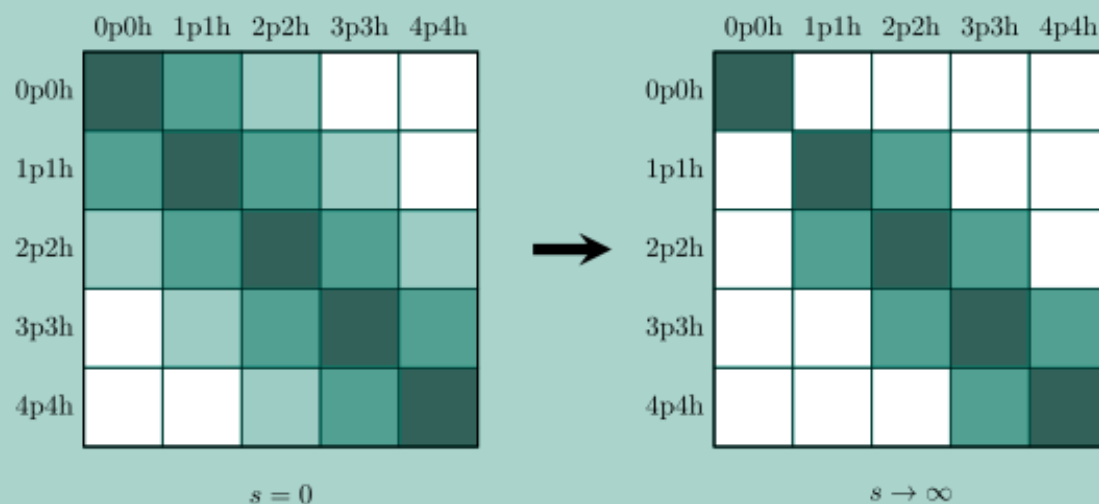

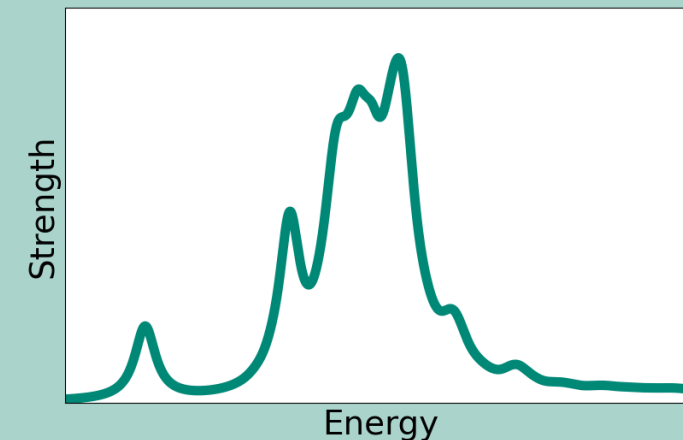


Collective Excitations in Open-Shell Nuclei: Strength Functions in the In-Medium CI

Michelle Müller



(S)RPA
CI-LS

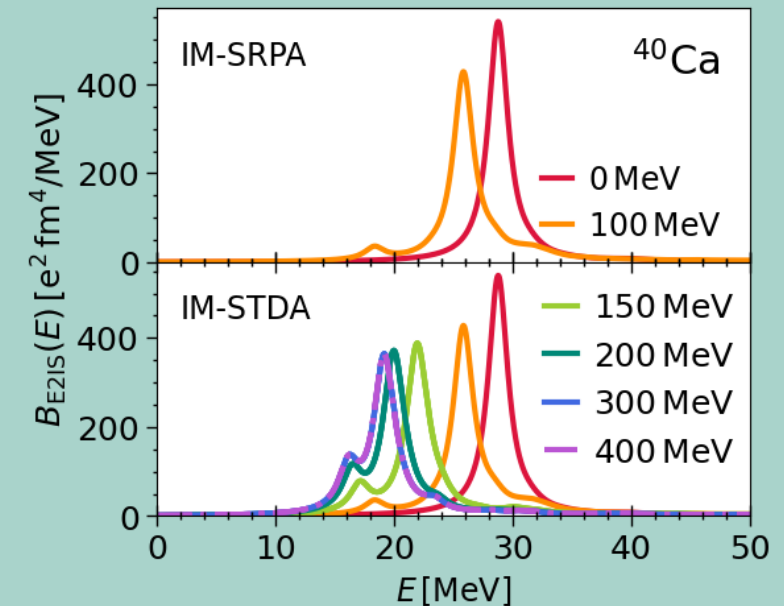
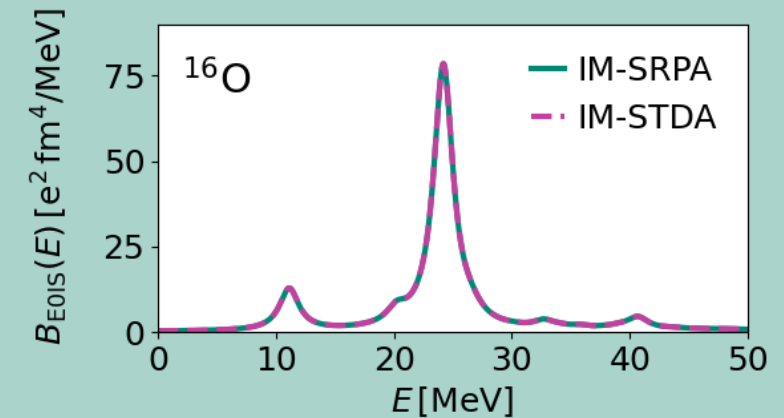



