Three-Body Corrections and Applications of the In-Medium NCSM

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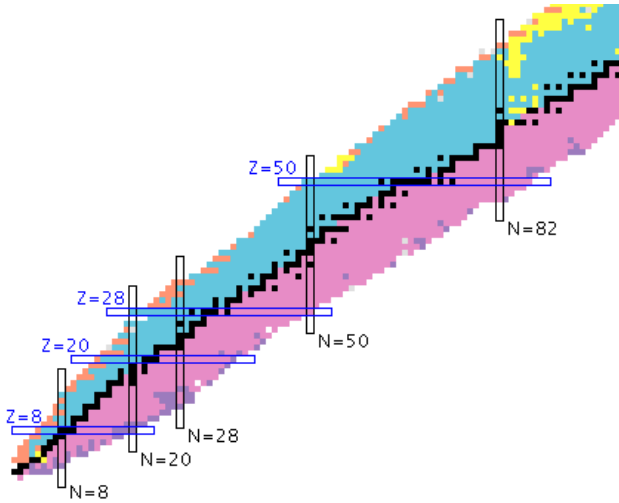
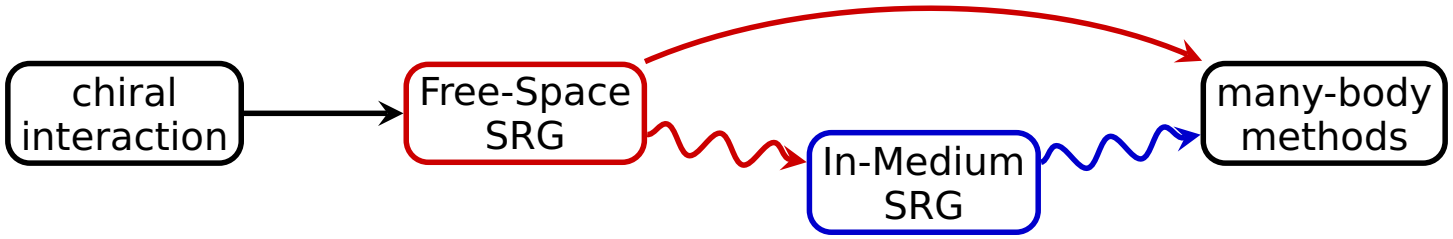
Overview

- family of non-local chiral NN+3N interactions up to N3LO optimized to medium mass nuclei
- In-Medium No-Core Shell Model
- applications to carbon isotopic chain including electromagnetic properties
- leading-order three-body correction to transformed operators





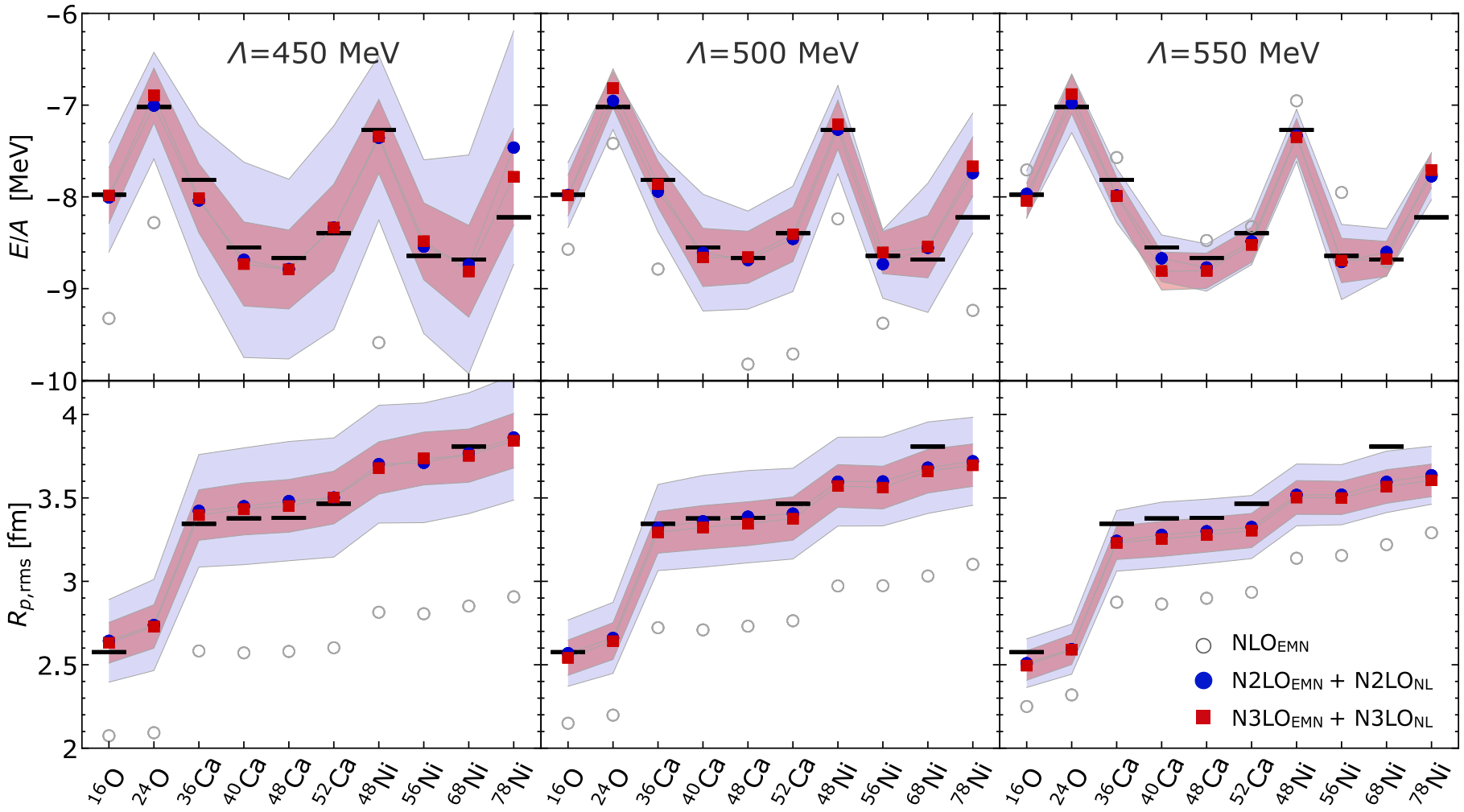
Family of Chiral Interactions up to N3LO

