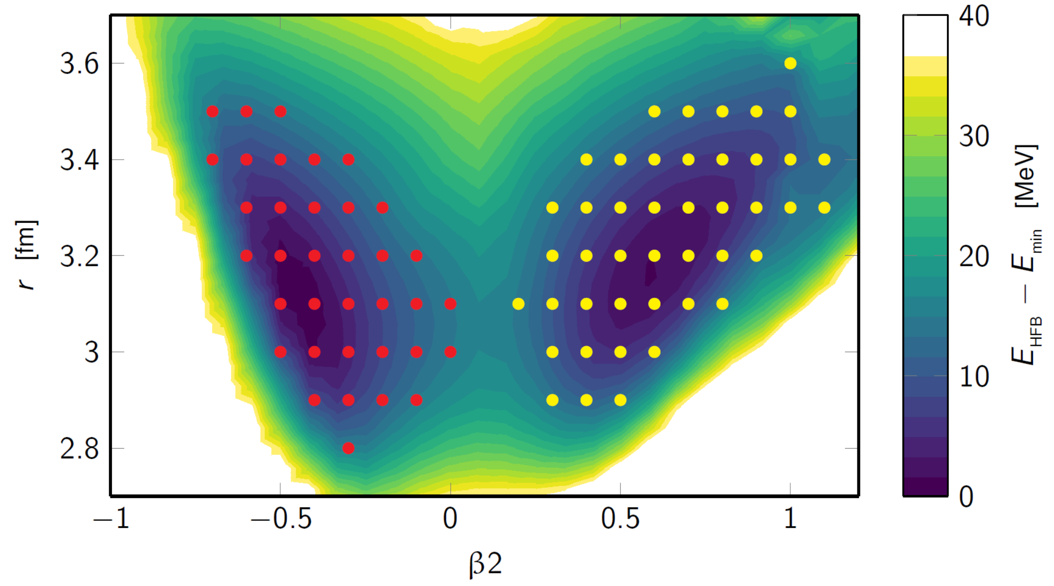
Strong static correlations

1 Constrained HFB solutions

$|\Phi(q)\rangle$

Generator coordinates

(q can be any coordinate)



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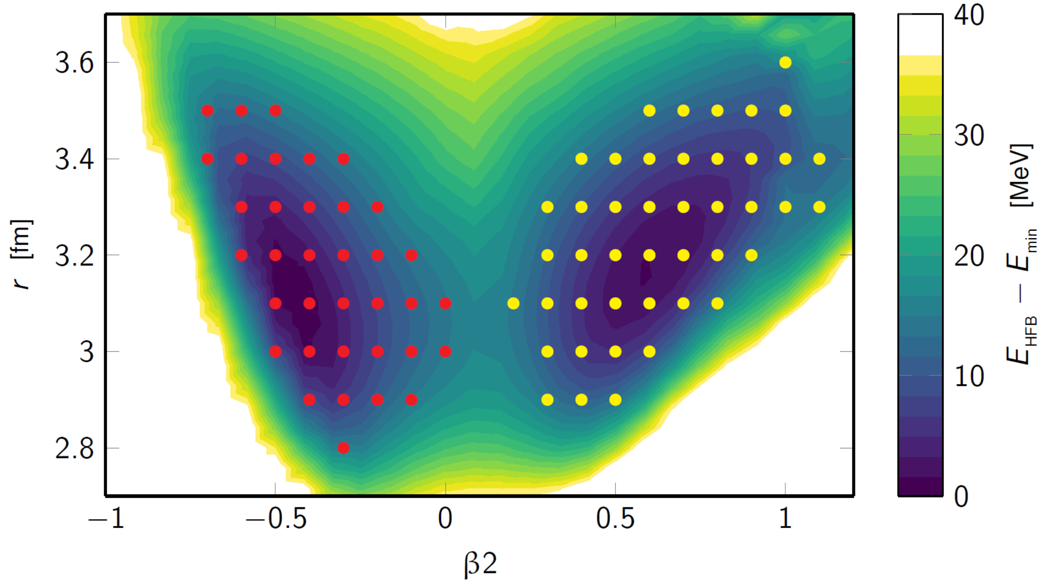

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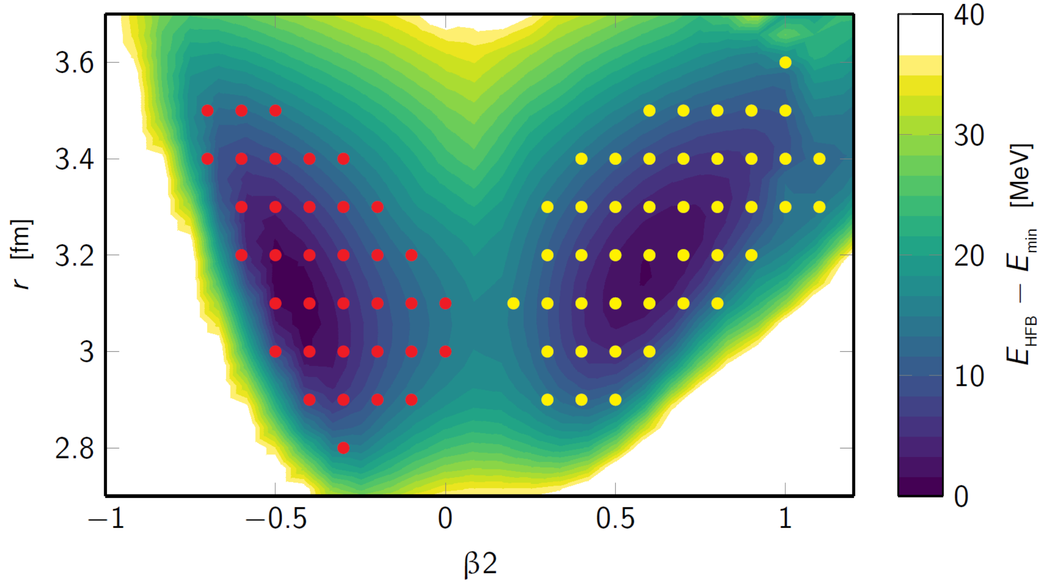

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Open-shell systems → Strong static correlations ← Symmetry-breaking reference states

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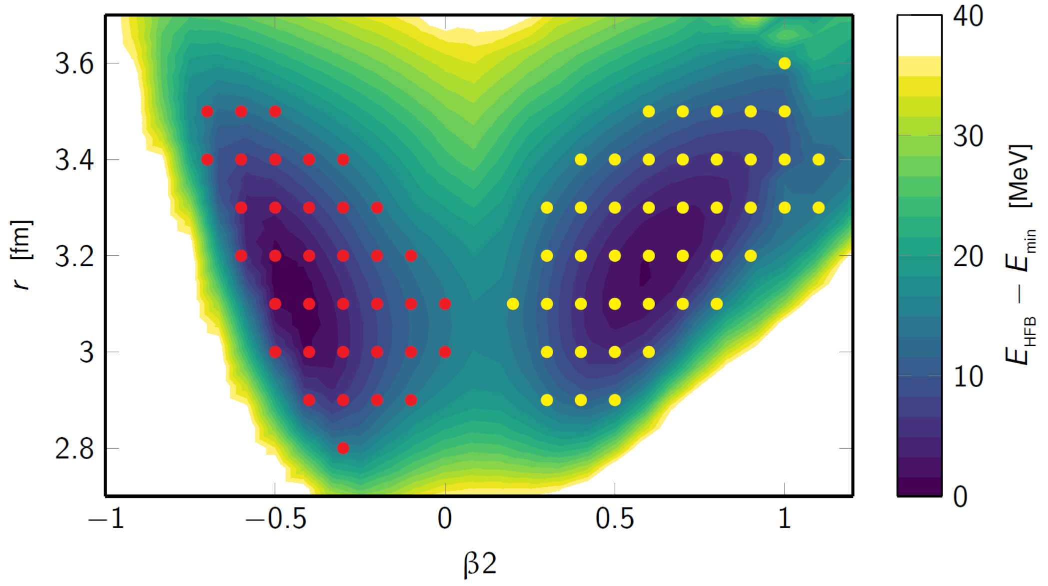
$$\delta \frac{\langle\Psi_n|H|\Psi_n\rangle}{\langle\Psi_n|\Psi_n\rangle} = 0$$



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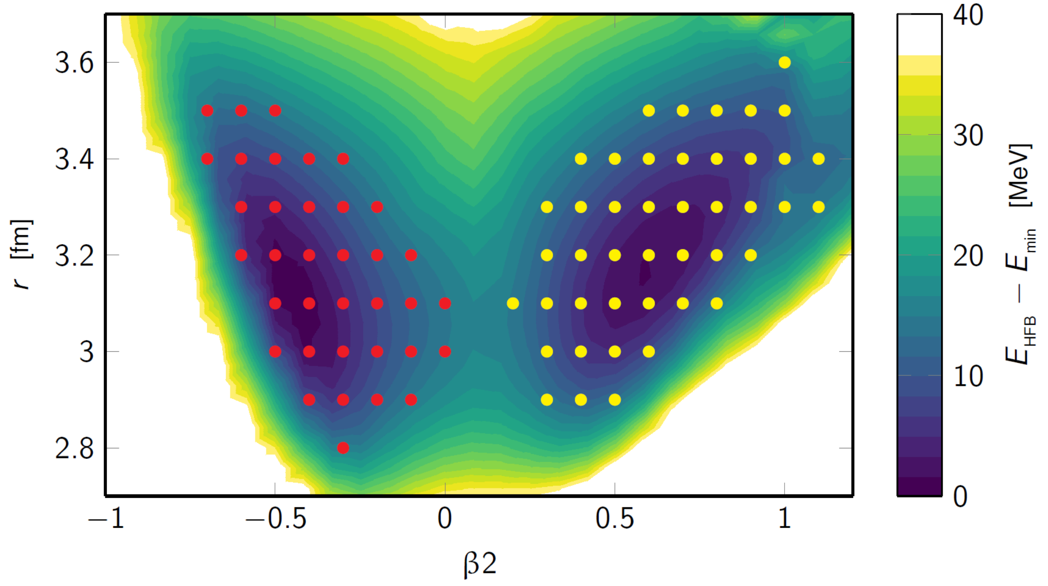

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Kernels evaluation

$$\mathcal{H}(p,q) \equiv \langle\Phi(p)|H|\Phi(q)\rangle$$
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[Porro and Duguet, EPJA, 2022]

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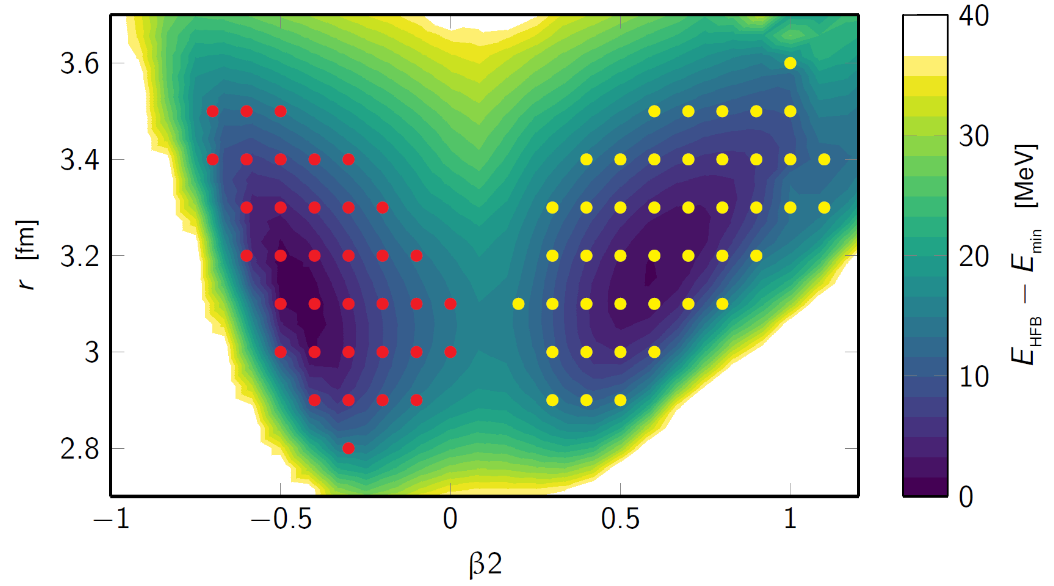
Schrödinger equation $H\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$

Diagonalization in a physically-informed
reduced Hilbert space



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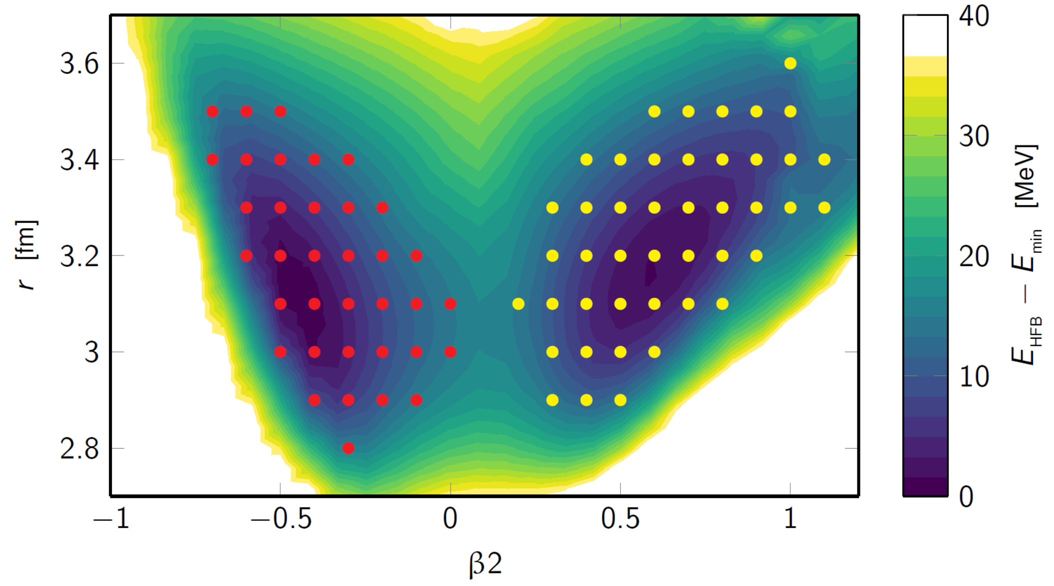

