Fully Open-Shell Nuclei and Electromagnetic Observables from the In-Medium NCSM

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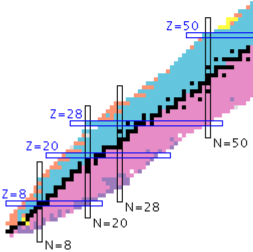
Motivations

- ab initio many-body method for the description of ground and excited states in open-shell nuclei

- No-Core Shell Model (NCSM)
  ⇝ limited by basis dimension, scaling with particle number

- medium-mass methods:
  - In-Medium Similarity Renormalization Group (IM-SRG)
  - Coupled Cluster
  - Perturbation Theory (PT)
  - ...

  ⇝ basic formulations limited to ground states



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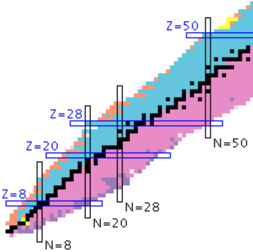
- our approach for overcoming limitations:
  No-Core Shell Model based hybrid methods



In-Medium No-Core Shell Model: Concept

NCSM

- NCSM calculation in small model space defines reference state

$$|\Psi\rangle = \sum_i c_i \, |\Phi_i\rangle$$

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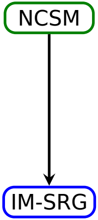

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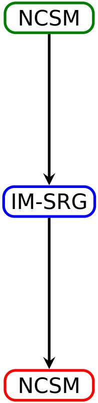
$$|\Psi\rangle = \sum_i c_i \, |\Phi_i\rangle$$

- perform **multi-reference** IM-SRG aiming at decoupling reference state from generalized ph-excitations $\tilde{a}^{p_1}_{q_1} |\Psi\rangle$, $\tilde{a}^{p_1 p_2}_{q_1 q_2} |\Psi\rangle$, ...

$$\hat{H}(\infty) \; |\Psi\rangle = E(\infty) \; |\Psi\rangle$$

In-Medium No-Core Shell Model: Concept



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- use IM-SRG-evolved Hamiltonian $\hat{H}(s)$ as input for subsequent NCSM calculation
- convergence of NCSM calculation massively improved w.r.t. N_{max}

IM-SRG: Key Ingredients

- IM-SRG(2): truncate operators at NO2B level throughout evolution

$$\hat{H}(s) \equiv E(s) + \sum_{pq} f^p_q(s)\ \{\hat{p}^\dagger \hat{q}\}_{|\Psi\rangle} + \frac{1}{4}\sum_{pqrs} \Gamma^{pq}_{rs}(s)\,\{\hat{p}^\dagger \hat{q}^\dagger \hat{s}\hat{r}\}_{|\Psi\rangle}$$

- perform unitary transformation via SRG flow equation approach:

$$\frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s), \hat{H}(s)\right]$$

- generator $\hat{\eta}(s)$ defines decoupling behavior/pattern ⇝ tailor for specific applications

- induced many-body terms up to the A-body level

$$\hat{H}(s) = \hat{H}^{[0]}(s) + \hat{H}^{[1]}(s) + \ldots + \hat{H}^{[A]}(s)$$

IM-SRG: Commutator Evaluation

- evaluation of $\frac{\mathrm{d}}{\mathrm{d}s}\hat{H}(s) = \left[\hat{\eta}(s), \hat{H}(s)\right]$ via (generalized) Wick's theorem

$$\{\hat{A}_1 \ldots\}\{\hat{B}_1 \ldots\} = \sum_{\text{ext. contr.}} \{\hat{A}_1 \ldots \hat{B}_1 \ldots\}$$

- single-particle transformed into natural-orbital basis (eigenbasis of $\gamma^{(1)}$, $\gamma^p_q \rightarrow n_p \delta_{pq}$)