T. Hüther *et al.*, Phys. Lett. B 808, 135651 (2020)

- chiral NN interaction by Entem, Machleidt & Nosyk
  - LO to N3LO
  - non-local regulator
  - cutoff 450, 500 & 550 MeV
- supplement non-local 3N interaction at N2LO and N3LO
  - non-local regulator
  - cutoff 450, 500 & 550 MeV
- fix c_E in few-body sector, keep c_D as parameter
  - c_E fit to triton binding energy
  - alternative: c_E from combined fit to ^{3}H, ^{4}He energy and radius
- explore dependence of many-body observables on c_D
- fix c_D via ^{16}O groundstate energy

Performance in Medium-Mass Calculations

T. Hüther *et al.*, Phys. Lett. B 808, 135651 (2020)

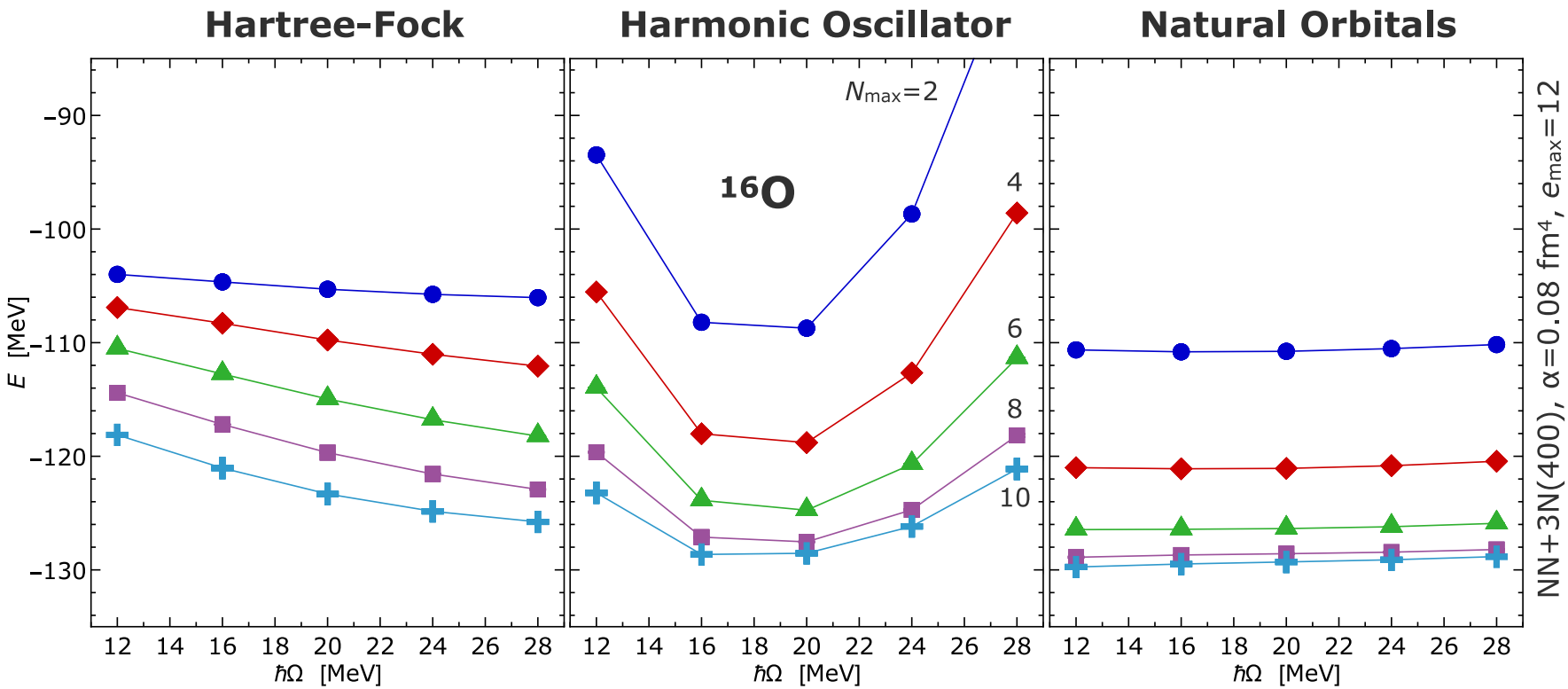


IM-SRG(M2), natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, e_{max}=12, $E_{3\mathrm{max}}$=16,
error bands show interaction + many-body uncertainties

Natural-Orbital Basis

A. Tichai *et al.*, Phys. Rev. C 99, 034321 (2019)

- eigenbasis of the one-body density matrix obtained from second-order MBPT calculation
- optimization of all single-particle states due to inclusion of correlated ground-state



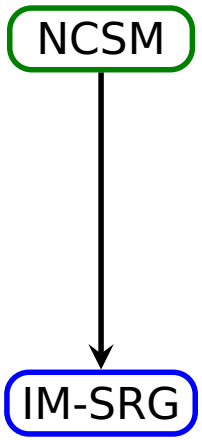
In-Medium No-Core Shell Model

NCSM

- NCSM calculation in small model space defines reference state

$$|\Psi_{\text{ref}}\rangle = \sum_i c_i |\Phi_i\rangle$$

In-Medium No-Core Shell Model



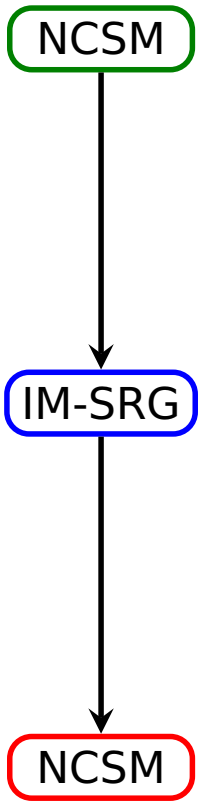
- NCSM calculation in small model space defines reference state

$$|\Psi_{\text{ref}}\rangle = \sum_i c_i |\Phi_i\rangle$$

- perform **multi-reference** IM-SRG aiming at decoupling reference state from generalized ph-excitations in a magnus formalism

$$\frac{d}{ds}\hat{\Omega}(s) = \sum_{k=0}^{\infty} \frac{B_k}{k!} \left[\hat{\Omega}(s), \hat{\eta}(s)\right]_k, \quad \hat{O}(s) = \sum_{k=0}^{\infty} \frac{1}{k!} \left[\hat{\Omega}(s), \hat{O}(0)\right]_k$$