Random-Phase and Tamm-Dancoff Approximation

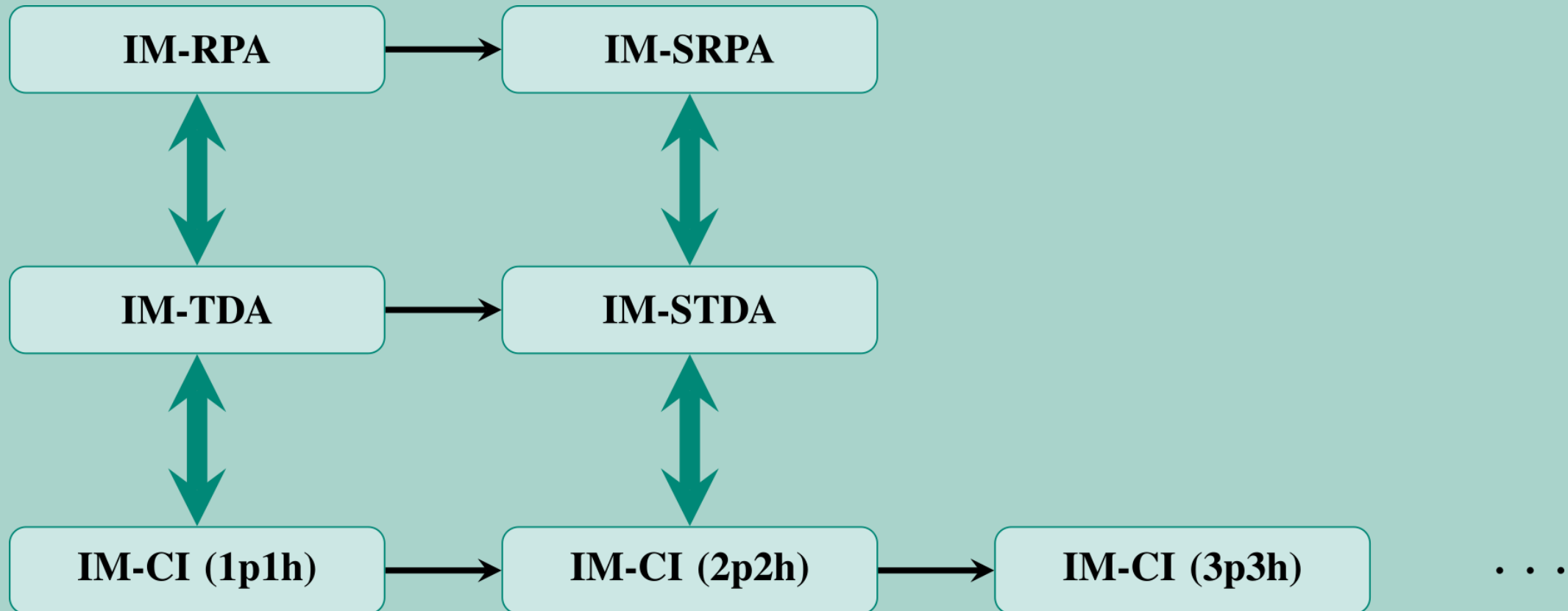
- standard methods to describe giant resonances in closed-shell nuclei
- **(S)TDA**: excited states built on Hartree-Fock ground state via 1p1h (+2p2h) excitations
- **(S)RPA**: excited states built on correlated ground state via 1p1h (+2p2h) excitations and de-excitations
but: typically, ground state is replaced by Hartree-Fock state via quasi-boson approximation

Combining In-Medium SRG with (S)RPA

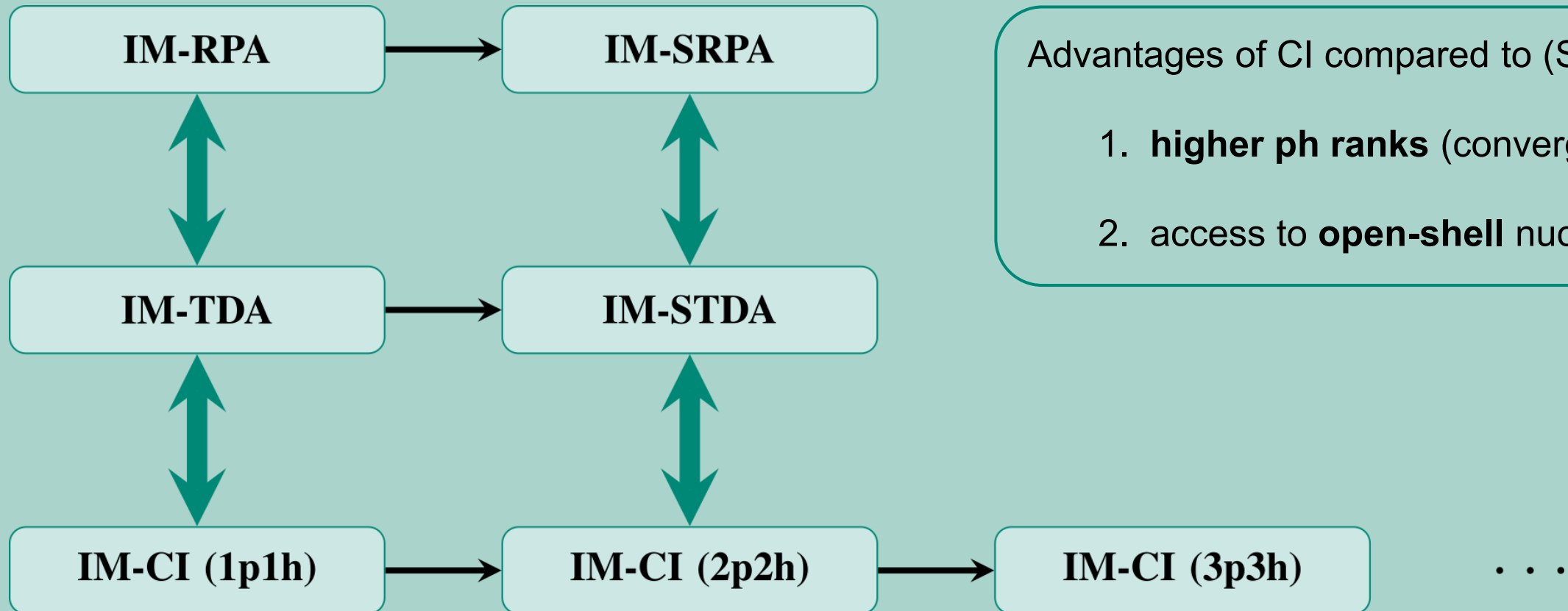
- IM-SRG: reference state is decoupled from ph excitations
- idea: implementing IM-SRG evolved matrix elements in (S)RPA
 - improved treatment of correlations *beforehand* (i.e. in IM-SRG), while maintaining simple structure of the formalism
- for IM-(S)RPA, all contributions from de-excitations vanish
 - IM-(S)RPA is reduced to IM-(S)TDA
 - improvement in computational effort
 - access to converged results for heavier nuclei, e.g. ^{40}Ca or ^{48}Ca