- result: coupled system of first-order ordinary differential equations

$$\frac{\mathrm{d}}{\mathrm{d}s}E(s) = \sum_{pq} (n_p - n_q)\ \eta^p_q(s)\ f^q_p(s) + \frac{1}{4} \sum_{pqrs} \left(\eta^{pq}_{rs}(s)\ \Gamma^{rs}_{pq}(s)\ n_p n_q \bar{n}_r \bar{n}_s - [\eta \leftrightarrow \Gamma]\right) + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}f^1_2(s) = \sum_p \left(\eta^1_p\ f^p_2\ - [\eta \leftrightarrow f]\right) + \ldots + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$\frac{\mathrm{d}}{\mathrm{d}s}\Gamma^{12}_{34}(s) = \sum_p \left(\left(\eta^1_p\ \Gamma^{p2}_{34} - f^1_p\ \eta^{p2}_{34}\right) - [1 \leftrightarrow 2]\right) + \ldots$$

- neglection of $\lambda^{(3)}$, only scalar part of $\lambda^{(2)}$ considered ($\rightsquigarrow$ restriction to even nuclei)

- express in terms of reduced matrix elements ($\rightsquigarrow$ rank of spherical tensor operators)

- solve this system of ordinary differential equations numerically

Magnus Expansion & Observables

- unitary transformation $\hat{H}(s) \equiv \hat{U}^\dagger(s)\hat{H}(0)\hat{U}(s)$ can be written as

$$\hat{U}(s) = \exp(\hat{\Omega}(s))$$

- derive differential equation for $\hat{\Omega}(s)$ associated with unitary transformation $\hat{U}(s)$

$$\frac{\mathrm{d}}{\mathrm{d}s}\hat{\Omega}(s) = \sum_{k=0}^{\infty} \frac{B_k}{k!}\left[\hat{\Omega}(s)\,,\hat{\eta}(s)\right]_k \qquad = \sum_{k=0}^{\infty} \frac{B_k}{k!} \underbrace{\left[\hat{\Omega}(s), \left[\hat{\Omega}(s), \left[\,\ldots \left[\hat{\Omega}(s), \left[\hat{\Omega}(s),\right.\right.\right.\right.\right.}_{\text{k-times}} \hat{\eta}(s)\left.\left.\left.\left.\left.\right]\right]\right]\right]\right]$$

- solve flow equations for matrix elements of anti-hermitian $\hat{\Omega}(s)$

- Magnus(2): truncate all operators involved at two-body level

- apply unitary transformation via Baker-Campbell-Hausdorff series

$$\hat{O}(s) = \exp(-\hat{\Omega}(s))\hat{O}(0)\exp(\hat{\Omega}(s)) = \sum_{k=0}^{\infty} \frac{1}{k!}\left[\hat{\Omega}(s)\,,\hat{O}(0)\right]_k$$

- much more efficient than simultaneous evolution via $\frac{\mathrm{d}}{\mathrm{d}s}\hat{O}(s) = \left[\hat{\eta}(s)\,,\hat{O}(s)\right]$

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- Magnus(2): truncate all operators ir
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an efficient
commutator evaluation machinery
is crucial for the IM-SRG!