In-Medium No-Core Shell Model



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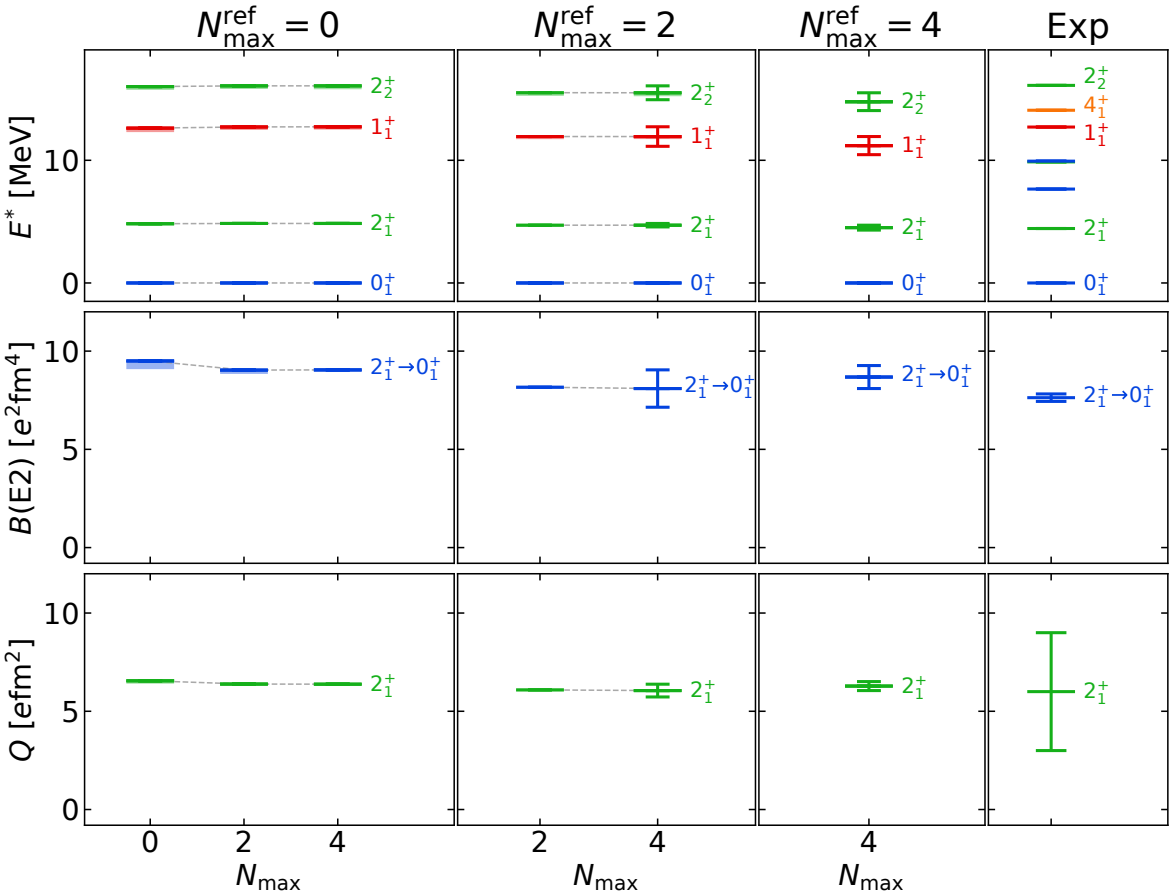
- use IM-SRG-evolved (non-scalar) operators $\hat{O}(s)$ as input for subsequent NCSM calculation
- convergence of NCSM calculation massively improved

Advantages of the IM-NCSM

- ab initio calculations with quantified truncation uncertainties
- direct calculations for all J = 0 nuclei
- odd isotopes accessible using a particle attached - particle removed scheme
- excitation spectrum comes automatically with the diagonalization
- access to all observables known in the NCSM
- electromagnetic observables possible via BCH series
- orders of magnitude more efficient than standard NCSM