From IM-(S)TDA to IM-CI



From IM-(S)TDA to IM-CI



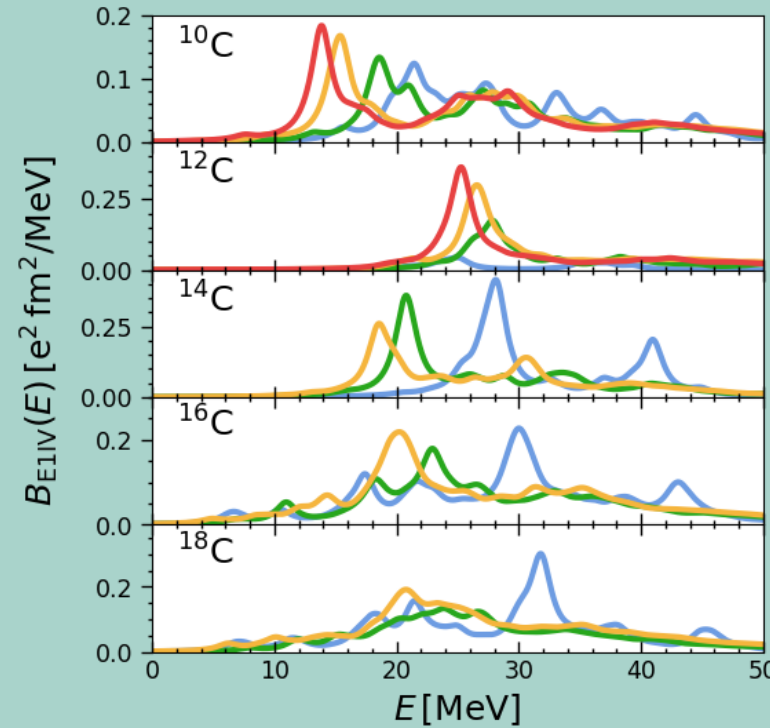
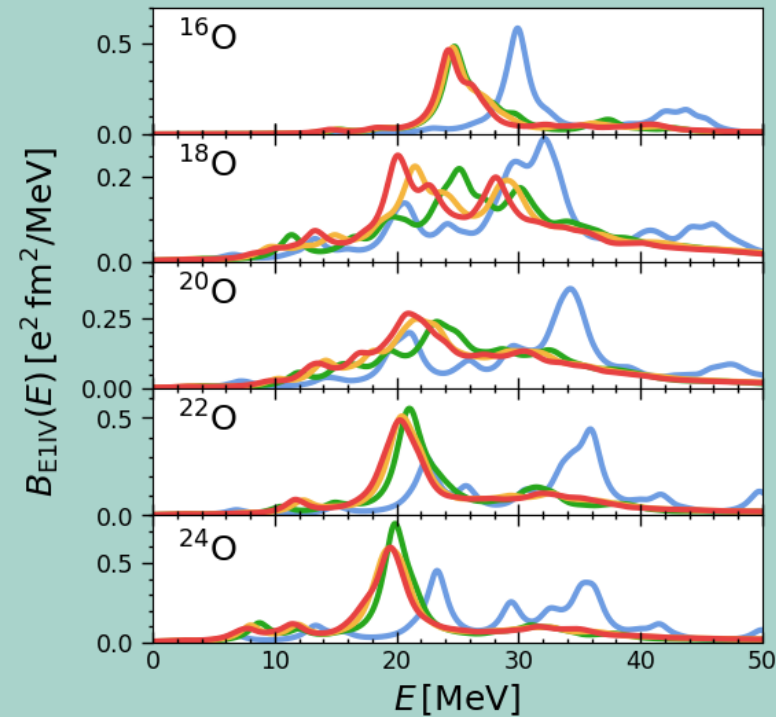
Advantages of CI compared to (S)RPA :

1. **higher ph ranks** (convergence!)
2. access to **open-shell** nuclei

In-Medium CI with Lanczos Strength-Function Method

Oxygen Isotopes

Carbon Isotopes



- IM-CI(1p1h) \approx IM-RPA
- IM-CI(2p2h) \approx IM-SRPA
- IM-CI(3p3h)
- IM-CI(4p4h)