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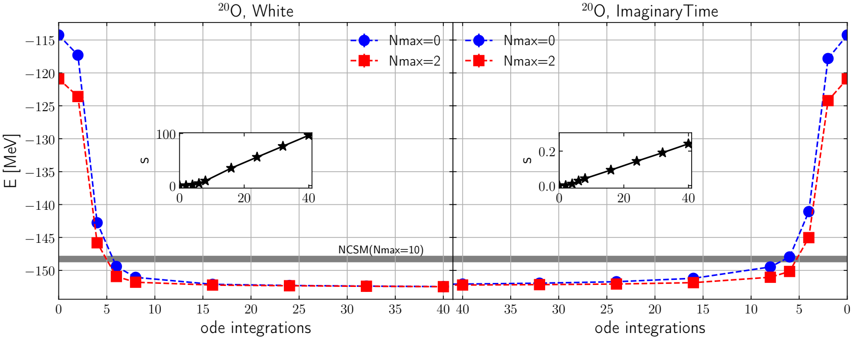
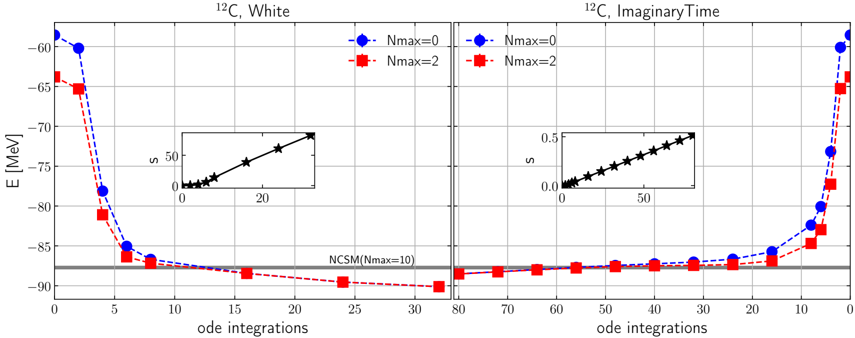
Generator and Single-Particle Basis Optimizations

^{20}O: All seems well...



- initially: strong couplings of N=0 space to basis states at higher N
  $\rightsquigarrow$ high N_{max} necessary for converged results
- finally: $N_{\text{max}} = 0$ space decoupled $\rightsquigarrow$ converged results at $N_{\text{max}} = 0$.
- both generators yield same results (note difference in numerical efficiency)

^{12}C: But it isn't...

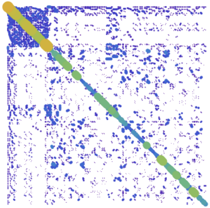


- impact of neglected many-body contributions beyond NO2B level
- explore different (simpler) decoupling patterns?

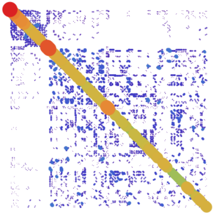
IM-SRG: Decoupling & Generators

- partition Hamiltonian $\hat{H} = \hat{H}^{\mathrm{d}} + \hat{H}^{\mathrm{od}}$, suppress $\hat{H}^{\mathrm{od}}$
  ⇝ define decoupling pattern
- generator types: White, Imaginary-Time, Wegner,...
  ⇝ define decoupling behavior
- decouple reference state $|\Phi\rangle$ from $|\Phi^{p_1}_{q_1}\rangle, |\Phi^{p_1 p_2}_{q_1 q_2}\rangle, \ldots$
  ⇝ reference state $|\Psi\rangle$ becomes ground-state of $\hat{H}(\infty)$
- reference state $|\Psi\rangle$ doesn't need to be decoupled from other $N_{\mathrm{max}} = 0$ eigenstates (⇝ induced couplings)
- only suppress couplings between different N spaces
  ⇝ "loosen up" decoupling pattern
- label as White', Imaginary-Time'