^{12}C - $N_{\max}$ Convergence

A. D'Alessio, TM, *et al.*, Phys. Rev. C 102, 011302(R) (2020)

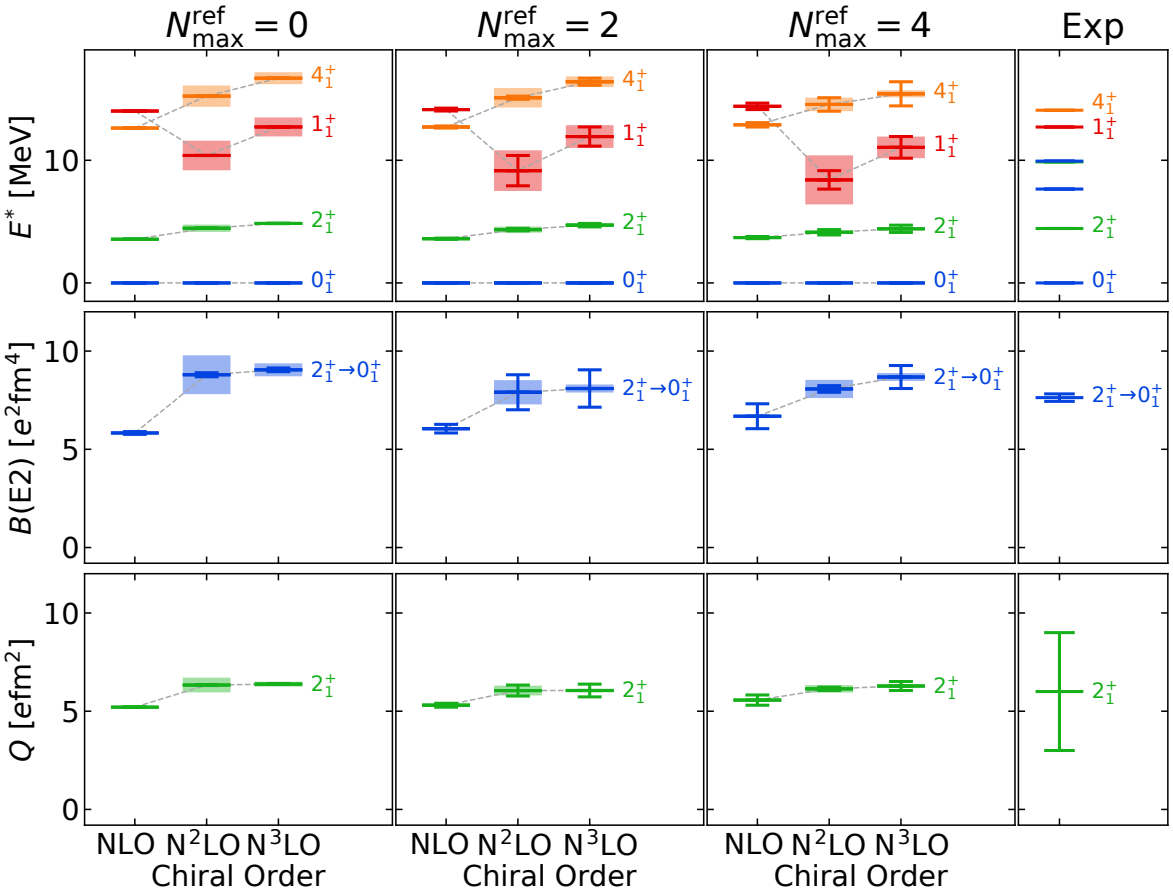


IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, $e_{\max}$=12, $E_{3\max}$=14,
many-body error bars

- spectrum, B(E2) transition strength and quadrupole moment vs. $N_{\max}$
- error bars indicate many-body uncertainties
- very good agreement with experiment

^{12}C - Order-by-Order Convergence

A. D'Alessio, TM, *et al.*, Phys. Rev. C 102, 011302(R) (2020)

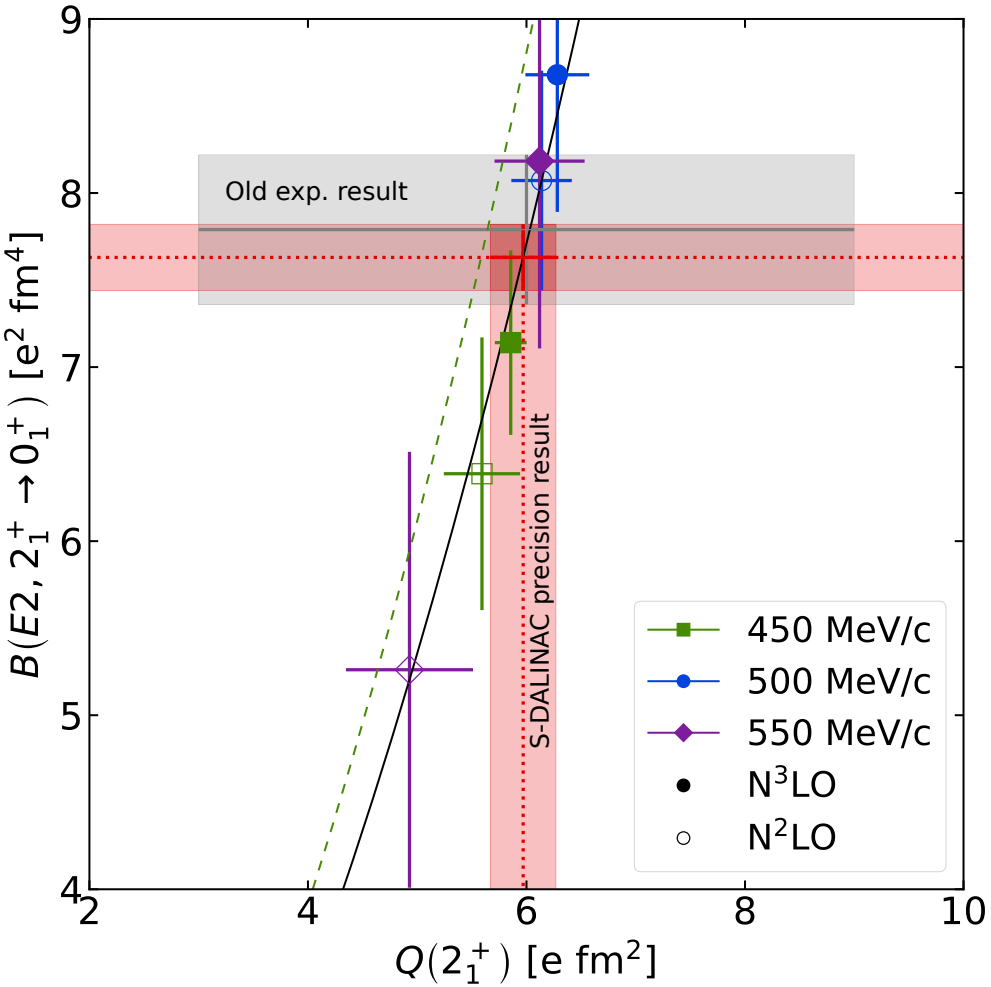


IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, e_{max}=12, E_{3max}=14,
many-body error bars, interaction error bands

- spectrum, B(E2) transition strength and quadrupole moment vs. interaction order
- error bars indicate many-body uncertainties, error bands interaction uncertainties
- very good agreement with experiment regarding combined many-body and interaction uncertainties