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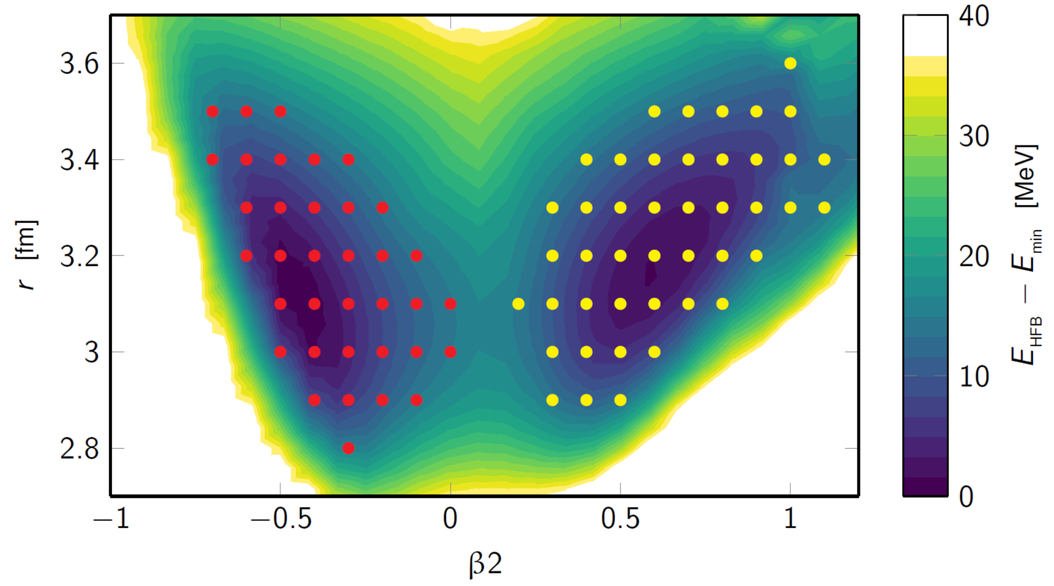

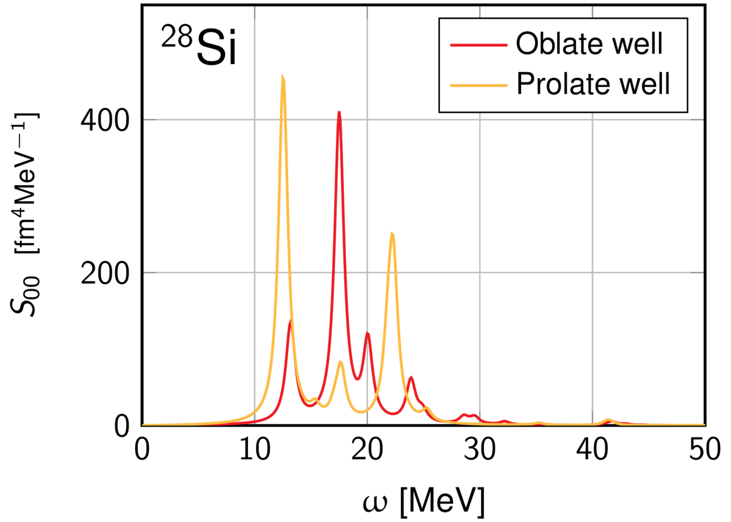

Ab-initio PGCM numerical settings (systematic study in ^{46}Ti)

- Quantities expanded on harmonic oscillator basis (characterised by **ħω**, e_{max}, e_{3max})
- Family of chiral NN + in-medium 3N interactions (NLO, N2LO and N3LO)
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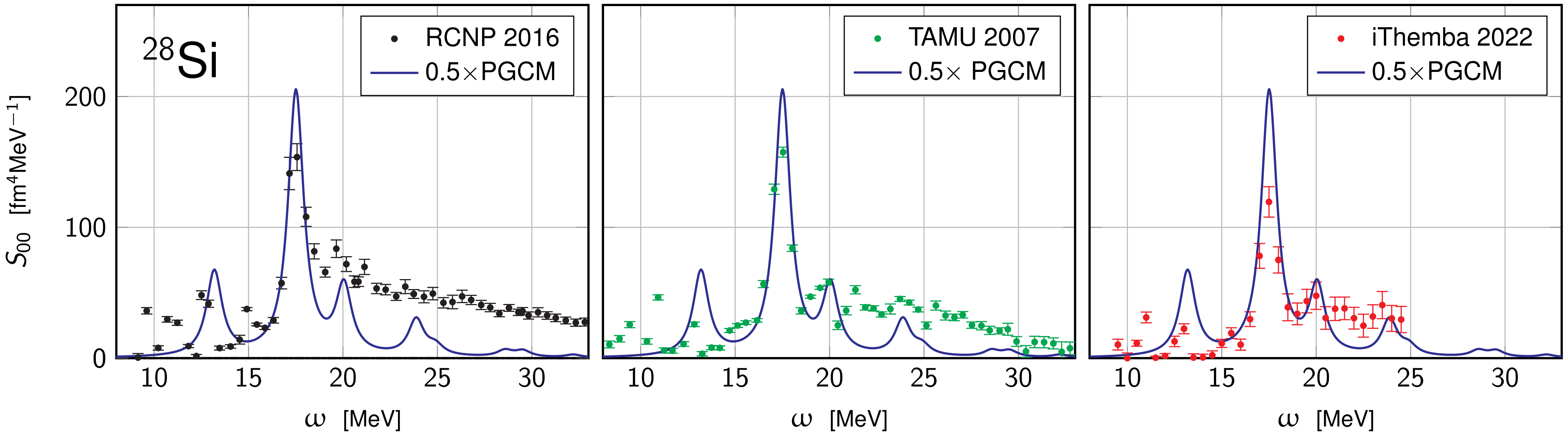
Good agreement with experimental data



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

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→ Ground state only ← Identity resolution

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

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Complexity shifted to operator structure

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

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

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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]

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

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

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

$$\equiv \langle \Psi_0 | M_k(Q_\lambda) | \Psi_0 \rangle$$

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

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

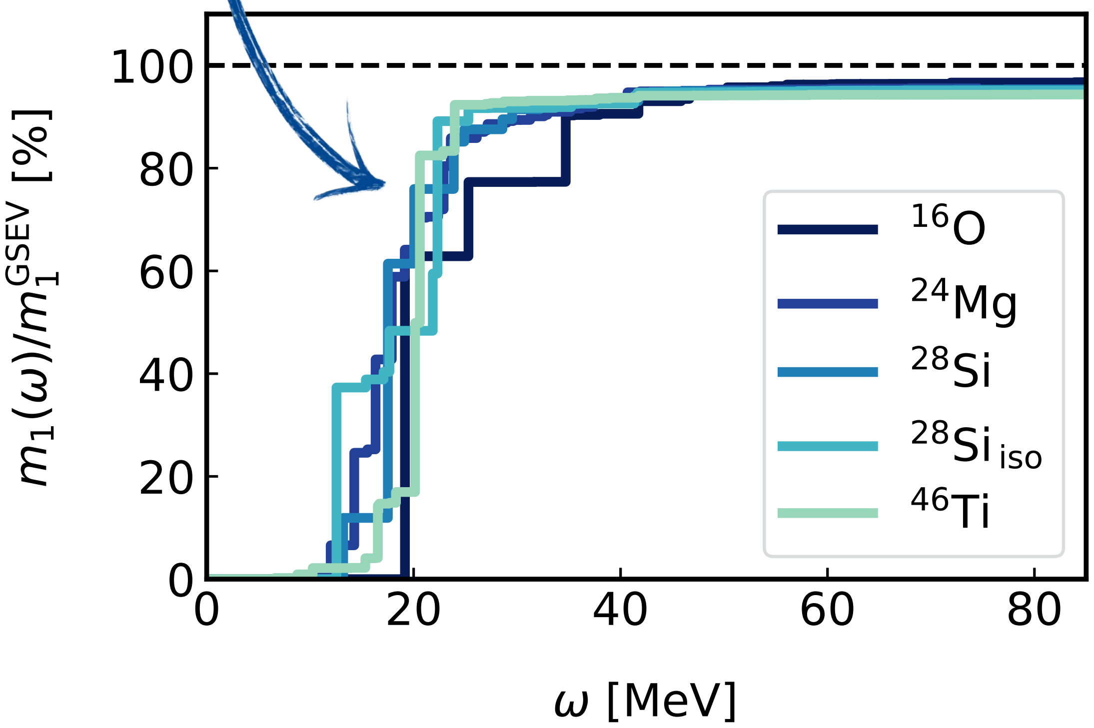
- Exact treatment for exc states
- Many-body truncation only GS

"Exact sum rules with approximate ground states"

[Johnson et al. , JPG, 2020]

First application within the PGCM

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



[EPJA (2024) 60, 155]

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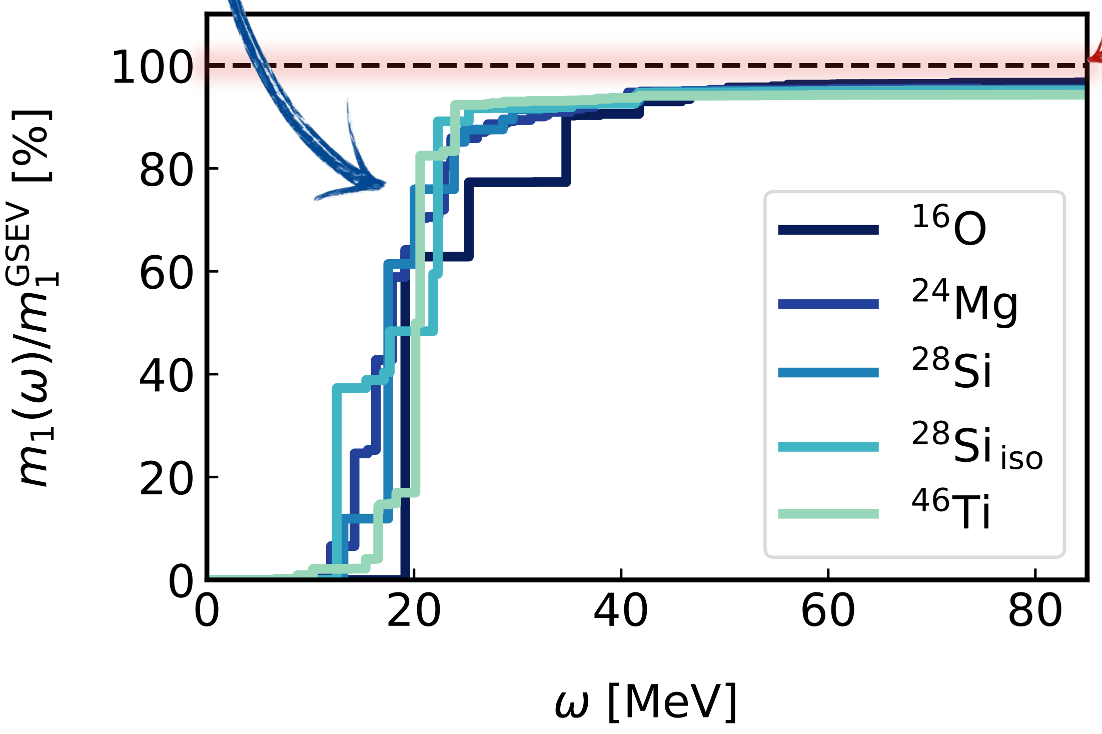

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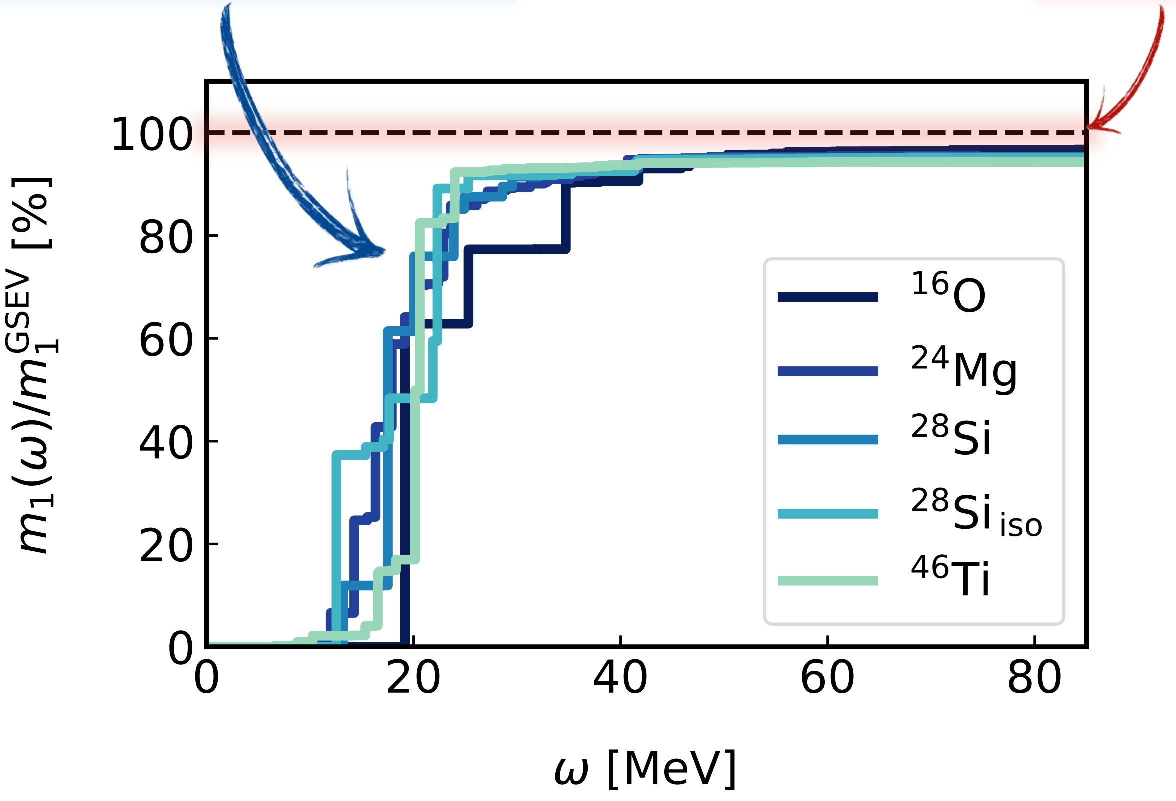