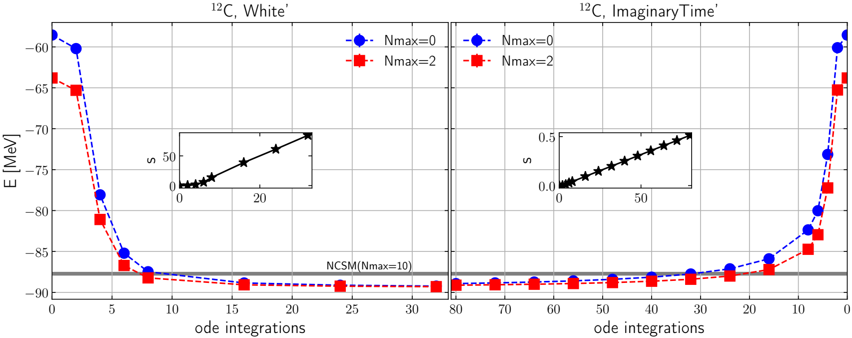
initial



final

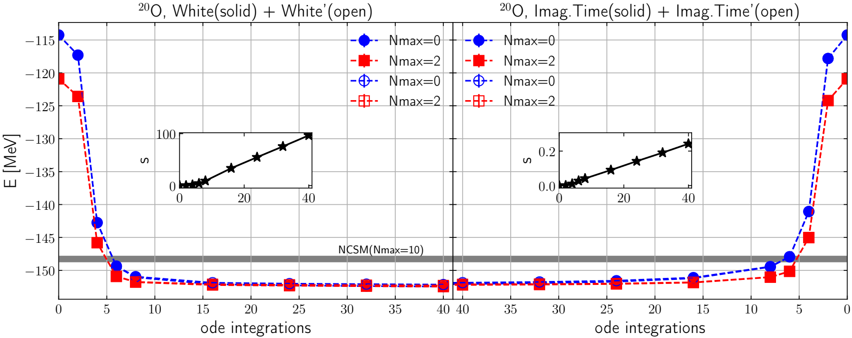


^{12}C: Converged Results



- flow stabilizes ⇝ generator modifications sucessful!
- both modified generators yield similar results

^{20}O: Backwards Compatibility



- all generators practically yield the same result
- generator modifications are "backwards compatible"

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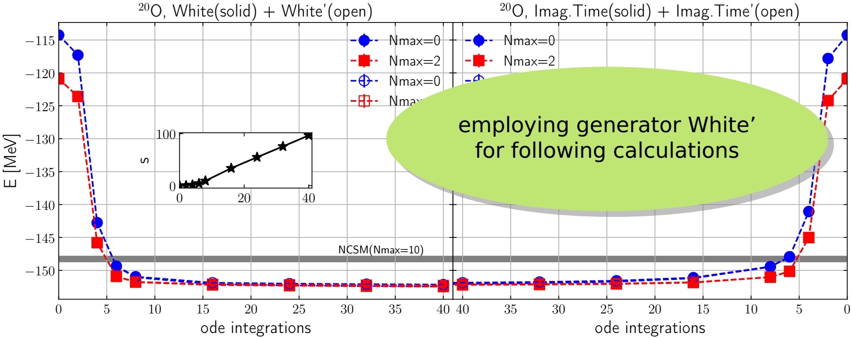

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Natural Orbitals

- use natural-orbital basis
  ⇝ eigenbasis of one-body density from, e.g., second-order Perturbation Theory
- original motivation: boost $N_{\max}$ convergence and eliminate $\hbar\Omega$ dependency
  ⇝Robert's talk
- motivation here: improve reference state description

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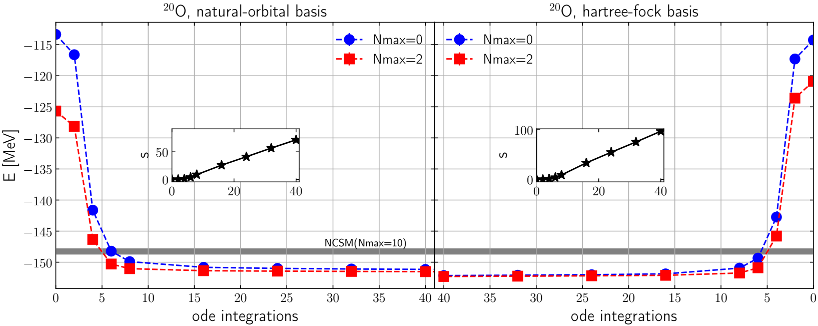