Oxygen

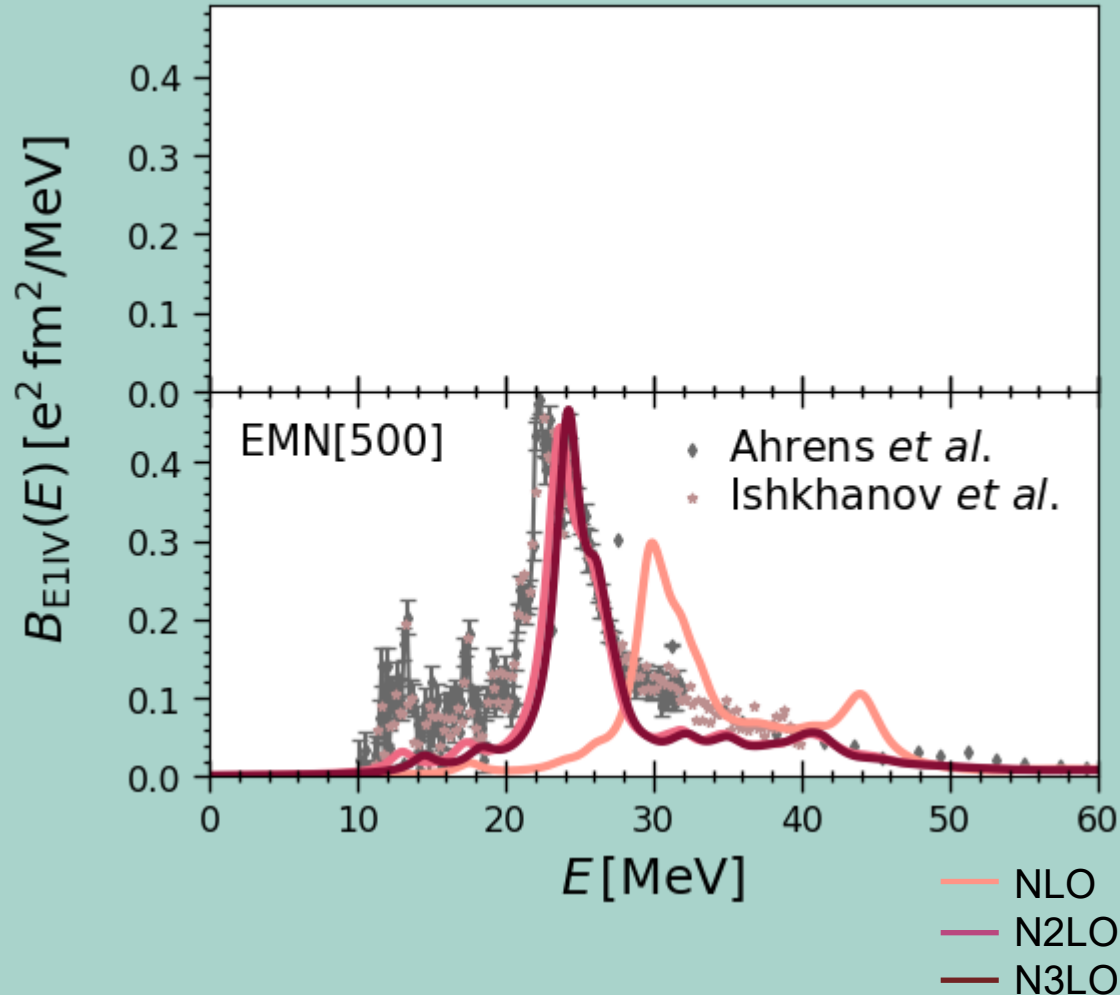
- 2p2h contributions close to convergence for most isotopes
- convergence at 3p3h truncation for most isotopes
- higher contributions required for ^{18}O

Carbon

- slower convergence behavior
- higher contributions required

Impact of Interaction Cutoffs and Chiral Orders

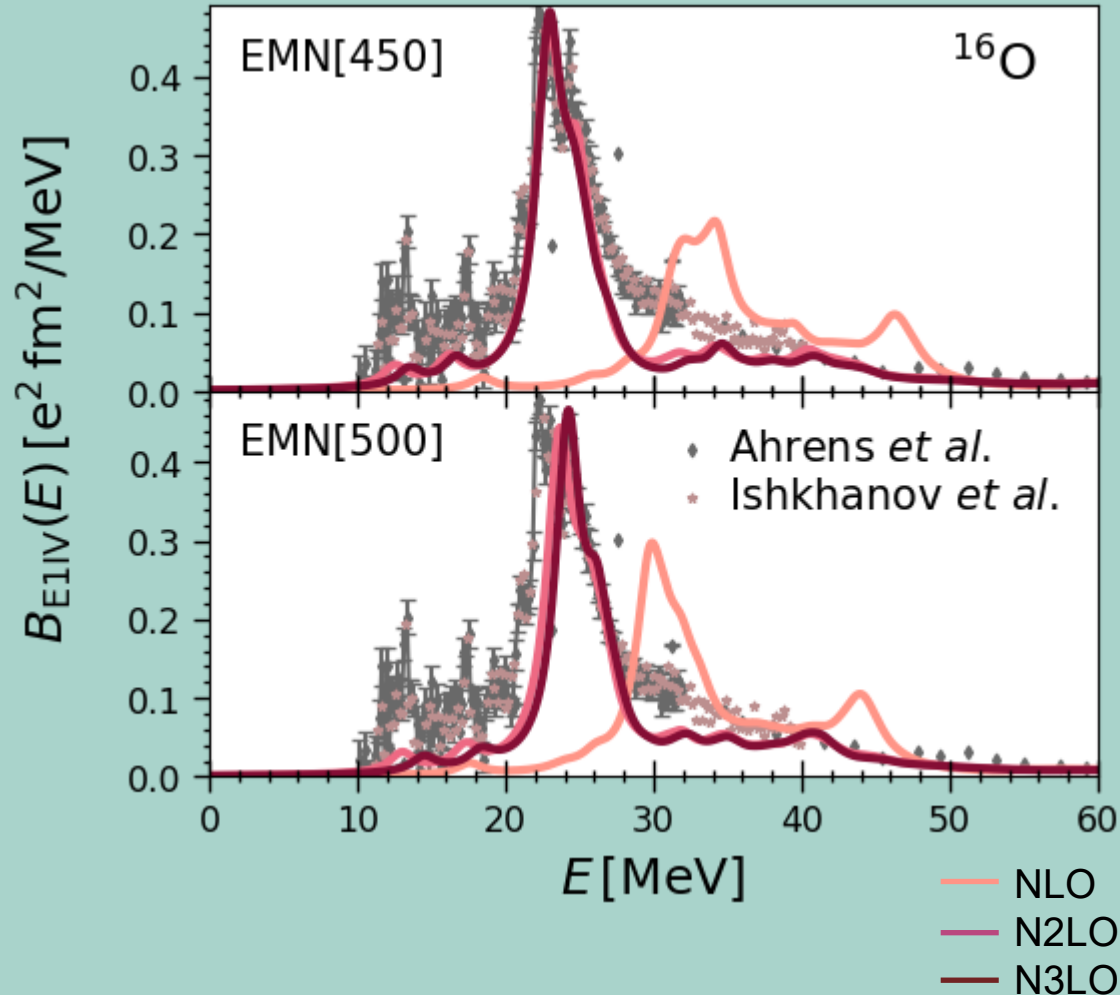
^{16}O



- interaction applied in plots throughout the talk:
chiral NN+3N interactions with cutoff of 500 MeV
NN: Entem, Machleidt, Nosyk, Phys. Rev. C 96, 024002 (2017)
3N: Hübner, Vobig, Hebeler, Machleidt, Roth, Phys. Lett. B 808, 135651 (2020)
→ reasonable results for ground-state observables
- comparing different chiral orders at 4p4h truncation
- N2LO and N3LO yield similar strength distributions
- strengths at higher energies compared to experiment
→ also found for other transition modes and nuclei