^{12}C - B(E2) vs. Q Correlation

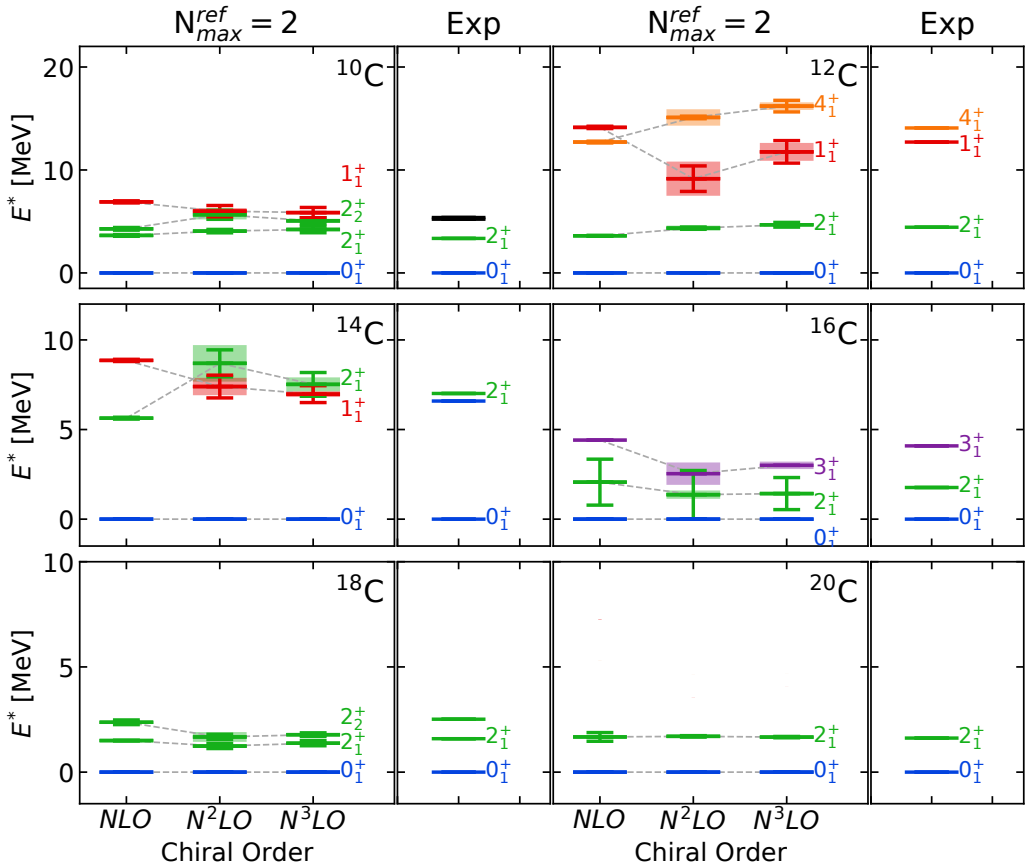
A. D'Alessio, TM, *et al.*, Phys. Rev. C 102, 011302(R) (2020)
A. Calci, R. Roth, Phys. Rev. C 94, 014322 (2016)



IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, e_{max}=12, E_{3max}=14,
combined many-body and interaction error bars

- correlation between B(E2) and quadrupole moment
- combined uncertainties
- strong correlation behaviour
- quadrupole moment from Bohr Mottelson fit $Q(2^+)$ = (5.97 ± 0.30) efm^2

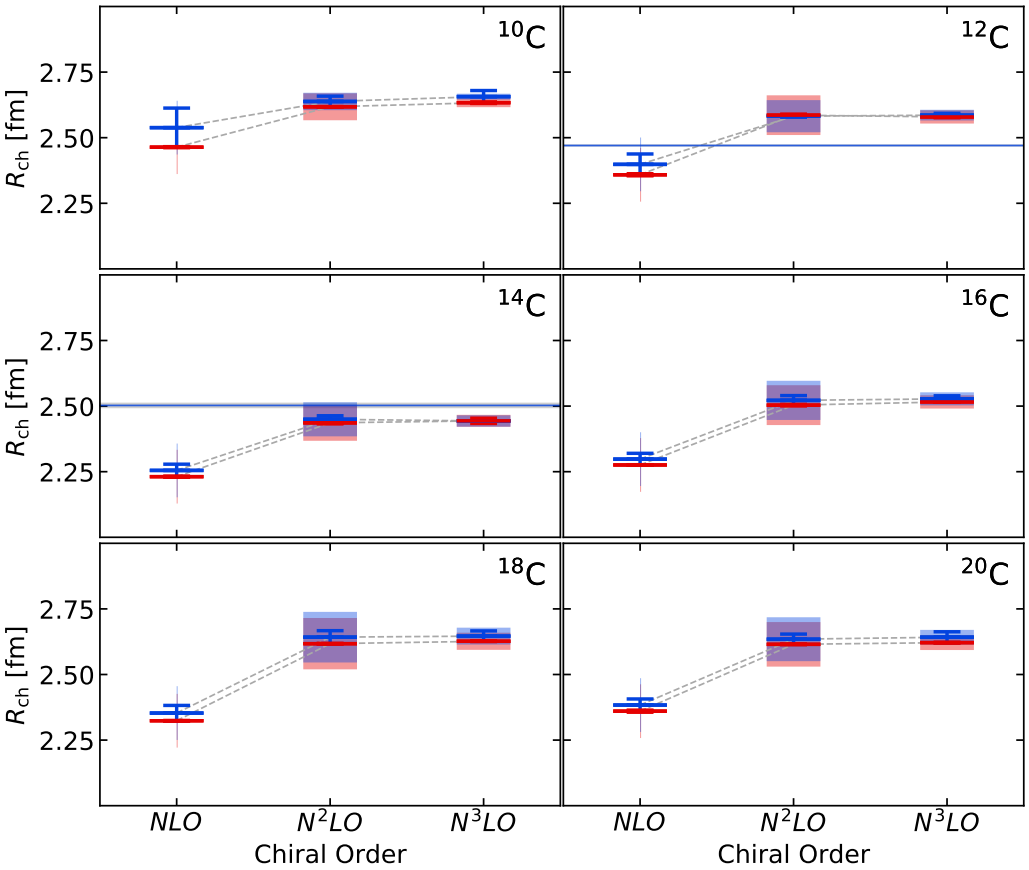
Carbon Isotopes: Spectra



IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, $e_{\max}$=12, $E_{3\max}$=14,
many-body error bars, interaction error bands