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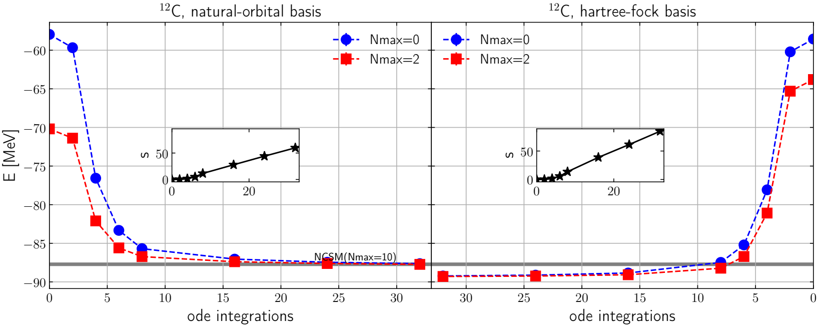

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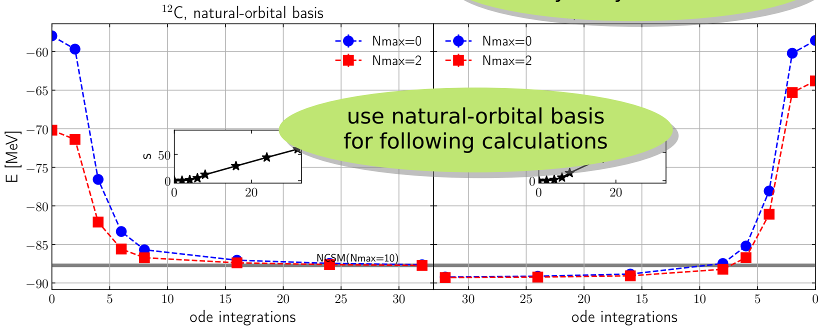
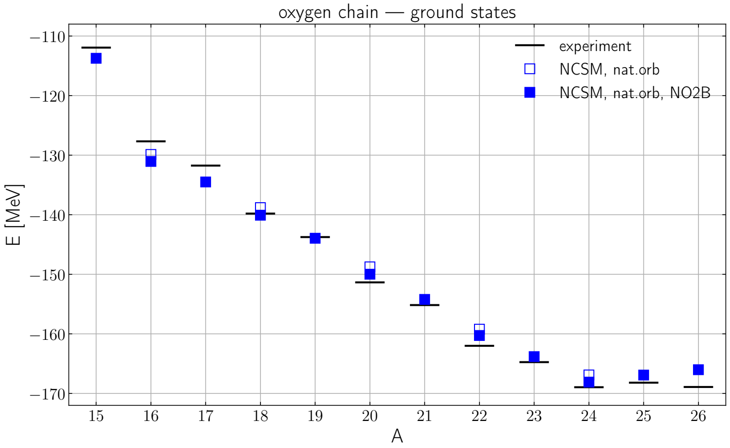
seemingly less induced many-body interactions



use natural-orbital basis for following calculations

Open-Shell Nuclei:
Ground and Excited states

IM-NCSM: Oxygen Chain



NN at N^3LO, 3N at N^2LO ($\Lambda = 400$ MeV), free-space SRG $\alpha = 0.08\,\text{fm}^4$

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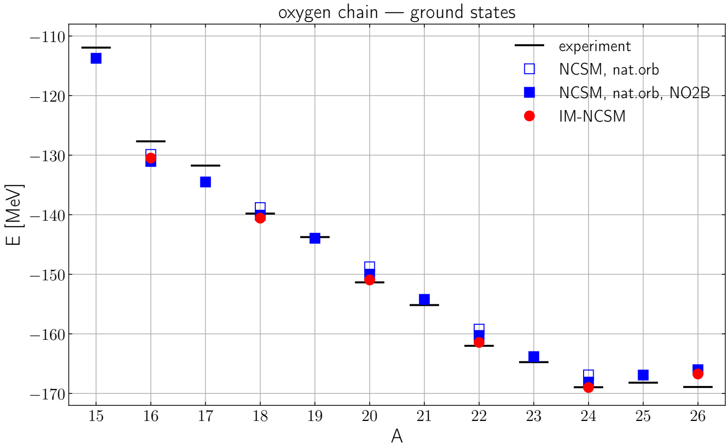