Impact of Interaction Cutoffs and Chiral Orders

^{16}O

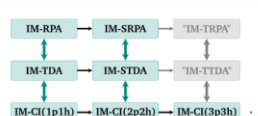


- chiral NN+3N interactions at two different cutoffs
 NN: Entem, Machleidt, Nosyk, Phys. Rev. C 96, 024002 (2017)
 3N: Hübner, Vobig, Hebeler, Machleidt, Roth, Phys. Lett. B 808, 135651 (2020)
- comparing different chiral orders at 4p4h truncation
- N2LO and N3LO yield similar strength distributions
- EMN[450] at N3LO consistent with experimental data
- similar behavior for other nuclei

Collective Excitations in Open-Shell Nuclei: Strength Functions in the In-Medium CI

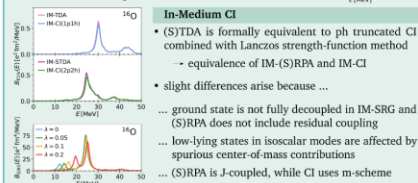


Michelle Müller, Robert Roth

Motivation	Random-Phase Approximation	Configuration Interaction
<ul style="list-style-type: none"> studying collective excitations reveals information on nuclear properties, e.g. deformation, incompressibility or polarizability two methods to investigate giant resonances <ol style="list-style-type: none"> (S)RPA (standard tool) CI with Lanczos strength-function method (relatively novel approach) CI allows describing open-shell nuclei and exploring convergence with respect to ph truncation improved treatment of correlations by including in-medium SRG evolved matrix elements for Hamiltonian and electromagnetic operators <i>ab initio</i> calculations: employing chiral NN+3N interactions with two different cutoffs <ul style="list-style-type: none"> exploring convergence with respect to chiral orders as well as cutoff dependence 	<ul style="list-style-type: none"> standard tool to describe giant resonances restricted to Slater determinant → closed-shell nuclei (S)RPA: excited states built on correlated ground state via 1p1h (+2p2h) excitations and de-excitations but: typically, ground state replaced by HF state (S)TDA: simplification of (S)RPA, excited states built on Hartree-Fock state via 1p1h (+2p2h) excitations 	<ul style="list-style-type: none"> giant resonances from ph truncated (TF)CI combined with Lanczos strength-function method [1, 2] two major advantages compared to (S)RPA: <ol style="list-style-type: none"> possibility to study higher ph ranks direct access to open-shell nuclei idea: iteratively constructing orthonormal basis in which the Hamiltonian matrix becomes tridiagonal clever choice of pivot vector using EM operator $v_1\rangle = \frac{1}{\sqrt{S}} \hat{T}_{E_1} \Psi_0\rangle, \quad S = \langle \Psi_0 \hat{T}_{E_1}^2 \Psi_0 \rangle$ <p style="text-align: center;">ground state calculated in CI</p> diagonalization of tridiagonal matrix yields approximations of Hamiltonian eigenpairs first coefficient provides transition matrix element $C_1^{(n)} = \langle \Phi_n v_1 \rangle = \frac{1}{\sqrt{S}} \langle \Phi_n \hat{T}_{E_1} \Psi_0 \rangle$

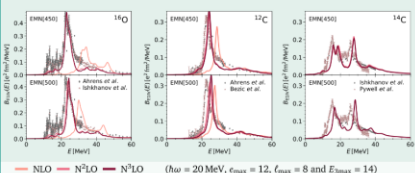
Merging In-Medium SRG with (S)RPA and CI

- In-Medium (S)RPA and (S)TDA**
- using IM-SRG evolved matrix elements in (S)RPA
 - improved treatment of correlations
 - IM-(S)RPA can be reduced to simpler IM-(S)TDA
 - significant improvement of computational costs
 - access to converged results for heavier nuclei



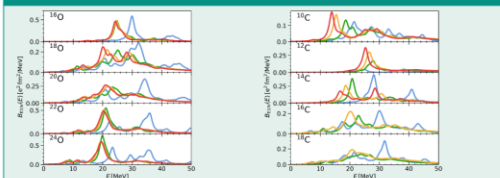
Impact and Convergence of Chiral Interactions

- strength distributions computed with IM-CI(4p4h) for ^{16}O , ^{12}C and ^{14}C
- SRG-evolved ($\alpha = 0.08 \text{ fm}^{-1}$) non-local chiral NN+3N interaction from [3, 4]



- N²LO and N³LO yield similar strength distributions
- EMN[500] produces results at higher energies compared to experimental strengths
- ^{16}O : EMN[450] is consistent with main peak of experimental data in N³LO
- $^{12,14}\text{C}$: strengths are not converged at 4p4h, but EMN[450] is close to experiment

Open-Shell Nuclei with IM-CI: Carbon and Oxygen Chains



- 1p1h yields results far from convergence
- already reasonable results at 2p2h level
- convergence at 3p3h for most isotopes
- both 1p1h and 2p2h distributions not converged
- large downward shifts for higher ranks
- distributions not even converged for 3p3h/4p4h

Conclusion and Outlook

Take-Home Messages

- equivalence of IM-(S)RPA, IM-(S)TDA and IM-CI
- IM-(S)TDA is computationally more efficient than IM-(S)RPA
 - enables calculation of heavier nuclei, e.g. Calcium
- IM-CI allows exploring ph convergence and open-shell nuclei
- convergence of strength distributions with respect to chiral orders
- EMN[450] yields strength distributions consistent with main peak of experimental data

What to do in the future?

- push Carbon isotopes to convergence
- test different interaction families and parameters
- consider heavier isotopic chains with IM-CI, e.g. Neon
 - explore deformation effects

References

- C. Lanczos, *J. Res. Natl. Bur. Stand. B* **48**, 255 (1950).
- C. Sturm, T. Wollgast, and R. Roth, (2017), arXiv:1709.05640.
- D. R. Entem, R. Machleidt, and Y. Nosyk, *Phys. Rev. C* **96**, 024004 (2017).
- T. Hübner et al., *Physics Letters B* **808** (2020), 10.1016/j.physletb.2020.136651.