6-7 % difference in PGCM

Motivation to test other many-body methods

[EPJA (2024) 60, 155]

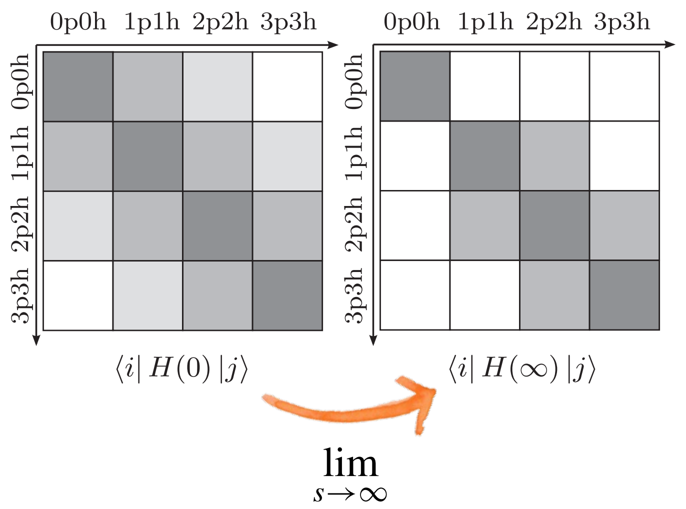
Strategy in the IMSRG framework

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



[Tsukiyama, Bogner and Schwenk, PRL, 2011]

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

Slater determinant

[Porro, Schwenk and Tichai, arXiv:2507.20665](https://arxiv.org/abs/2507.20665)

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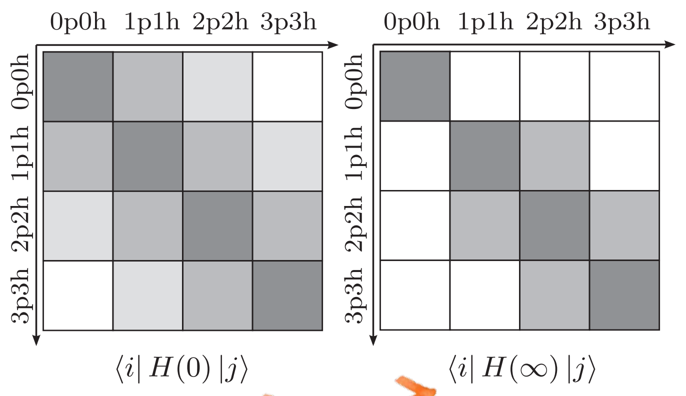

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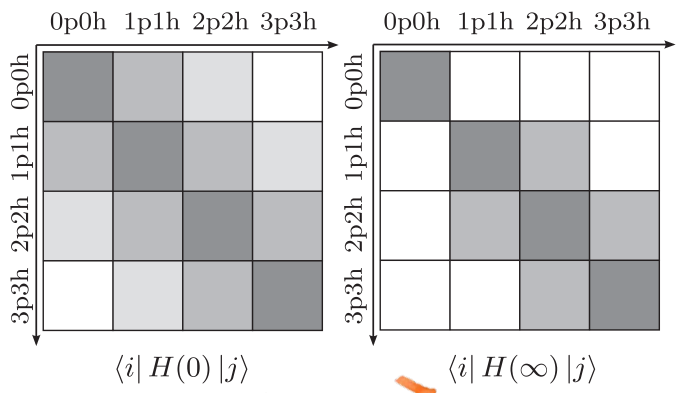

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J-scheme expressions of m_0 and m_1

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

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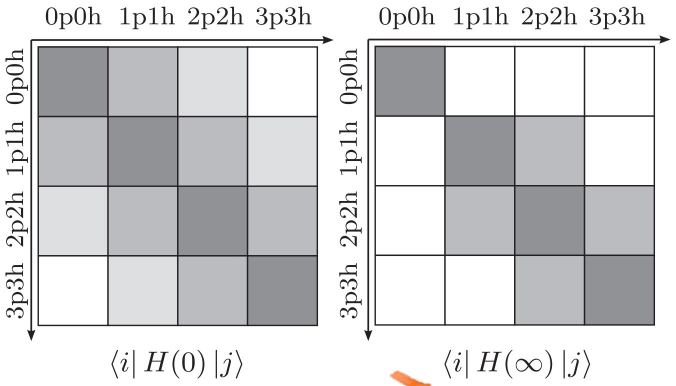

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Implemented within **imsrg++** code

[github.com/ragnarstroberg/imsrg]

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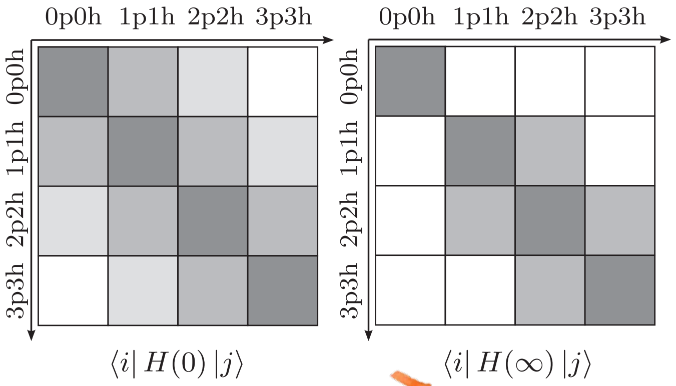

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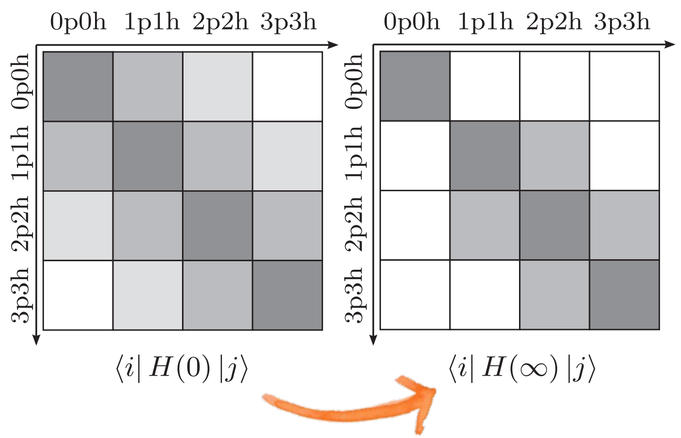

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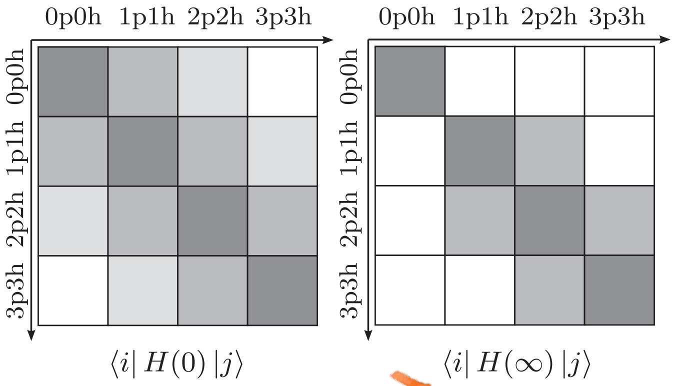

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Benchmarks

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

[Porro, Schwenk and Tichai, arXiv:2507.20665](https://arxiv.org/abs/2507.20665)

Dielectric theorem in the IMSRG

Add small perturbation to H

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

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

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

Numerically easier

Dielectric theorem in the IMSRG

Add small perturbation to H

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

$$H(\lambda)\left|\Psi(\lambda)\right\rangle = E(\lambda)\left|\Psi(\lambda)\right\rangle$$

$$m_{-1}(Q) = \sum_\nu \frac{|\langle \Psi_\nu | Q | \Psi_0 \rangle|^2}{E_\nu - E_0}$$

$$= -\frac{1}{2}\left[\frac{\partial \langle \Psi(\lambda)|Q|\Psi(\lambda)\rangle}{\partial \lambda}\right]_{\lambda=0}$$

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Numerically easier

Steps

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

Perturbation

$H(0,0)$ → $H(0,\lambda)$

IMSRG flow

IMSRG flow

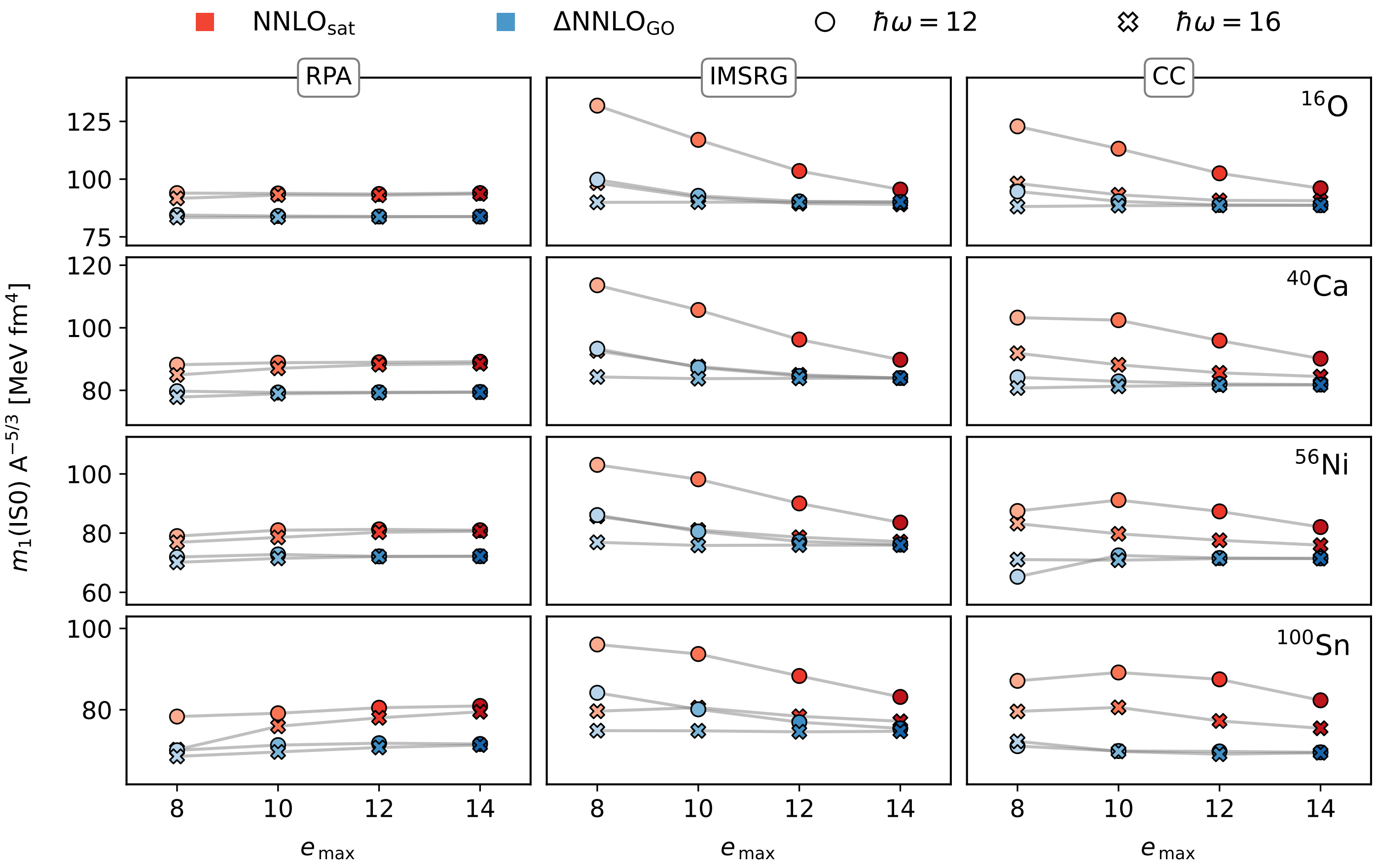
$H(s,0)$ $H(s,\lambda)$

Disclaimer: only scalar perturbations

IMSRG and CC results

Application to monopole moments

[CC results from Francesca Bonaiti and Sonia Bacca]