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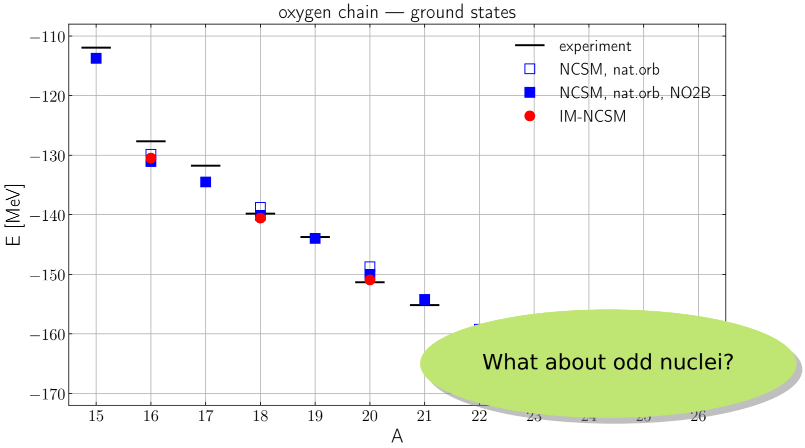
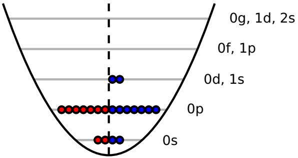
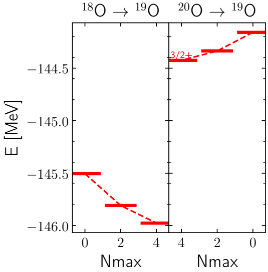


NN at N^3LO, 3N at N^2LO ($\Lambda = 400$ MeV), free-space SRG $\alpha = 0.08\,\mathrm{fm}^4$

IM-NCSM: Particle-Attached Particle-Removed

- perform IM-NCSM for ”parent“ nucleus
- take A_{eff} into account (⇝ kinetic energy)
- perform diagonalization for ”target“ nucleus
- several schemes possible:
  - attachment (^{18}O → ^{19}O, ...)
  - removal (^{20}O → ^{19}O, ...)
  - hybrid (^{20}Ne → ^{20}F, ...)
- IM-SRG only ”sees“ density matrices
  ⇝ partitioning into core, active and virtual space
- removal scheme is very robust
- attachment less robust for closed-shell parent
  ⇝ no information about active space
  ⇝ slow N_{max} convergence