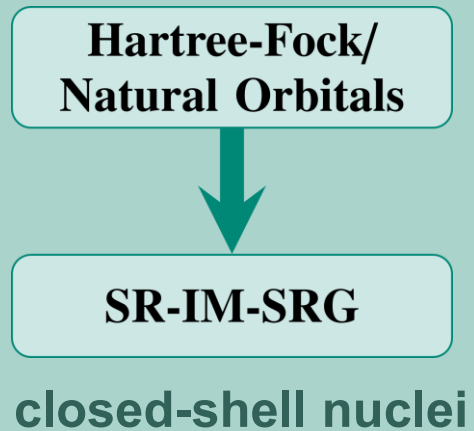
Thank you for your attention!

Find more information on my poster!

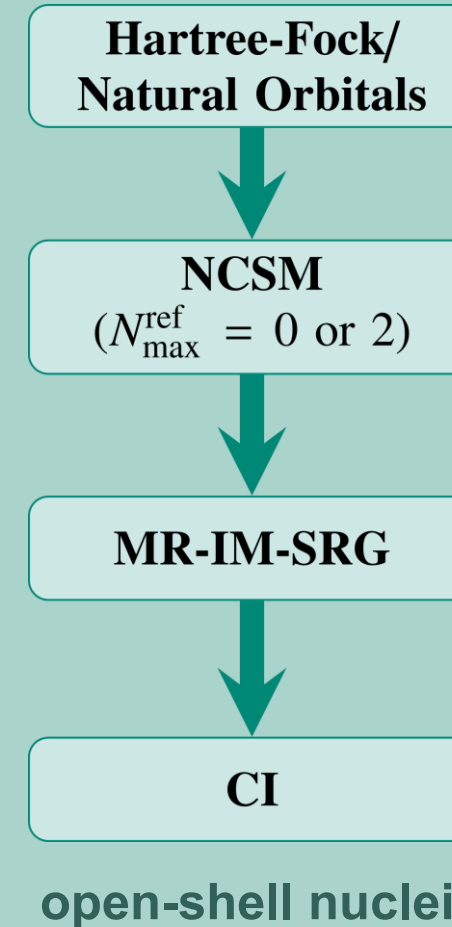
Backup Slides

In-Medium Similarity Renormalization Group

Single-Reference IM-SRG



Multi-Reference IM-SRG



CI with Lanczos Strength-Function Method

- relatively novel approach to calculate transition strengths
- idea: constructing orthonormal basis $V_p = (\vec{v}_1, \vec{v}_2, \dots, \vec{v}_p)$ in which Hamiltonian becomes tridiagonal
- recursive formulation of Lanczos vectors

$$\vec{v}_{i+1} = \frac{1}{\beta_i} (H\vec{v}_i - \beta_{i+1}\vec{v}_{i-1} - \alpha_i\vec{v}_i)$$

$$\alpha_i = \vec{v}_i^T H \vec{v}_i, \quad \beta_i = \|H\vec{v}_i - \beta_{i-1}\vec{v}_{i-1} - \alpha_i\vec{v}_i\|$$

- clever choice of **pivot vector**

$$|v_1\rangle = \frac{1}{\sqrt{S}} \hat{T}_{E\lambda} |\Psi_0\rangle, \quad S = \langle \Psi_0 | \hat{T}_{E\lambda}^\dagger \hat{T}_{E\lambda} | \Psi_0 \rangle$$



electric multipole operator

CI with Lanczos Strength-Function Method

- after p iteration steps, Hamiltonian can be rewritten in tridiagonal form:

$$H_p = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & \dots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \beta_{p-2} & \ddots & \beta_{p-1} \\ 0 & \dots & 0 & \beta_{p-1} & \alpha_p \end{pmatrix}$$

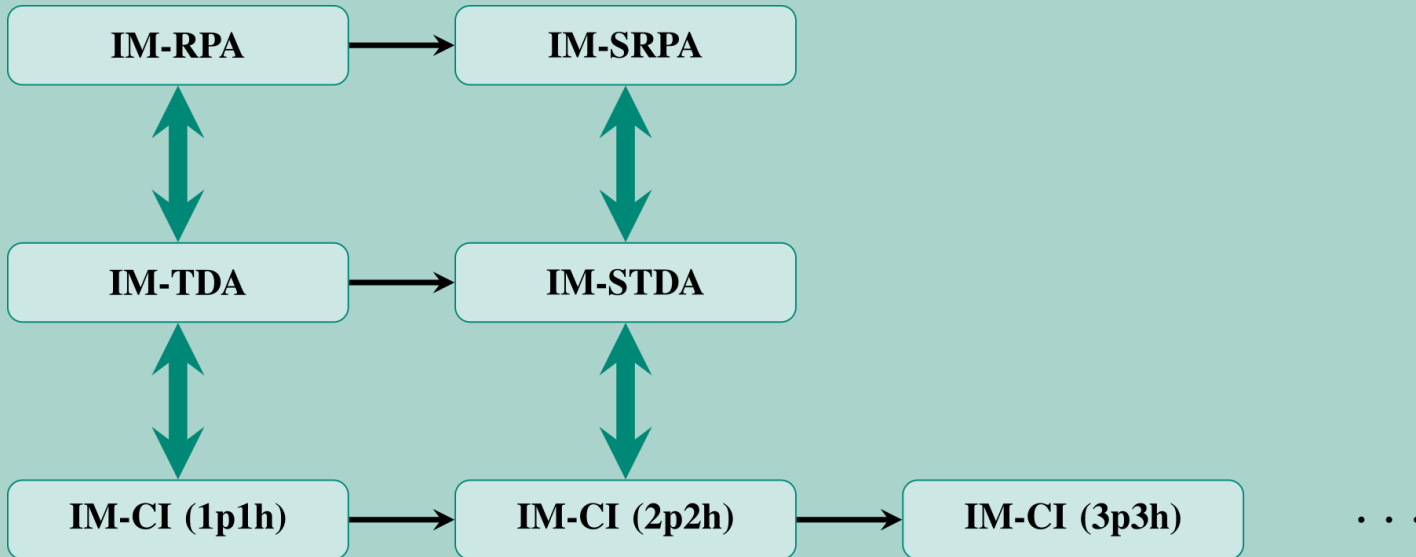
- diagonalization yields approximation of Hamiltonian eigenstates