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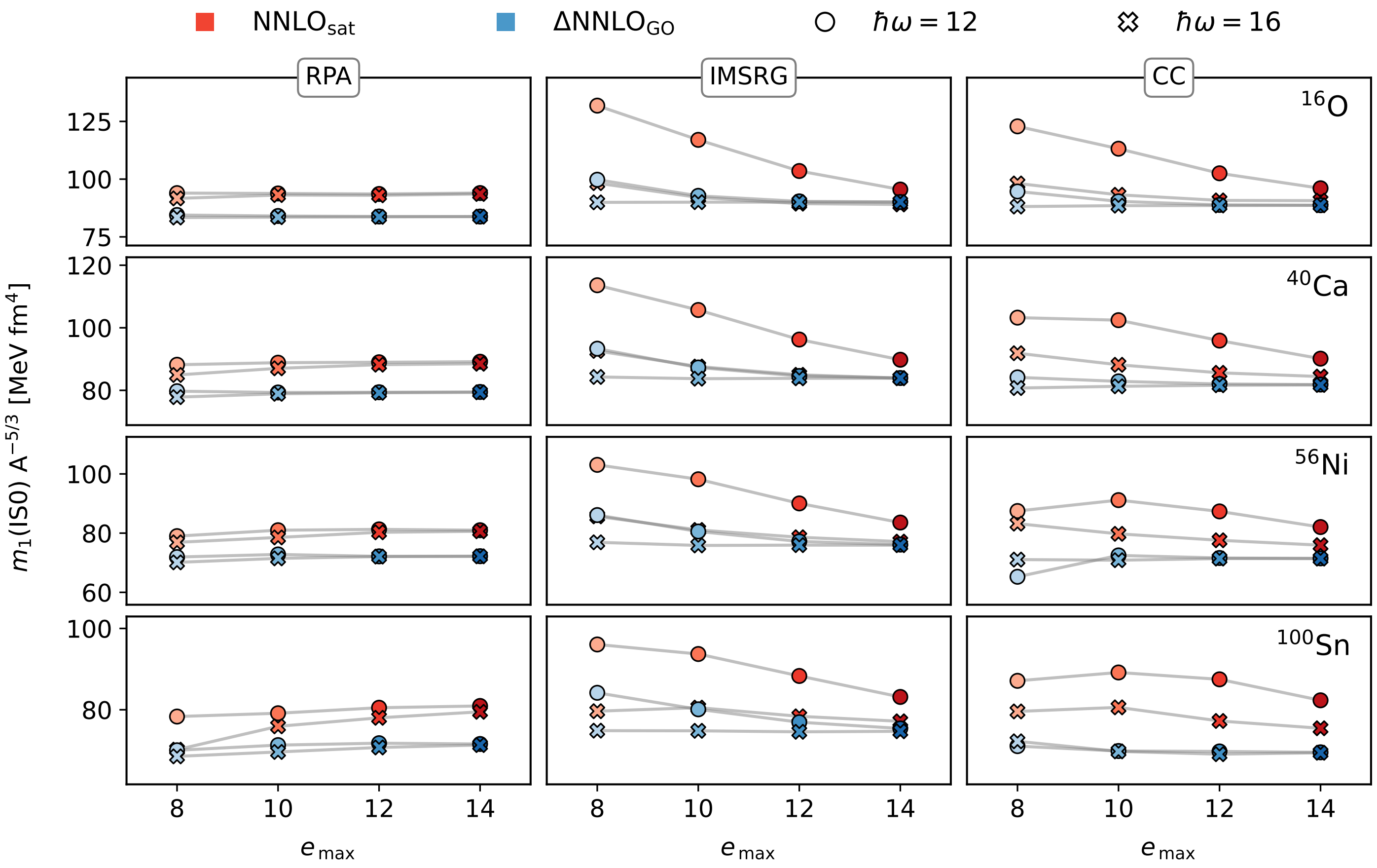

Application to monopole moments

Comparison to RPA and LIT-CC

Excited-states methods

Interaction comparison

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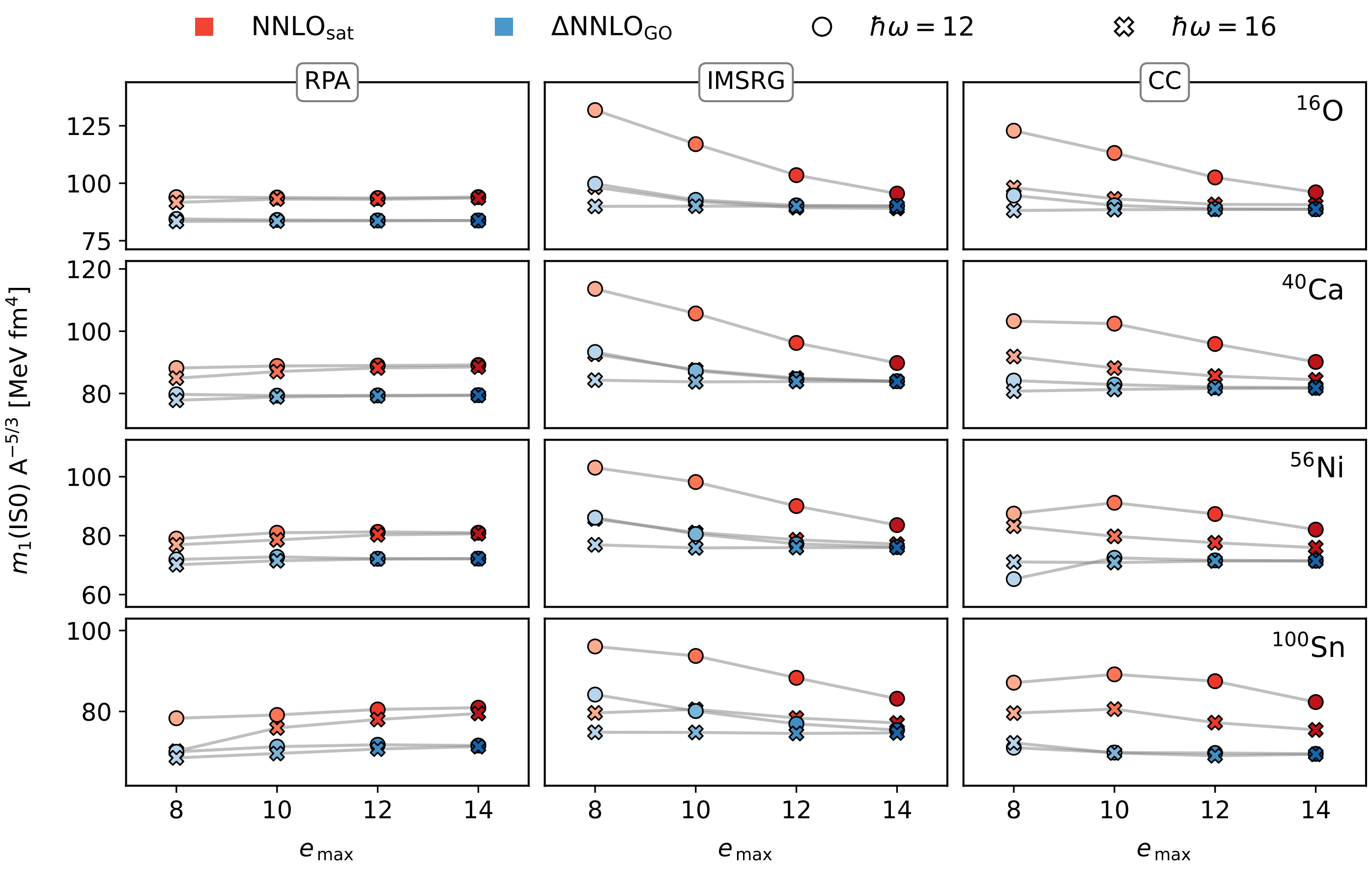

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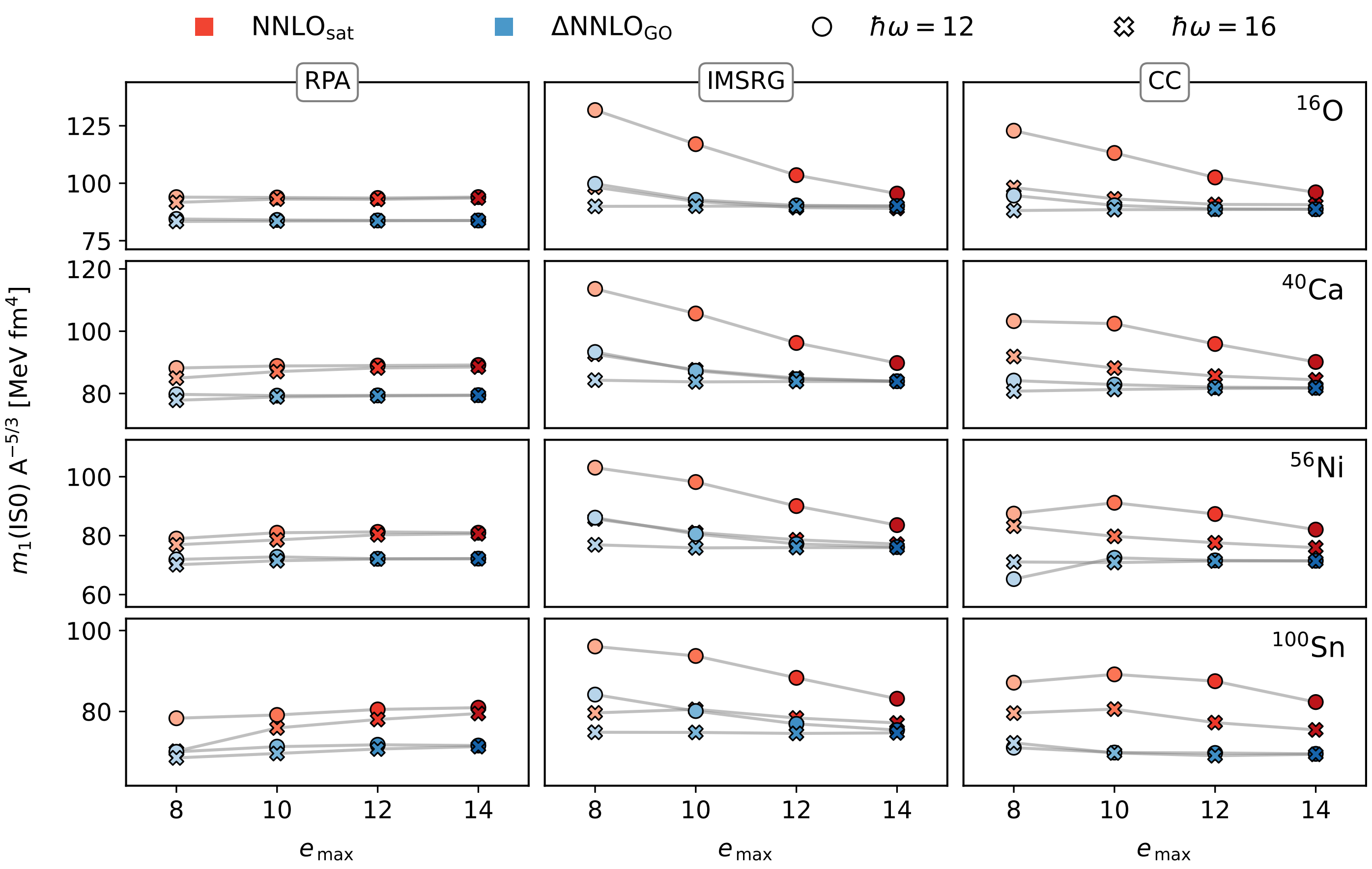

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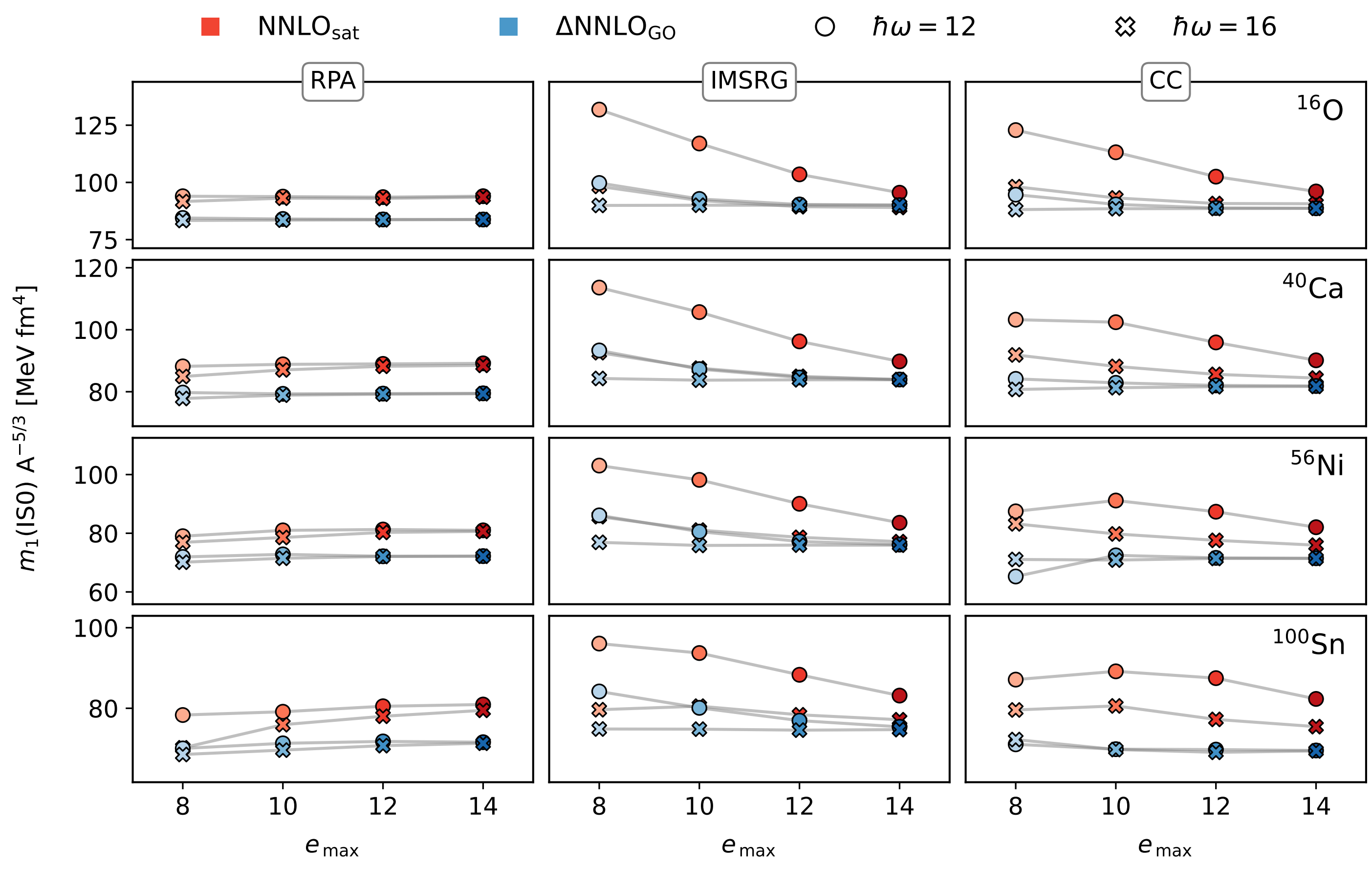