- spectrum of even carbon isotopes against the chiral interaction order
- good agreement with experimental values for all isotopes for both N^2LO and N^3LO
- N^2LO errors larger than N^3LO

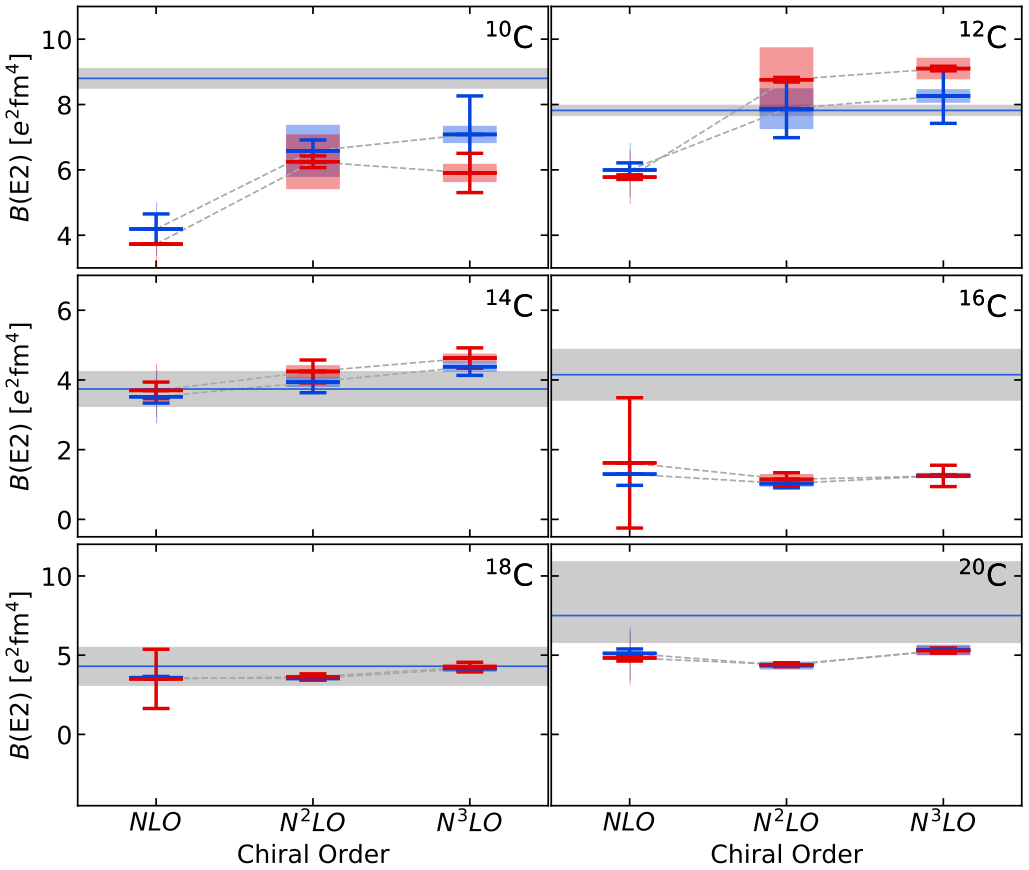
Carbon Isotopes: Charge Radii



IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, e_{max}=12, E_{3max}=14,
many-body error bars, interaction error bands

- charge radii for even carbon isotopes against chiral interaction order
- red: N^{ref}_{max}=0, blue: N^{ref}_{max}=2
- N2LO and N3LO ⇝ practically same result

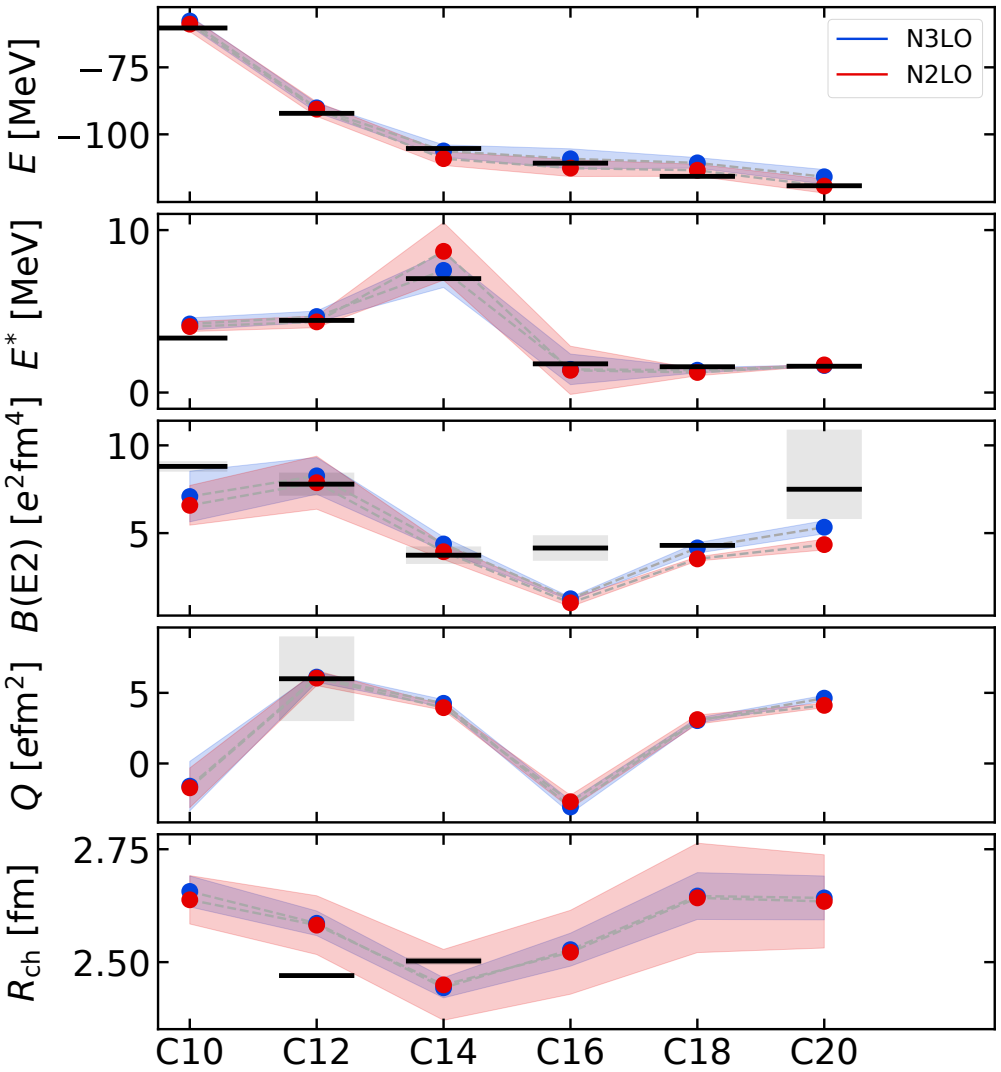
Carbon Isotopes: $B(\mathrm{E2}, 2_1^+ \rightarrow 0_1^+)$



IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, e_{max}=12, $E_{3\mathrm{max}}$=14,
many-body error bars, interaction error bands

- B(E2) transition strengths for even carbon isotopes against chiral interaction order
- red: $N_{\mathrm{max}}^{\mathrm{ref}}$=0, blue: $N_{\mathrm{max}}^{\mathrm{ref}}$=2
- good agreement for all isotopes compared to experimental values except for ^{16}C

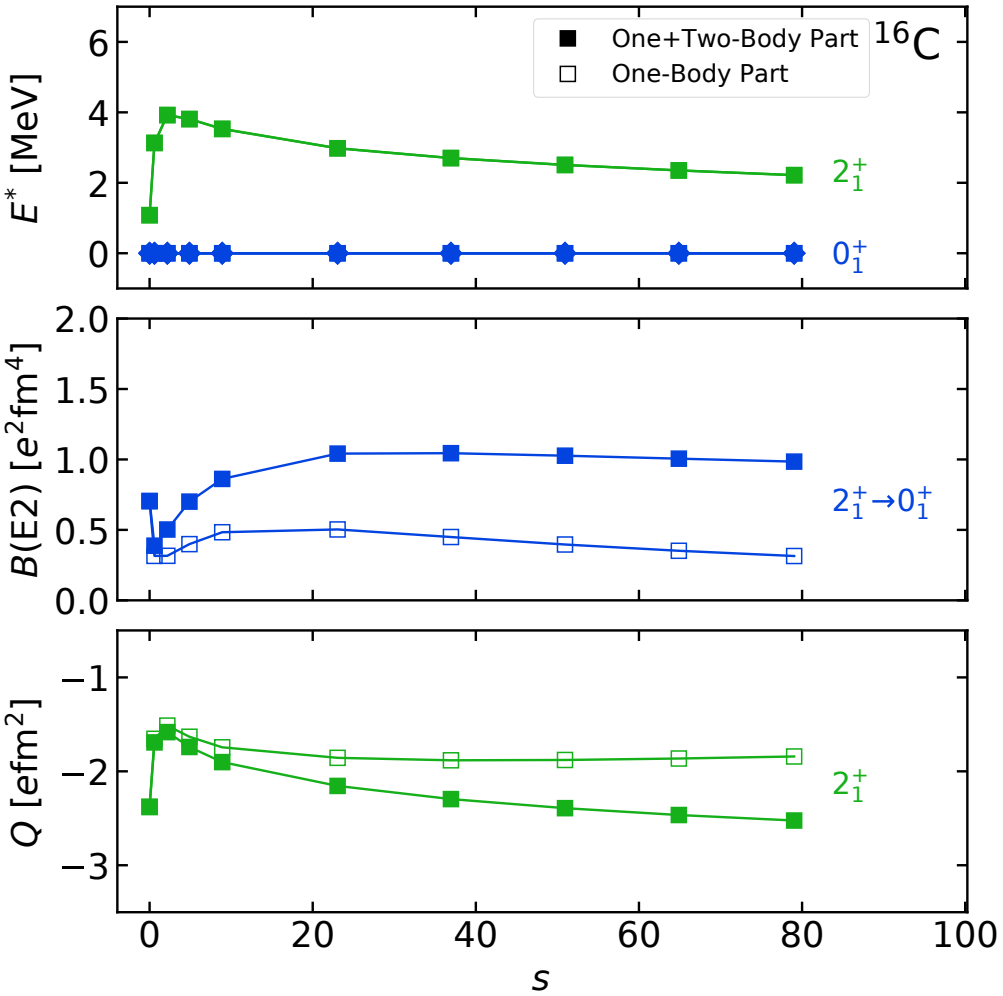
Carbon Isotopic Chain



IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, $e_{\max}$=12, $E_{3\max}$=14,
combined many-body and interaction error band

- ground state energy, first excited state, B(E2) transition strength, quadrupole moments and charge radii as function of A
- combined many-body and interaction uncertainties
- all observables → good agreement with experiments except $R_{\rm ch}$ for ^{12}C and B(E2) for ^{16}C

^{16}C - Hierarchy Inversion



IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, $e_{\max}$=12, $E_{3\max}$=14

- first excited state, B(E2) transition strength and electric quadrupole moment against the flow parameter s
- induced two-body contributions larger than one-body contribution for B(E2) transition strength
- what about three-body contributions?