$$|\Phi_n\rangle = \sum_{j=1}^p C_j^{(n)} |v_j\rangle$$

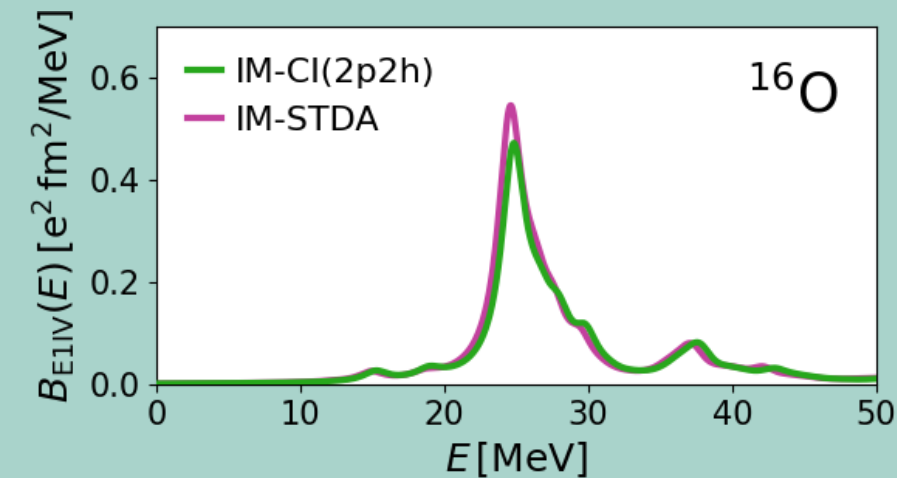
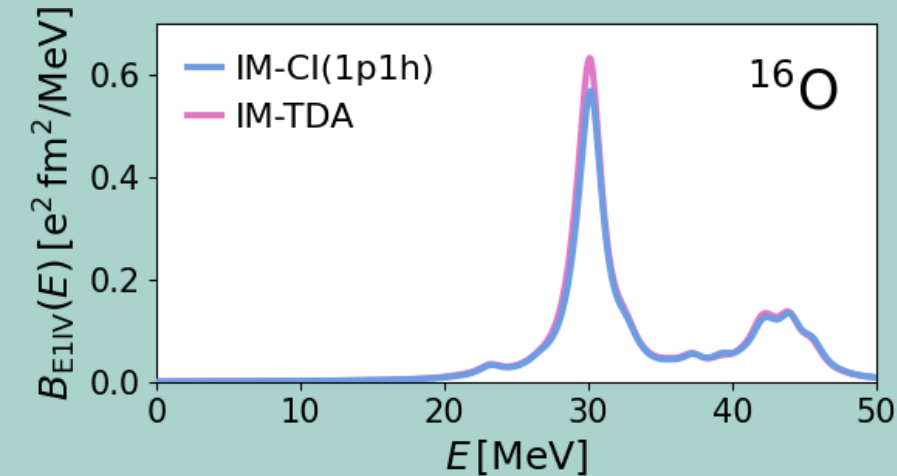
- choice of pivot vector: first coefficient provides **transition matrix element**

$$C_1^{(n)} = \langle \Phi_n | v_1 \rangle = \frac{1}{\sqrt{S}} \langle \Phi_n | \hat{T}_{E\lambda} | \Psi_0 \rangle \longleftarrow \text{ground state determined by preceding CI}$$