[Arthuis et al, arXiv:2401.06675]

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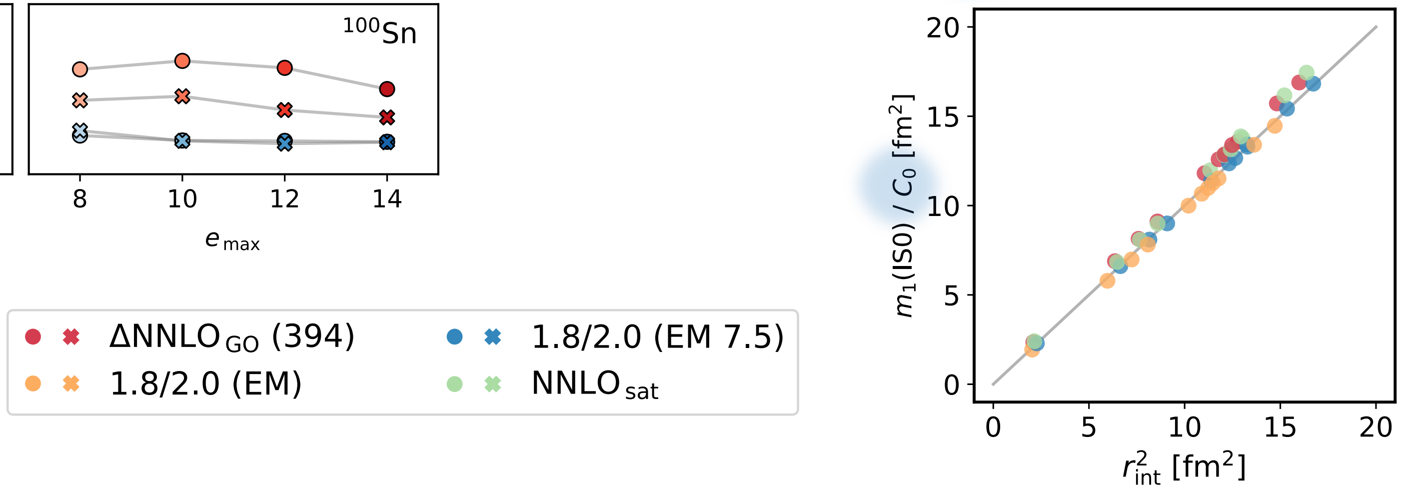

Link to nuclear matter

[Blaizot, Phys. Rep. 64, 1980]

Link to nuclear matter

Compression modulus in infinite systems

(thermodynamic limit)

$$K_\infty \equiv k_{F_0}^2 \left. \frac{\mathrm{d}^2 E/A}{\mathrm{d}k_F^2} \right|_{k_{F_0}}$$

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Average in nuclei

$$E_\mathrm{GMR} = \sqrt{\frac{m_1}{m_{-1}}}$$

[Blaizot, Phys. Rep. 64, 1980]

Extrapolation to infinite matter

Leptodermous expansion

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Doubly-closed-shell N=Z nuclei

^{16}O, ^{40}Ca, ^{56}Ni, ^{100}Sn

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Neglect Coulomb

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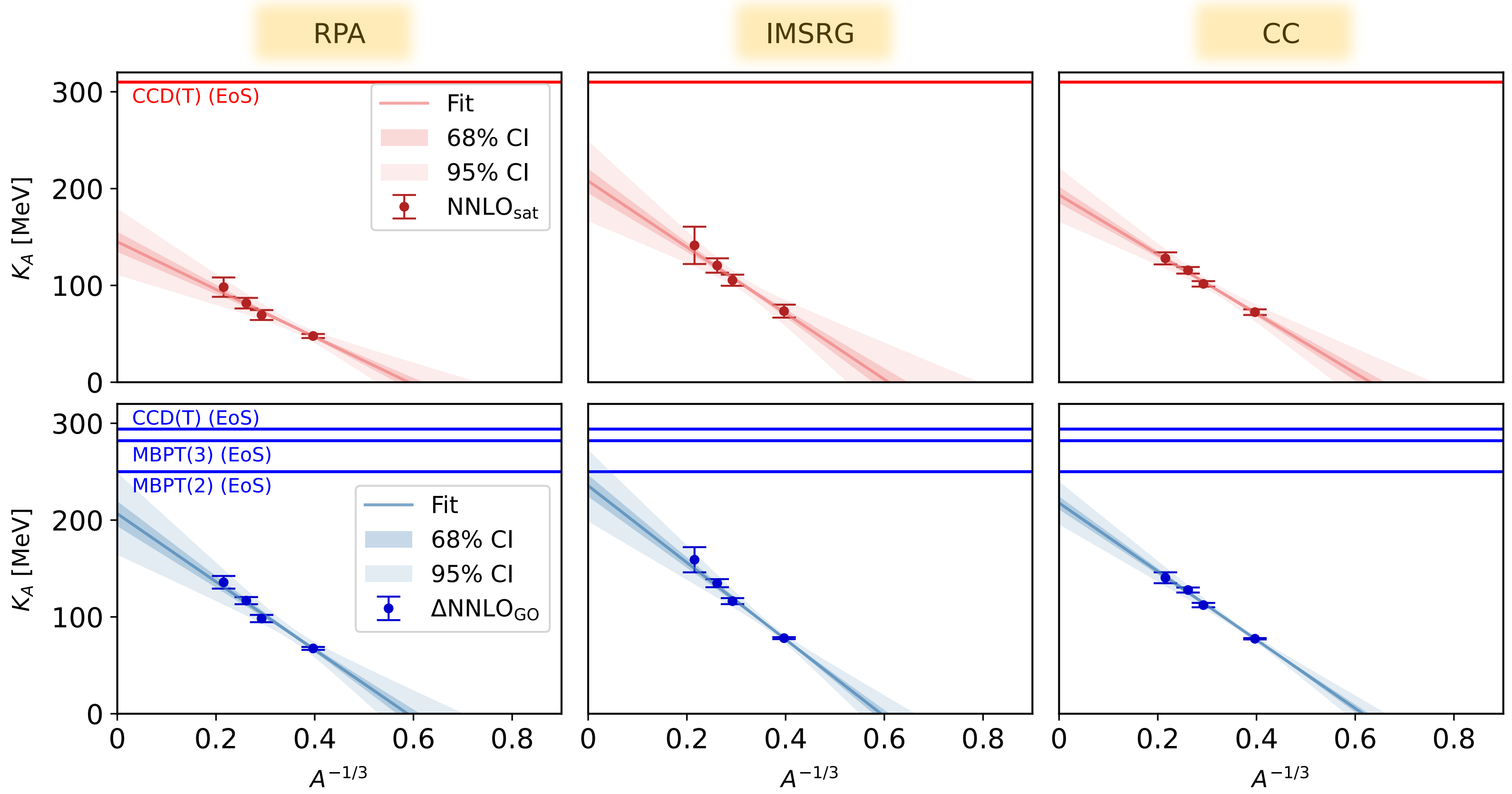

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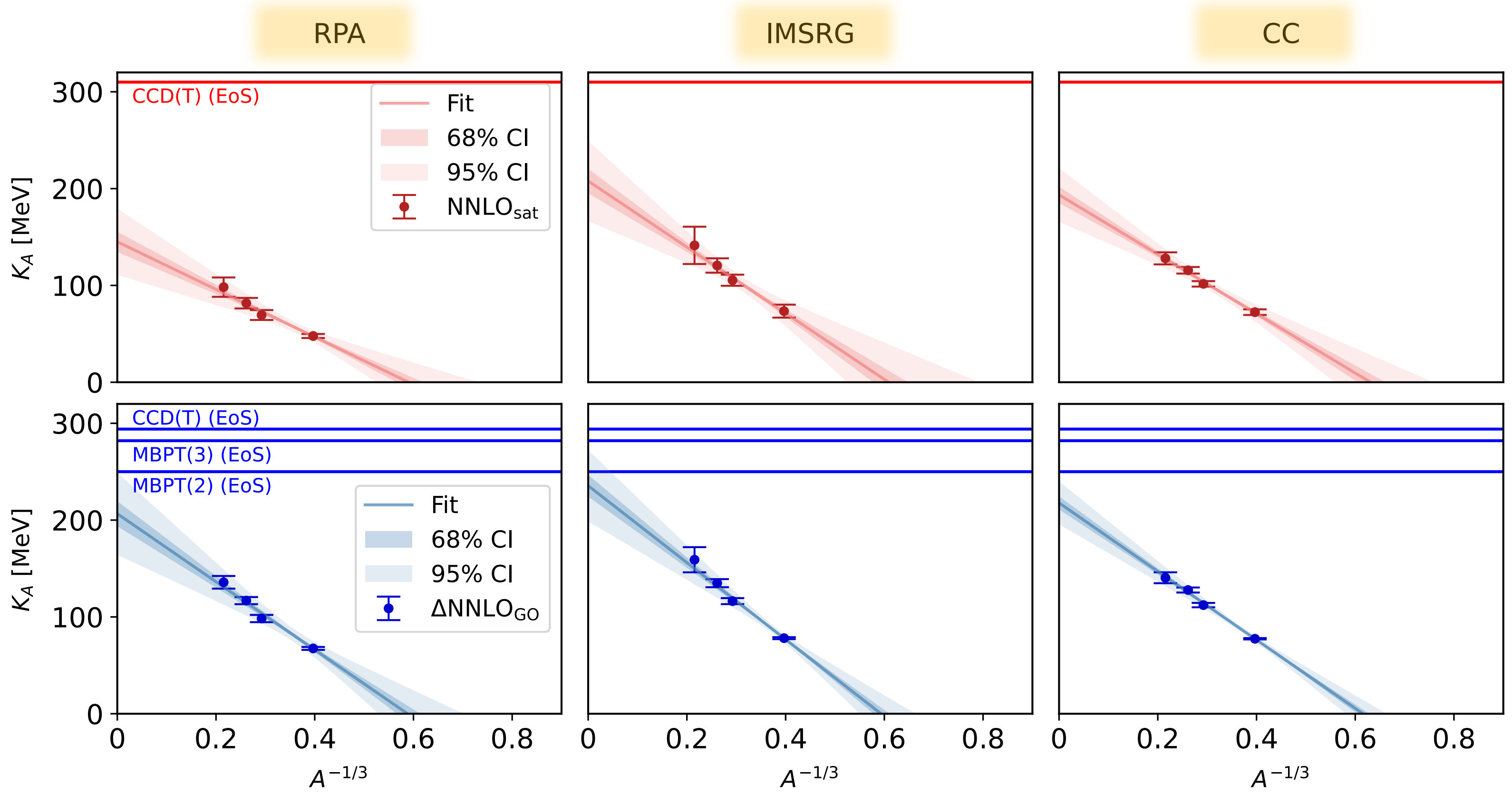

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Model space uncertainty

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[Jiang et al, PRC 102(5), 054301, 2020]

Extrapolation to infinite matter

Leptodermous expansion

$$K_A = (M/\hbar^2)\langle r^2\rangle E_{GMR}^2 \qquad E_{GMR} = \sqrt{\frac{m_1}{m_{-1}}}$$

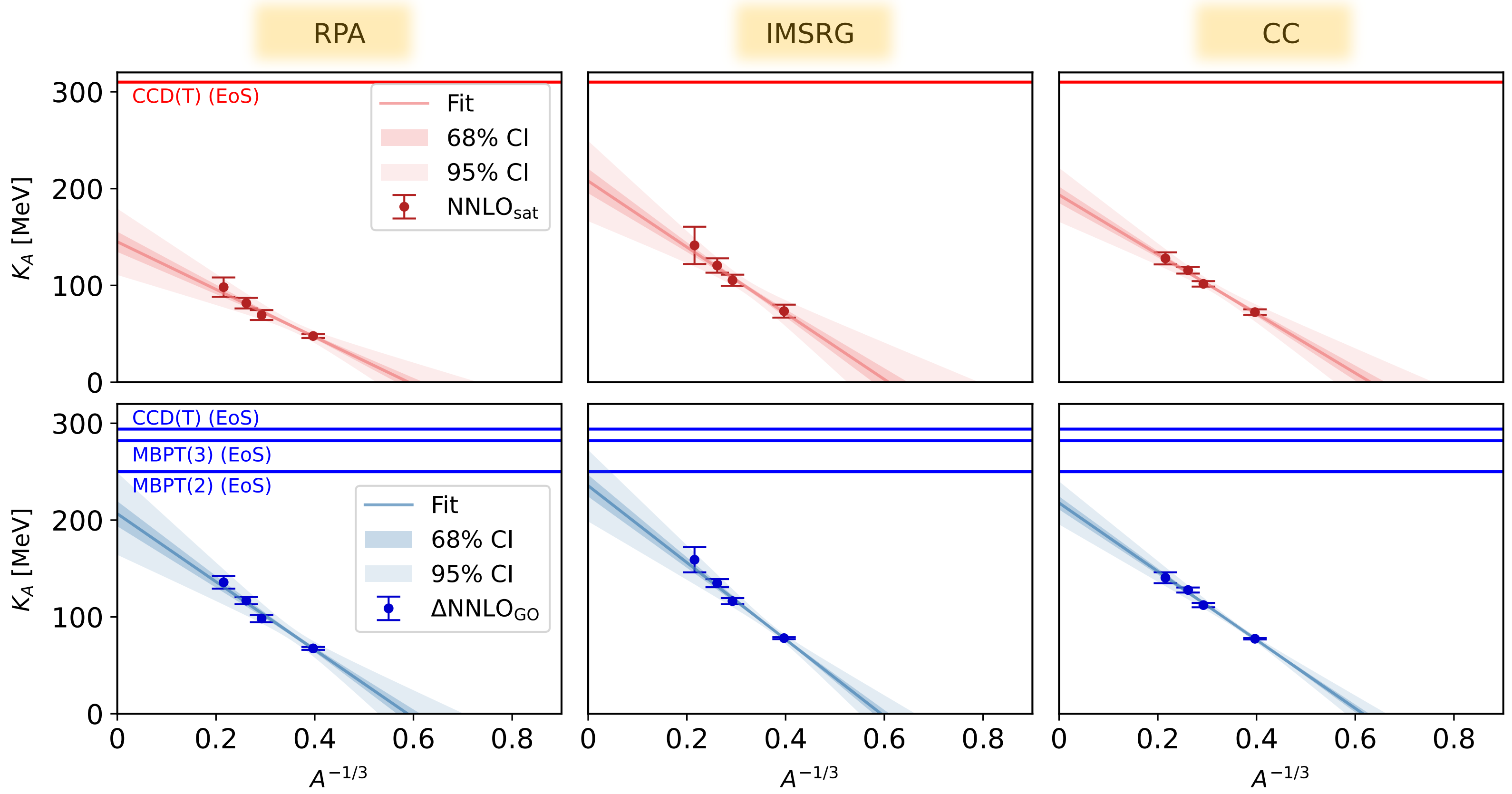
$$K_A = K_{vol} + K_{surf}A^{-1/3} + K_{Coul}Z^2A^{-4/3} + K_{sym}\beta^2$$