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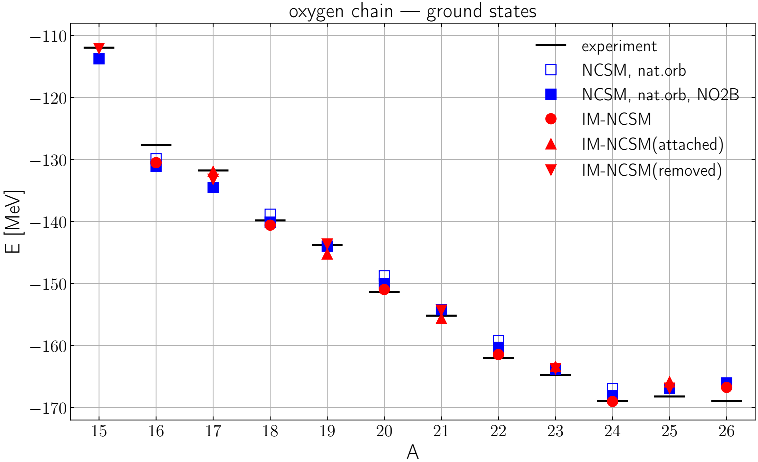
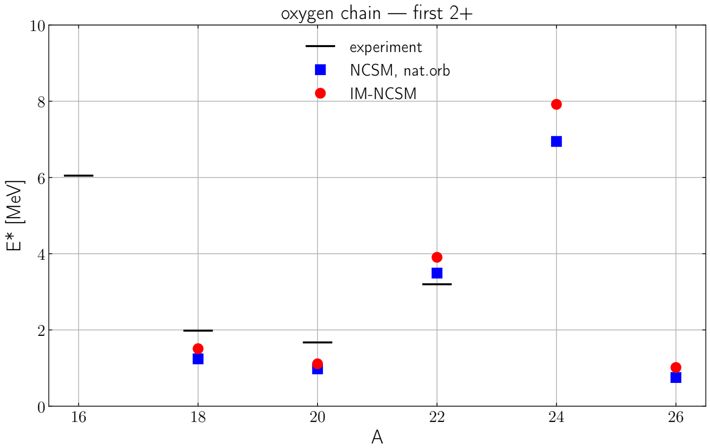
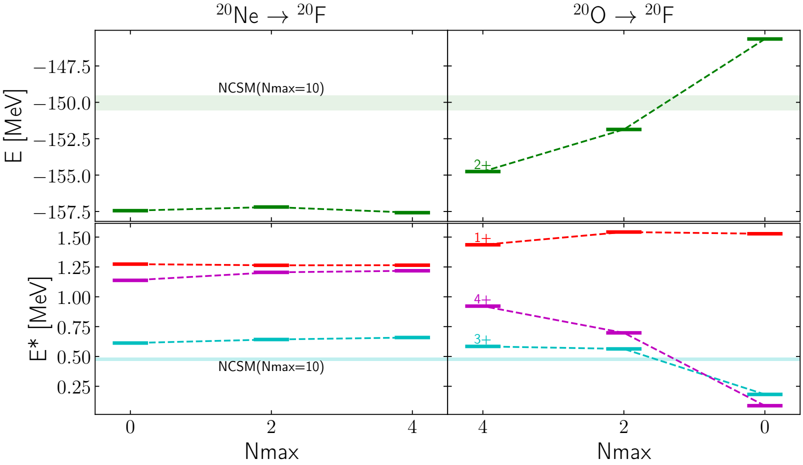


IM-NCSM: First 2+ in Oxygen Chain



IM-NCSM: ^{20}F



^{20}Ne → ^{20}F
^{20}O → ^{20}F
E [MeV]
−147.5
−150.0
−152.5
−155.0
−157.5
NCSM(Nmax=10)
2+
E* [MeV]
1.50
1.25
1.00
0.75
0.50
0.25
1+
4+
3+
NCSM(Nmax=10)
0
2
4
4
2
0
Nmax
Nmax

Electromagnetic Observables

IM-NCSM and Electromagnetic Observables

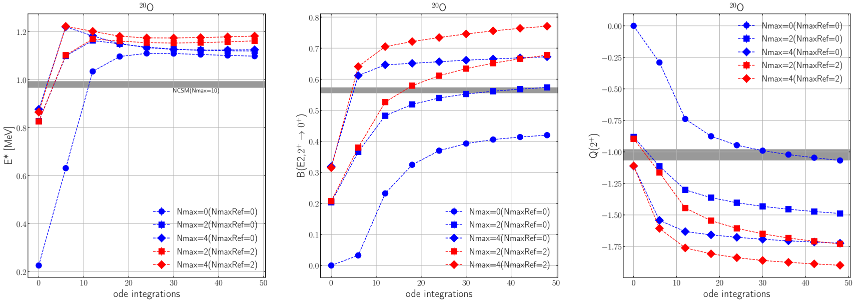
- MR-IM-SRG machinery was restricted to scalar operators
- study of electromagnetic observables
  ⇝ extend formalism to spherical tensor operators $\hat{B}^L_M(s)$ of arbitrary rank L
- use $\hat{\Omega}$ from Magnus expansion for transforming $\hat{B}^L_M(s)$ via BCH
- couple (diagramatically) and implement $\hat{C}^L_M(s) = \left[\hat{A}^0_0(s), \hat{B}^L_M(s)\right]$