IM-NCSM: Induced Three-Body Corrections

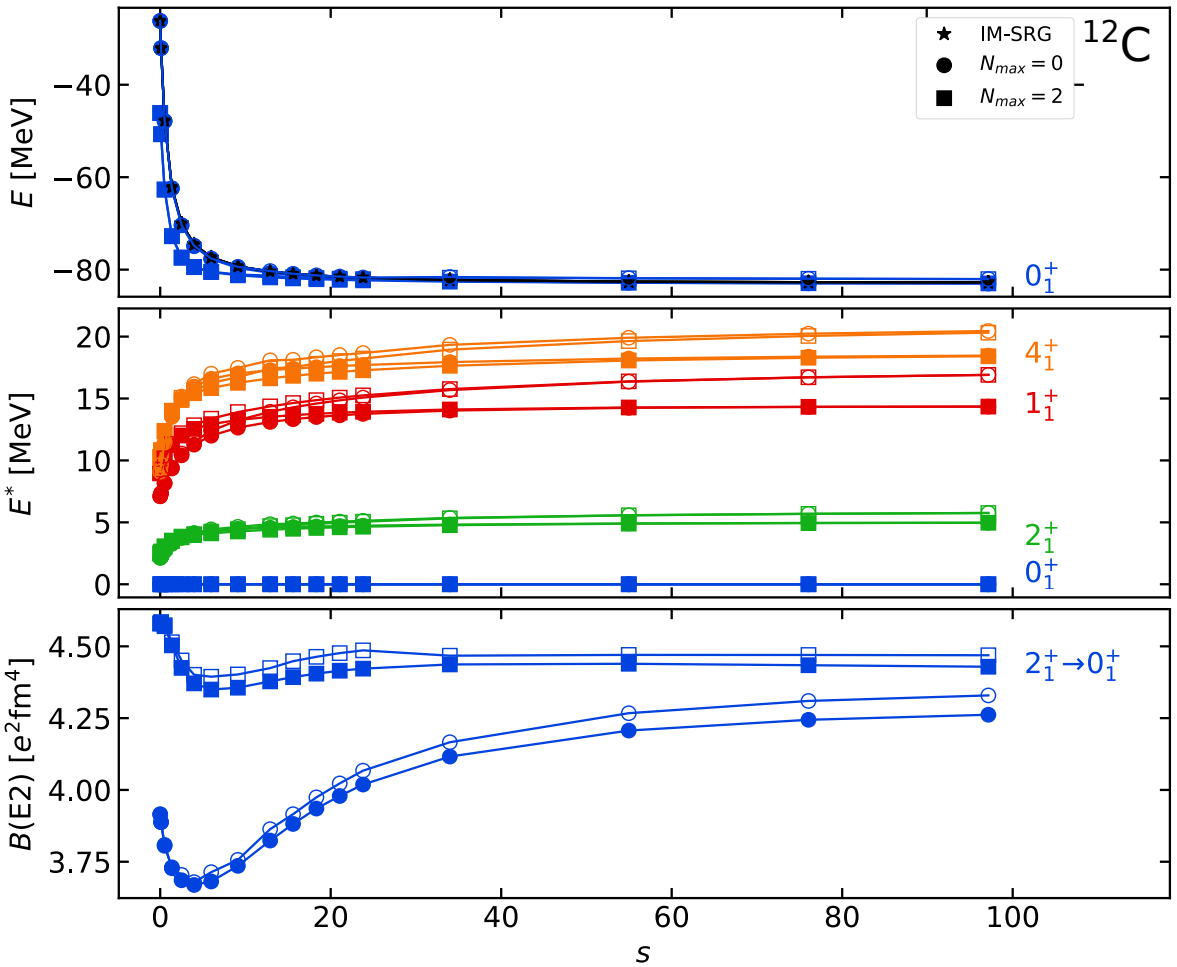
- IM-SRG flow equation yields $\hat{\Omega}^{[0]}$, $\hat{\Omega}^{[1]}$ and $\hat{\Omega}^{[2]}$
- transformation of operators via BCH series using 2B operators only

$$\hat{O}(s) = \left[\hat{\Omega}(s), \hat{O}(0)\right] + \frac{1}{2}\left[\hat{\Omega}(s), \left[\hat{\Omega}(s), \hat{O}(0)\right]\right] + \frac{1}{6}\left[\hat{\Omega}(s), \left[\hat{\Omega}(s)\left[\hat{\Omega}(s), \hat{O}(0)\right]\right]\right] + \ldots$$

- Leading-order three-body correction (LOTC): include intermediate 3B terms

$$\begin{aligned}\Delta\hat{O}^{\mathrm{LOTC}} = &+ \frac{1}{2}\left[\hat{\Omega}^{[1]}, \left[\hat{\Omega}^{[2]}, \hat{O}^{[2]}\right]_{\mathrm{3B}}\right]_{\mathrm{1B}} + \frac{1}{2}\left[\hat{\Omega}^{[1]}, \left[\hat{\Omega}^{[2]}, \hat{O}^{[2]}\right]_{\mathrm{3B}}\right]_{\mathrm{2B}} \\ &+ \frac{1}{2}\left[\hat{\Omega}^{[2]}, \left[\hat{\Omega}^{[2]}, \hat{O}^{[2]}\right]_{\mathrm{3B}}\right]_{\mathrm{0B}} + \frac{1}{2}\left[\hat{\Omega}^{[2]}, \left[\hat{\Omega}^{[2]}, \hat{O}^{[2]}\right]_{\mathrm{3B}}\right]_{\mathrm{1B}} \\ &+ \frac{1}{2}\left[\hat{\Omega}^{[2]}, \left[\hat{\Omega}^{[2]}, \hat{O}^{[2]}\right]_{\mathrm{3B}}\right]_{\mathrm{2B}}\end{aligned}$$

Results: Induced Three-Body Corrections



IM-NCSM, natural orbitals, $\hbar\Omega$=20 MeV,
α=0.04 fm^4, $e_{\max}$=4, $E_{3\max}$=14

- groundstate energy, spectrum and B(E2) transition strength vs. flow parameter s
- influence of the LOTC not very large for energies and electromagnetic observables in small model spaces

Conclusions & Outlook

- interaction family performs well for carbon isotopic chain
- electromagnetic observables well reproduced except for ^{16}C
- three-body correction ⇝ influence not very large for small model space sizes

- compute oxygen, neon, fluorine and calcium chain
- use other cutoffs and interaction families (LENPIC collaboration)
- develop a hybrid MPI/OpenMP parallelization for the LOTC to be able to use larger model spaces