Doubly-closed-shell N=Z nuclei

^{16}O, ^{40}Ca, ^{56}Ni, ^{100}Sn

$$\beta \equiv \frac{N-Z}{N+Z}$$

$$K_A = K_{vol} + K_{surf}A^{-1/3} + K_{Coul}Z^2A^{-4/3}$$



Neglect Coulomb

$$x \equiv A^{-1/3}$$

$$K_A = K_\infty + K_{surf}\,x$$

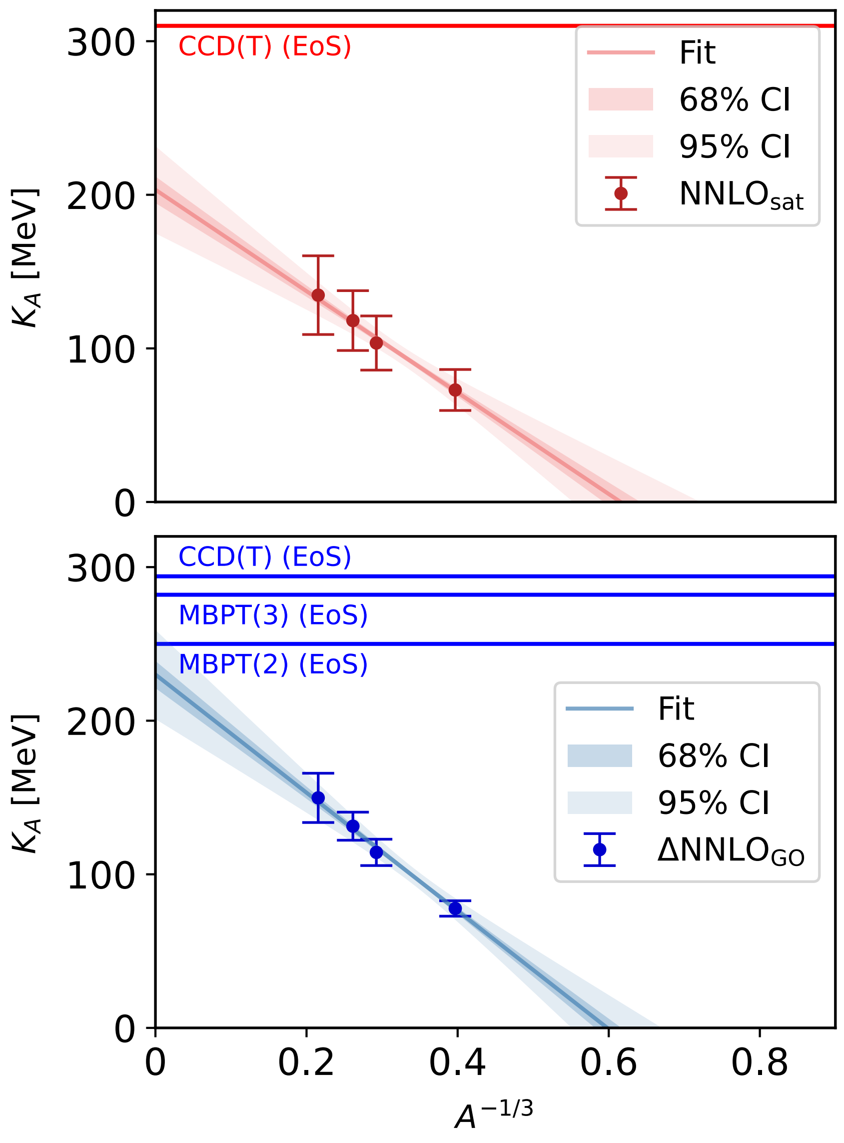
Model space uncertainty

Correlated values larger than HF

[Ekström et al, PRC 91(5), 051301, 2015]

[Jiang et al, PRC 102(5), 054301, 2020]

Extrapolation to infinite matter



$$K_{\mathrm{A}} = (M/\hbar^2)\langle r^2\rangle E_{\mathrm{GMR}}^2$$

$$E_{\mathrm{GMR}} = \sqrt{\frac{m_1}{m_{-1}}}$$

$$x \equiv A^{-1/3}$$

$$K_A = K_\infty + K_{\mathrm{surf}}\, x$$

Model space uncertainty

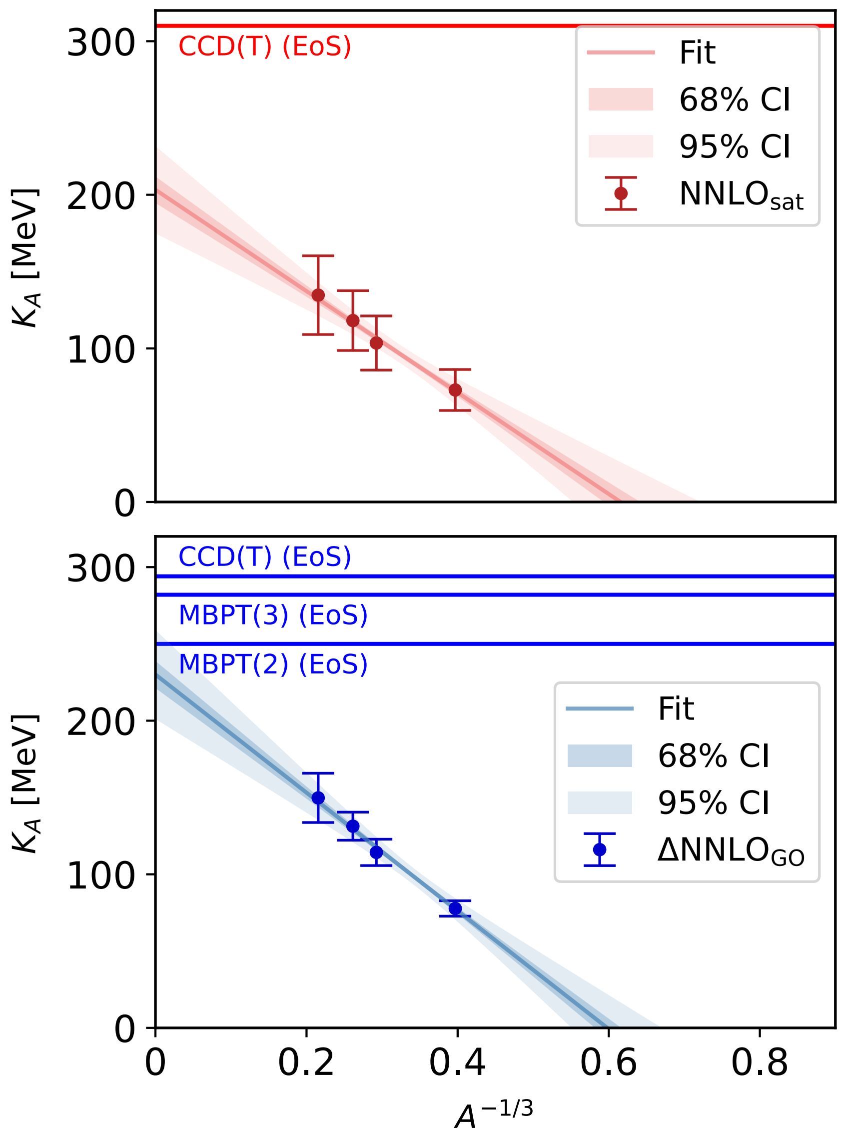
+

Many-body uncertainty

[Ekström et al, PRC 91(5), 051301, 2015]

[Jiang et al, PRC 102(5), 054301, 2020]

Extrapolation to infinite matter



$$K_\mathrm{A} = (M/\hbar^2)\langle r^2\rangle E^2_\mathrm{GMR}$$

$$E_\mathrm{GMR} = \sqrt{\frac{m_1}{m_{-1}}}$$

$$x \equiv A^{-1/3}$$

$$K_A = K_\infty + K_\mathrm{surf}\, x$$

Model space uncertainty

+

Many-body uncertainty

Agreement with accepted values K = 240 ± 20 MeV

Tension with nuclear matter calculations

[Ekström et al, PRC 91(5), 051301, 2015]

[Jiang et al, PRC 102(5), 054301, 2020]

Outline

Introduction

- Physics case
- The ab initio philosophy

PGCM – open-shell systems

- Theoretical insights
- Numerical results
- Comparison to experiment

IMSRG – closed-shell systems

- Strategy
- Numerical results
- Extrapolation to infinite matter

Challenges and opportunities

Conclusions and perspectives

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PGCM

- Reliable method for *ab initio* spectroscopy
- More systematic studies for heavier deformed isotopic chains

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- Average properties of the response (moments)
- Takes properly into account correlation effects

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- Benchmark for other methods (excited states)
- Systematic studies of H properties (e.g. incompressibility)

Conclusions and perspectives

PGCM

- Reliable method for *ab initio* spectroscopy
- More systematic studies for heavier deformed isotopic chains

IMSRG

- Average properties of the response (moments)
- Takes properly into account correlation effects
- Benchmark for other methods (excited states)
- Systematic studies of H properties (e.g. incompressibility)
- Extend the method to open-shell systems (VS, deformed, MR)

Thank you for the attention

Robert Roth
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Alexander Tichai

Thomas Duguet
Jean-Paul Ebran
Mikael Frosini
Vittorio Somà

Sonia Bacca

Francesca Bonaiti

Backup slides

Model-space convergence

Dipole response

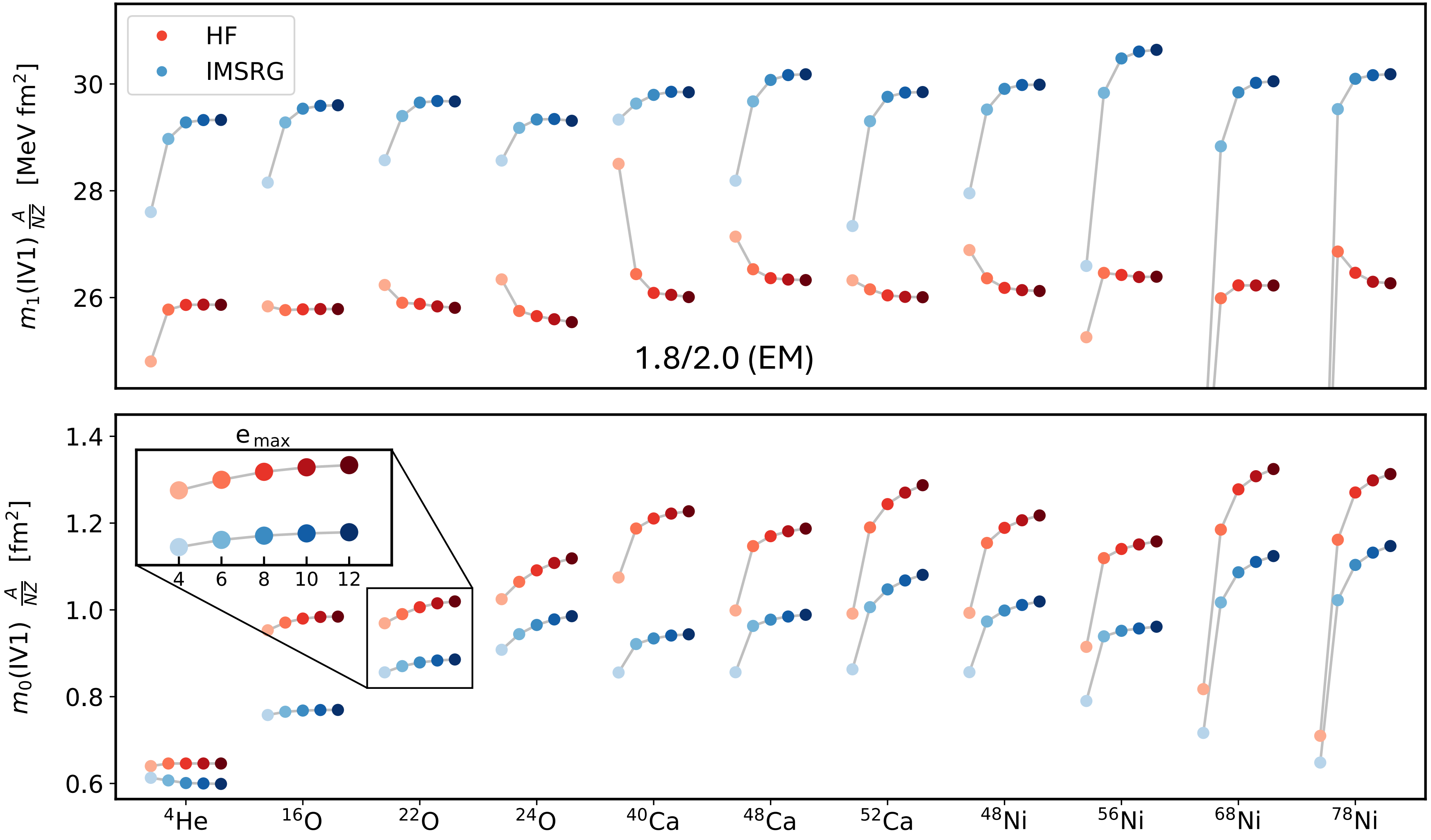
$$Q^{\mathrm{IV}}_{1\mu} = \frac{N}{A}\sum_{i=1}^{Z} r_i Y_{1\mu}(\hat{r}_i) - \frac{Z}{A}\sum_{i=1}^{N} r_i Y_{1\mu}(\hat{r}_i)$$