$$C^1_2 = \sum_p A^1_p \, B^p_2 + \ldots + \mathcal{F}\left(\lambda^{(2)}\right)$$

$$C^{12}_{34} = \sum_p A^1_p \, B^{p2}_{34} + \ldots$$

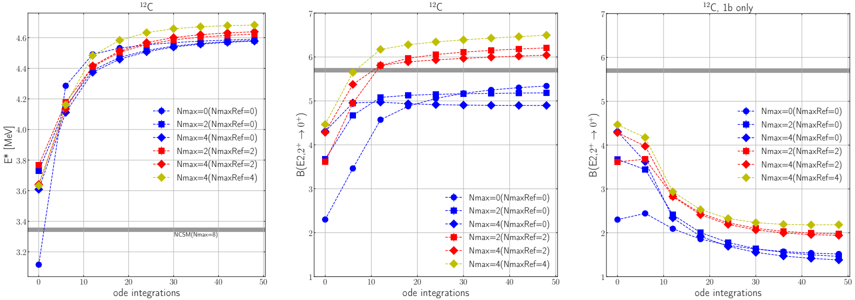
- significant increase in computational effort
- employing bare electromagnetic observables for following calculations

^{20}O: B(E2) and Q



- IM-NCSM results compatible with NCSM results at high N_{max}
- slight $N_{\text{max,ref}}$ dependency

^{12}C: B(E2), Q and Hierarchy Inversion



- again: compatible with NCSM calculation at high N_{max}
- difference between $N_{\text{max,ref}} = 0$ and $N_{\text{max,ref}} = 2, 4$
- significant shift into two-body part during IM-SRG flow

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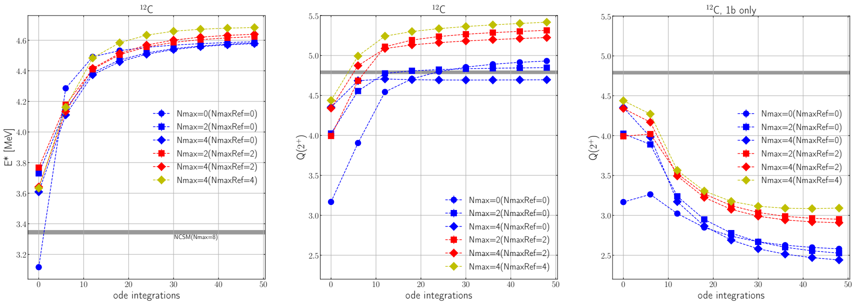

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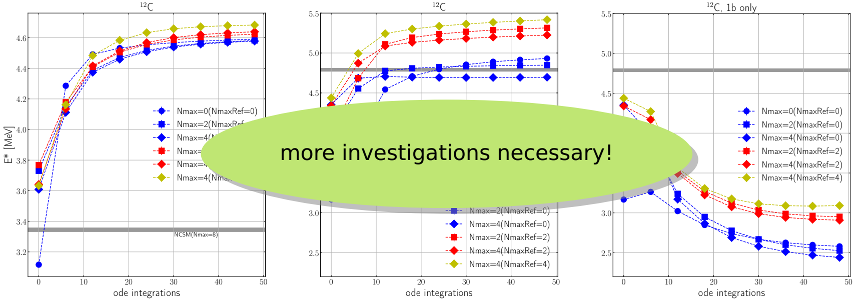

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Epilogue

- **Thanks to my group**
  - S. Alexa, T. Hüther, J. Müller, R. Roth, S. Schulz, C. Stumpf, R. Wirth

    Institut für Kernphysik, TU Darmstadt

- **Thank you for your attention!**

COMPUTING TIME

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LOEWE-CSC — CSC Center for Scientific Computing Frankfurt

LICHTENBERG — HRZ Hochschulrechenzentrum

SFB 1245

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