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

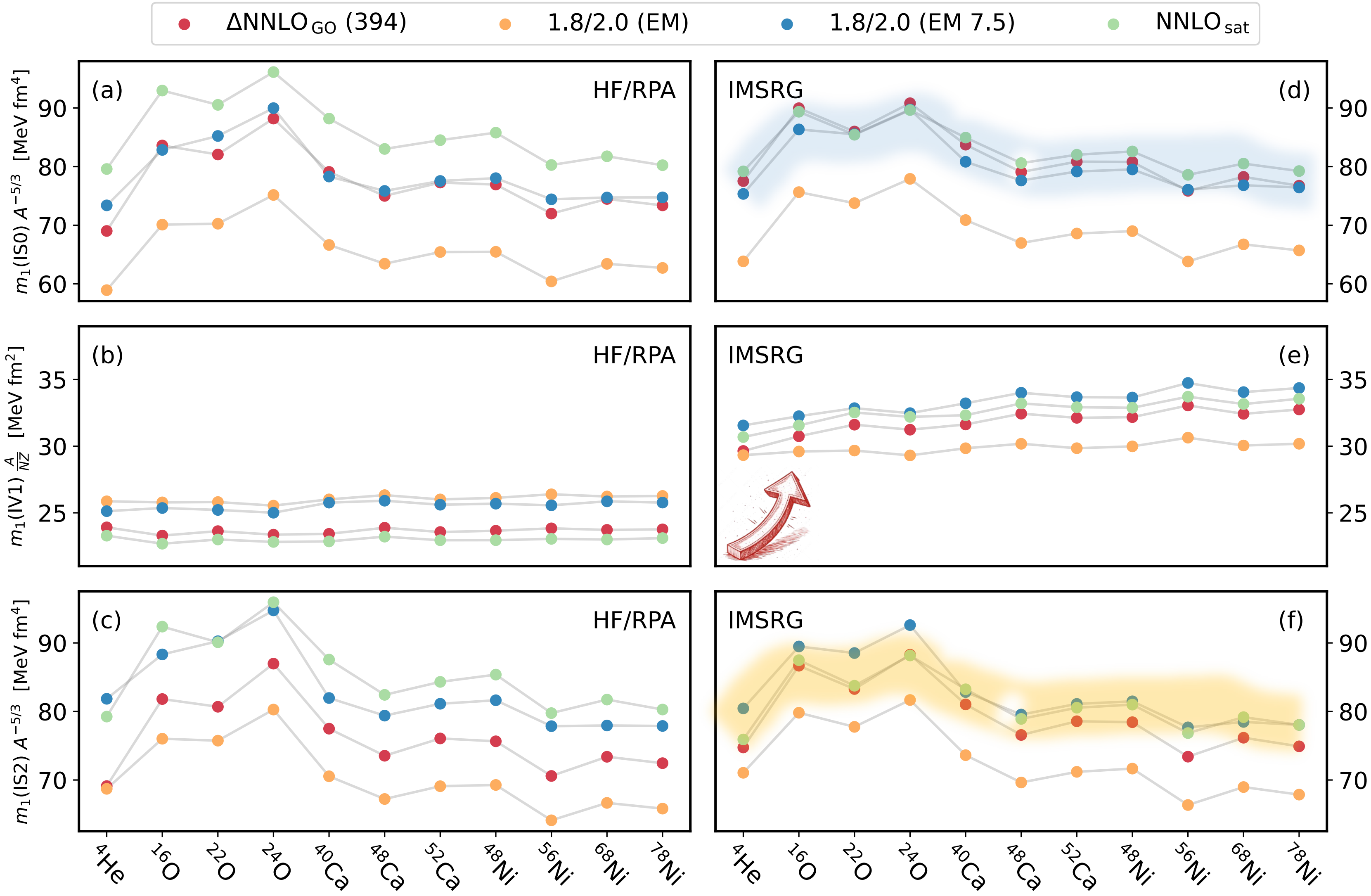
- Large correlation impact
- Relative difference ~0.2%
- Similar error for $\hbar\omega$ variations

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

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



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

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

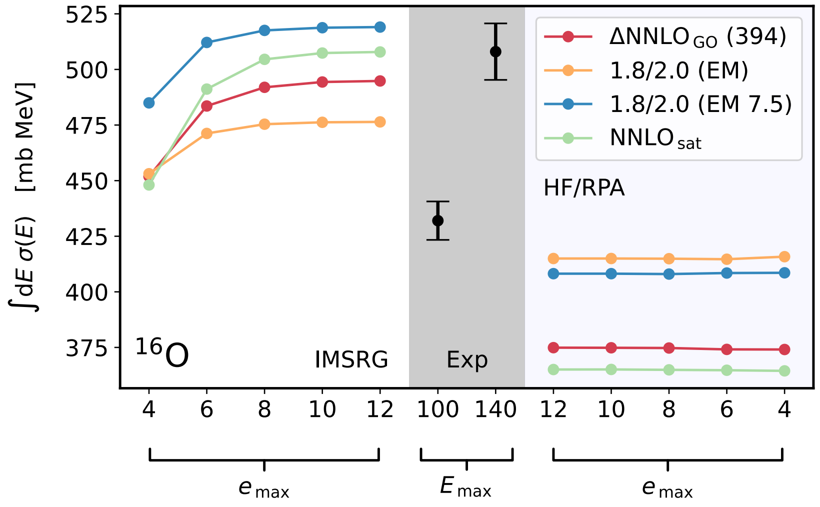
$$\approx 60\,\frac{NZ}{A}(1+\kappa)\quad \mathrm{mb}\cdot\mathrm{MeV}$$

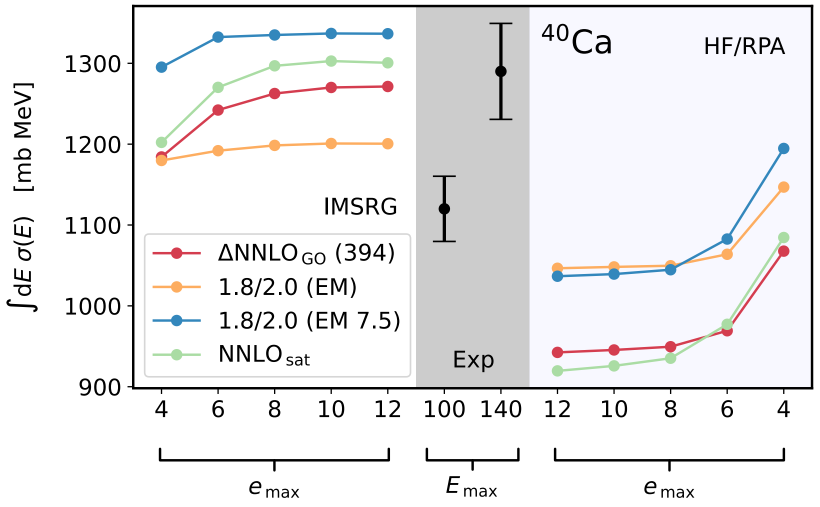
TRK sum rule

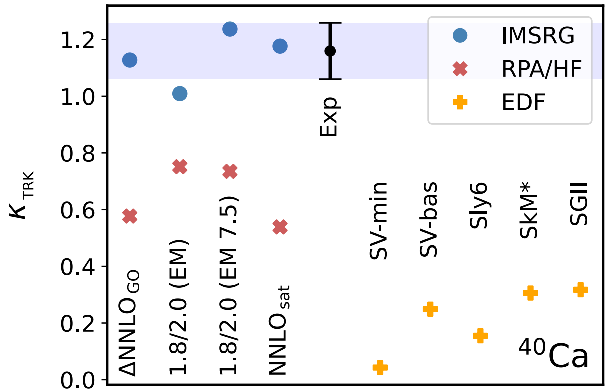
Pion-production threshold

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

[Ahrens et al., NPA, 1975]



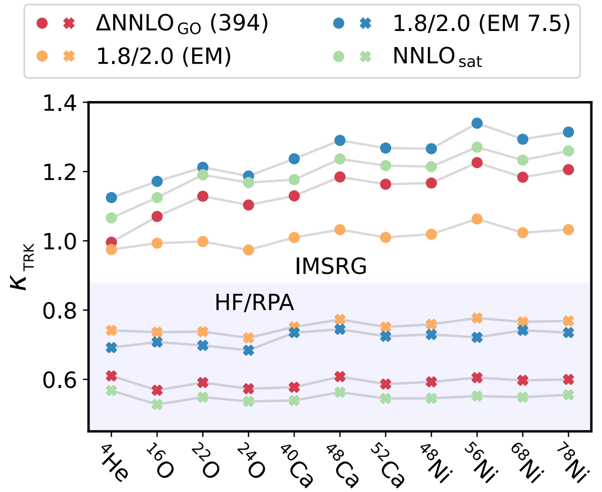




Comparison to EDF calculations

[Courtesy of P.-G. Reinhard]

Photoabsorption cross section



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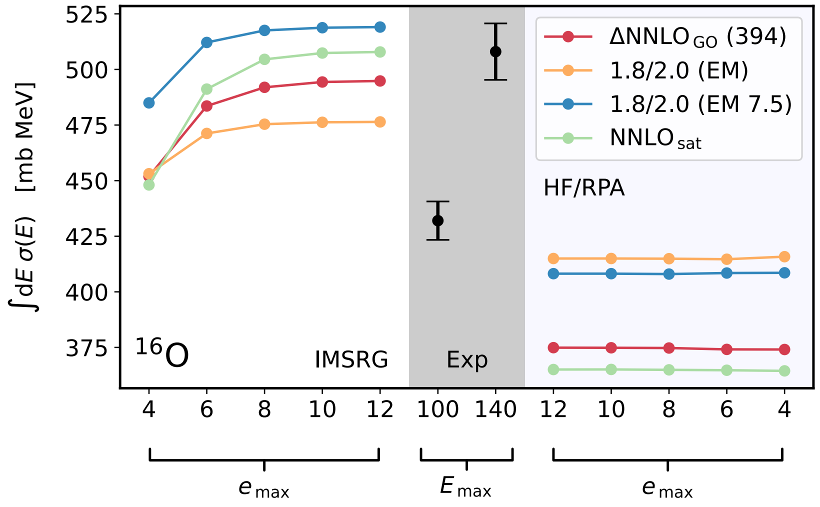
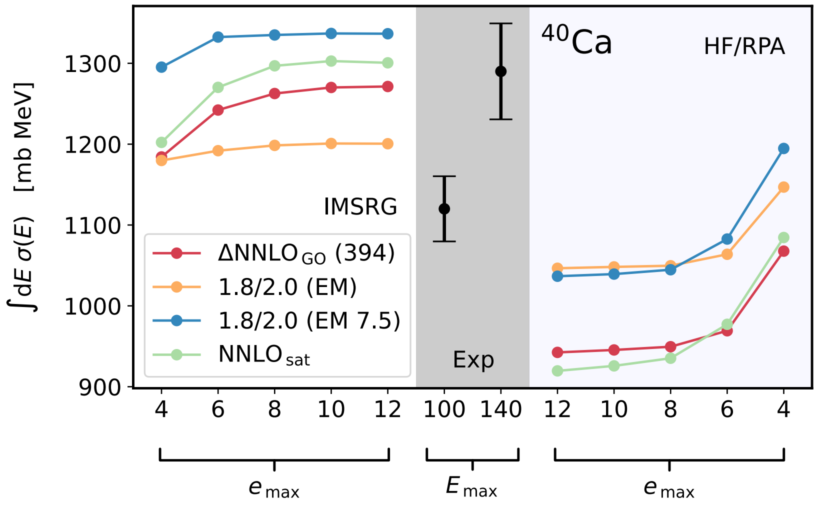
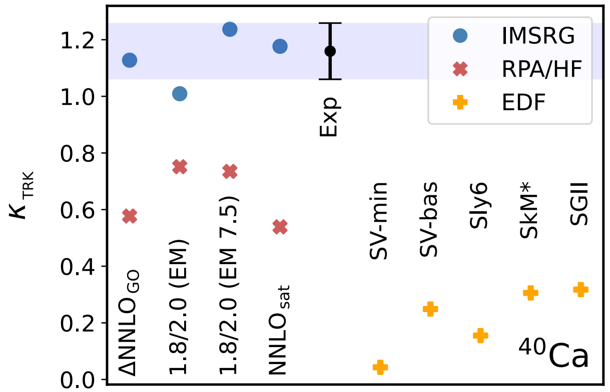






Both needed for consistent description

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

Comparison to EDF calculations

[Courtesy of P.-G. Reinhard]

Comparison to sum rules

Sum rules extensively studied in the past

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

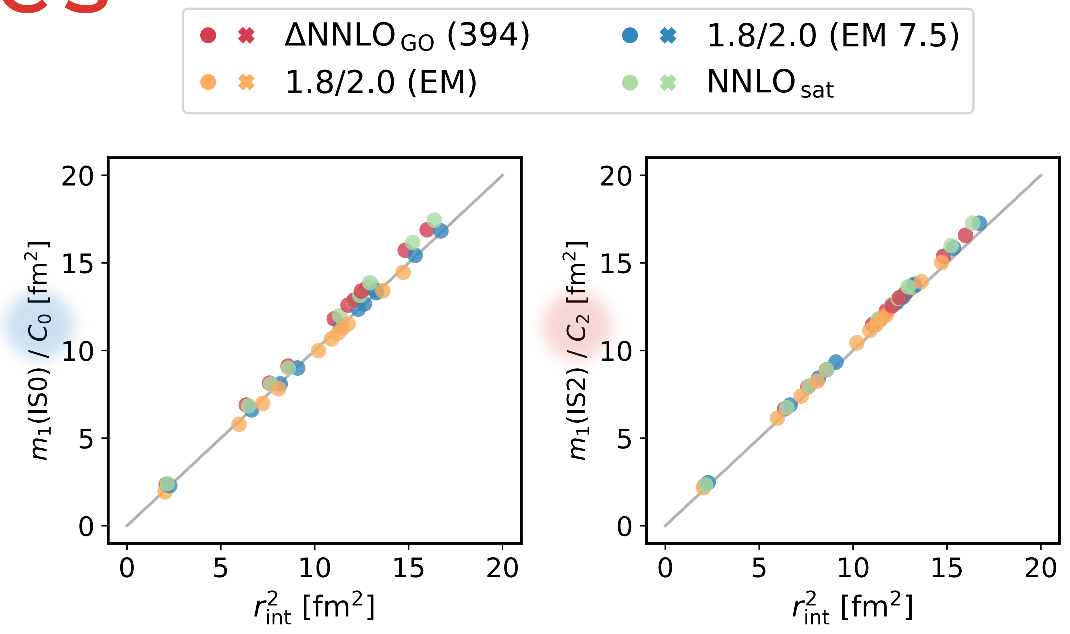
$$= \frac{1}{2}\langle\Psi_0|[Q_\lambda^\dagger(\vec{r}),[T,Q_\lambda(\vec{r})]]|\Psi_0\rangle$$

If V local

$$\mathrm{EWSR}_{\mathrm{int}}(r^2) = \frac{2\hbar^2}{m}\langle\Psi_0|r_{\mathrm{int}}^2|\Psi_0\rangle$$

$$\mathrm{EWSR}_{\mathrm{int}}(Q_2) = \frac{25}{4\pi}\frac{\hbar^2}{m}\langle\Psi_0|r_{\mathrm{int}}^2|\Psi_0\rangle$$

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



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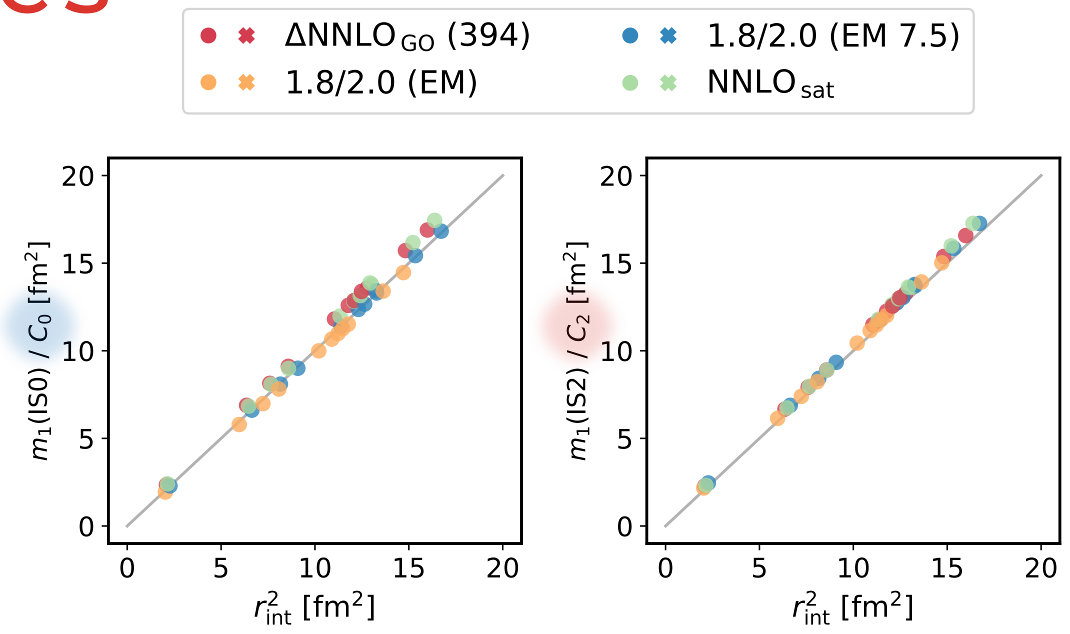
True if continuity Eq is only 1B

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

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

If V local



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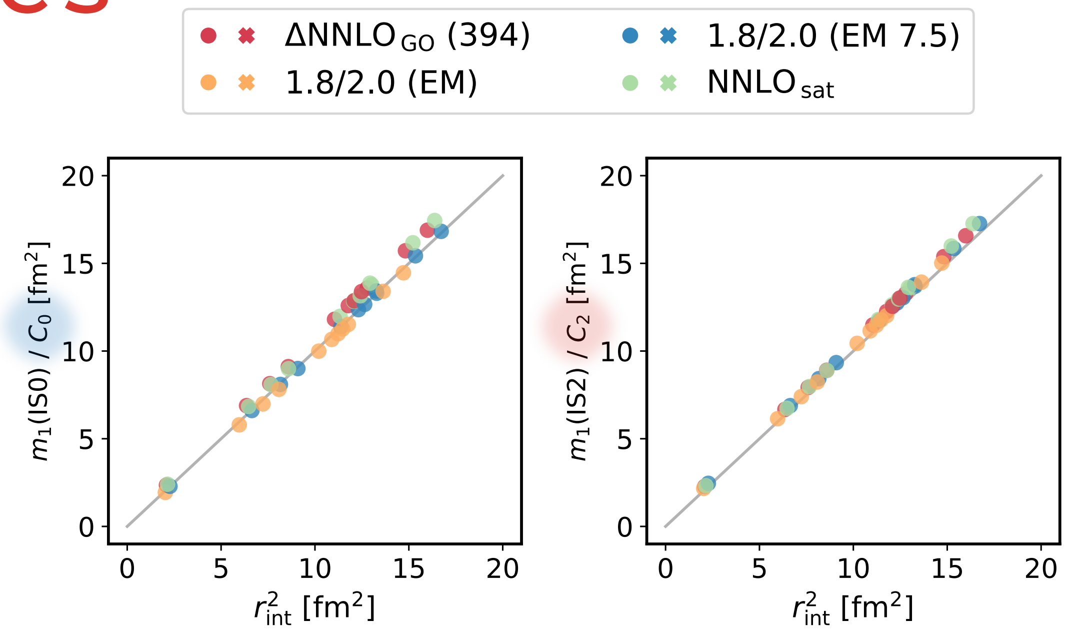

But many-body currents can be there !

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

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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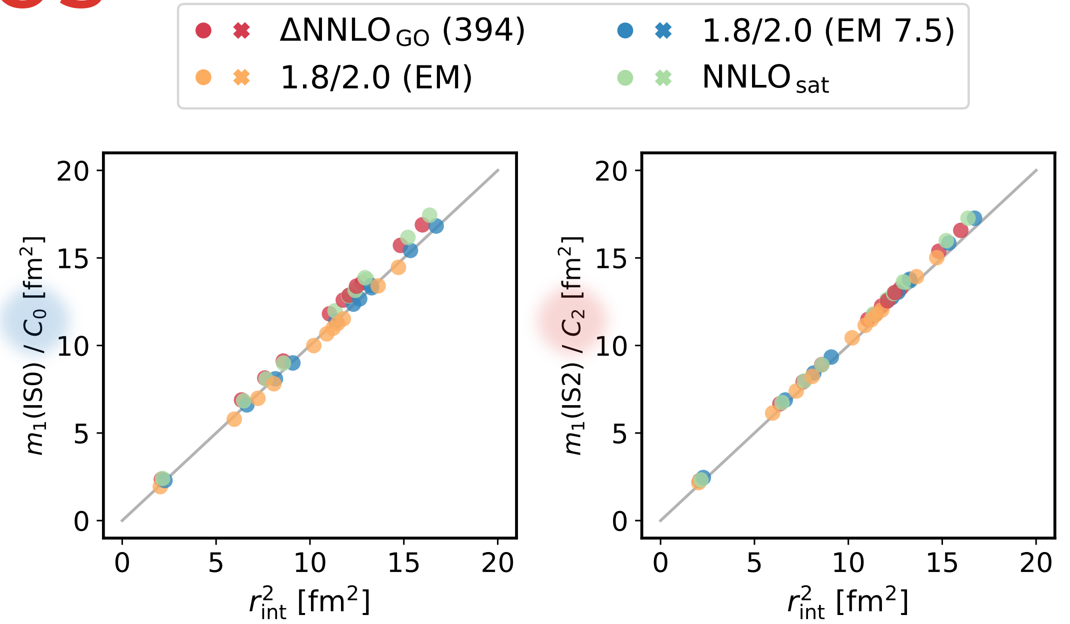

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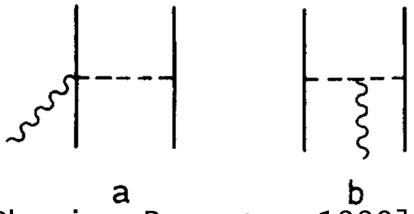
$$\vec\nabla \cdot \vec j_{[\nu]}(\vec r) + \frac{i}{\hbar}\sum_{\mu=1}^{\nu}[H_{[\nu+1-\mu]}, \rho_{[\mu]}(\vec r)]_{[\nu]} = 0$$

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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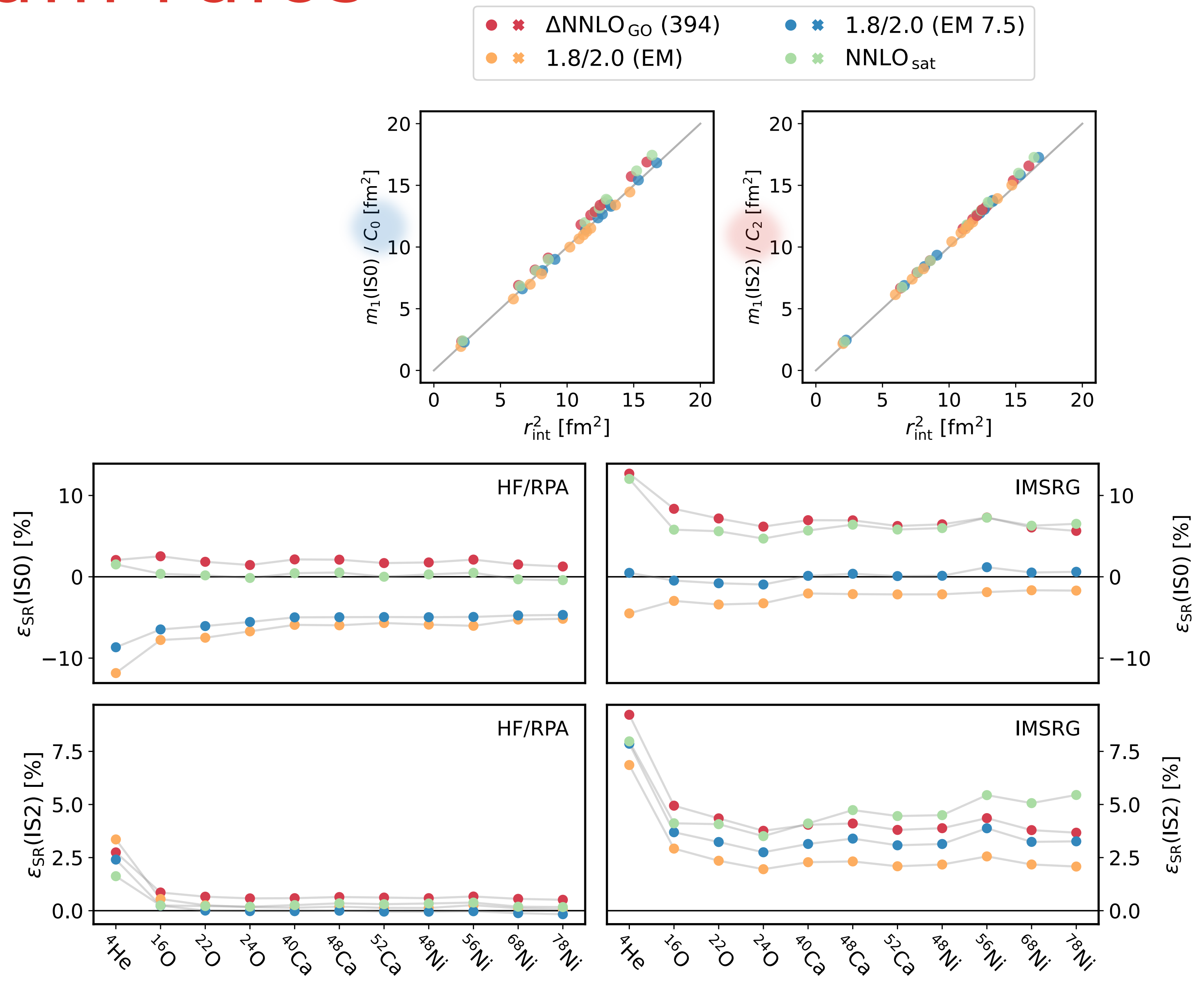

Let's look more closely

Relative difference

$$\varepsilon_{\mathrm{SR}}(Q_\lambda)[\%] \equiv \frac{m_1(Q_\lambda) - \mathrm{EWSR}(Q_\lambda)}{\mathrm{EWSR}(Q_\lambda)} \times 100$$

Differences from EWSR

- Nonlocalities
- Two-body currents

m1 from moments is better !

Going open-shell

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