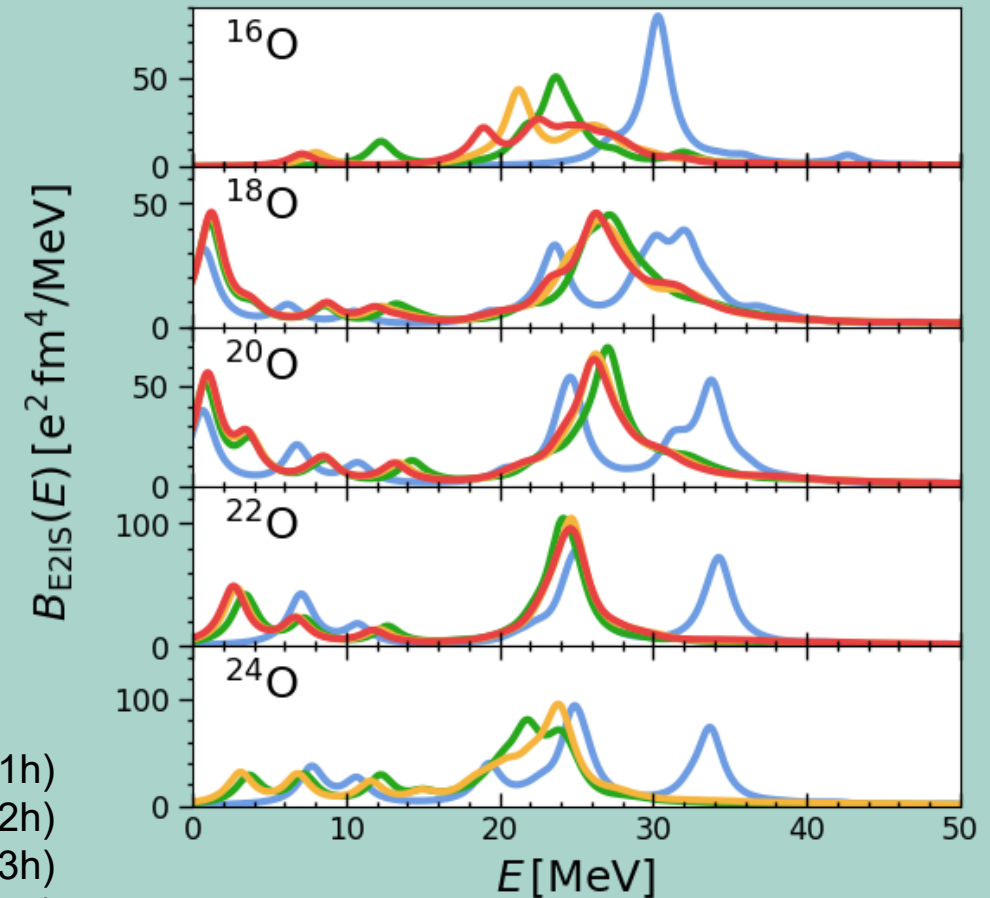
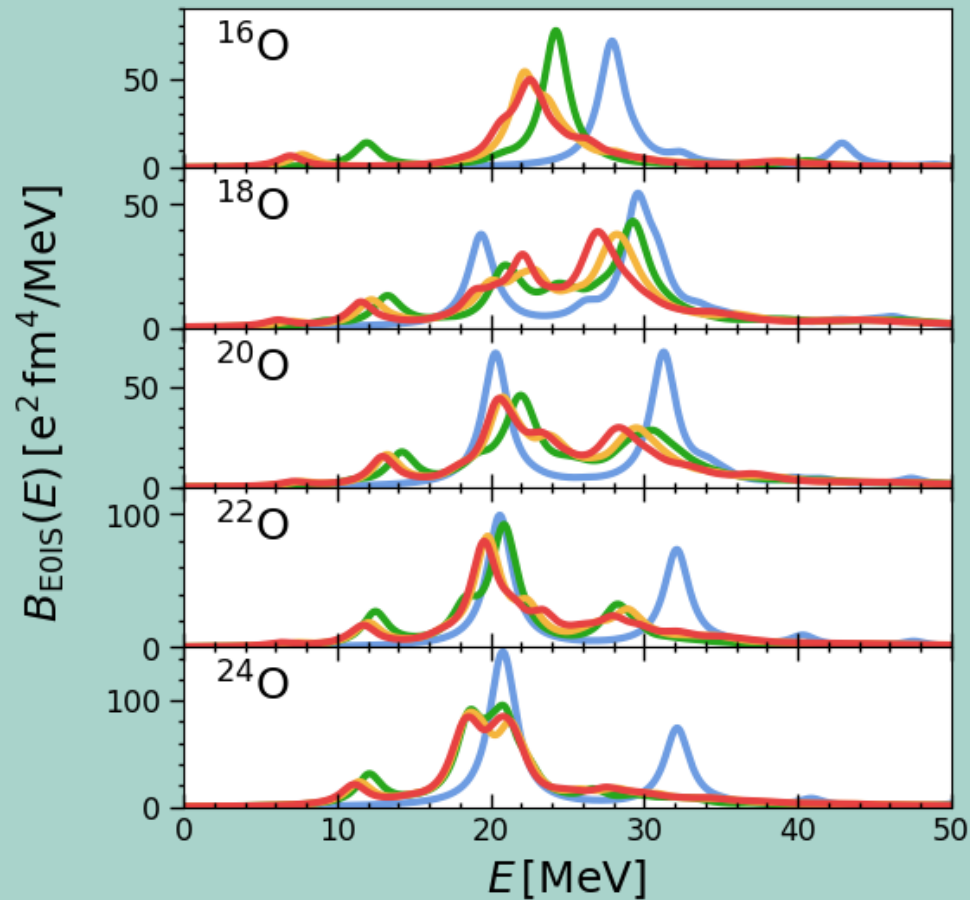
In-Medium CI with Lanczos Strength-Function Method



- two major advantages of CI compared to (S)RPA and (S)TDA:
 - possibility to study **higher ph ranks** (convergence!)
 - access to **open-shell** nuclei

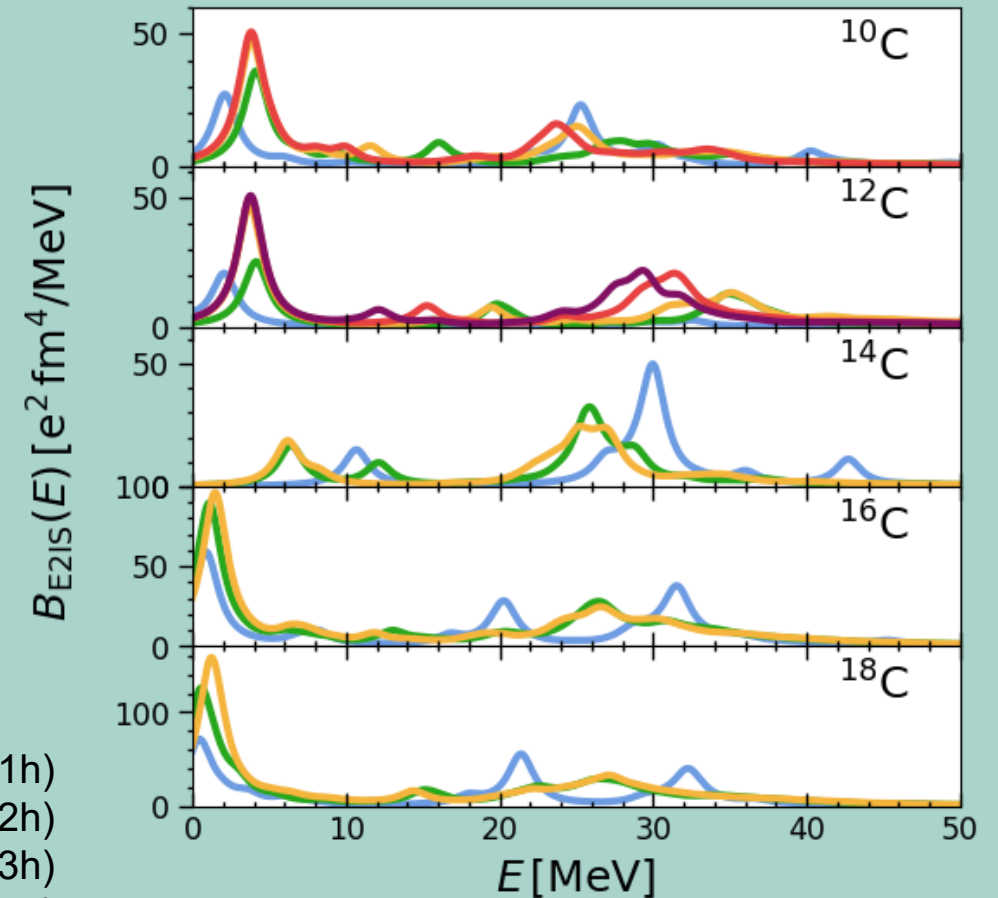
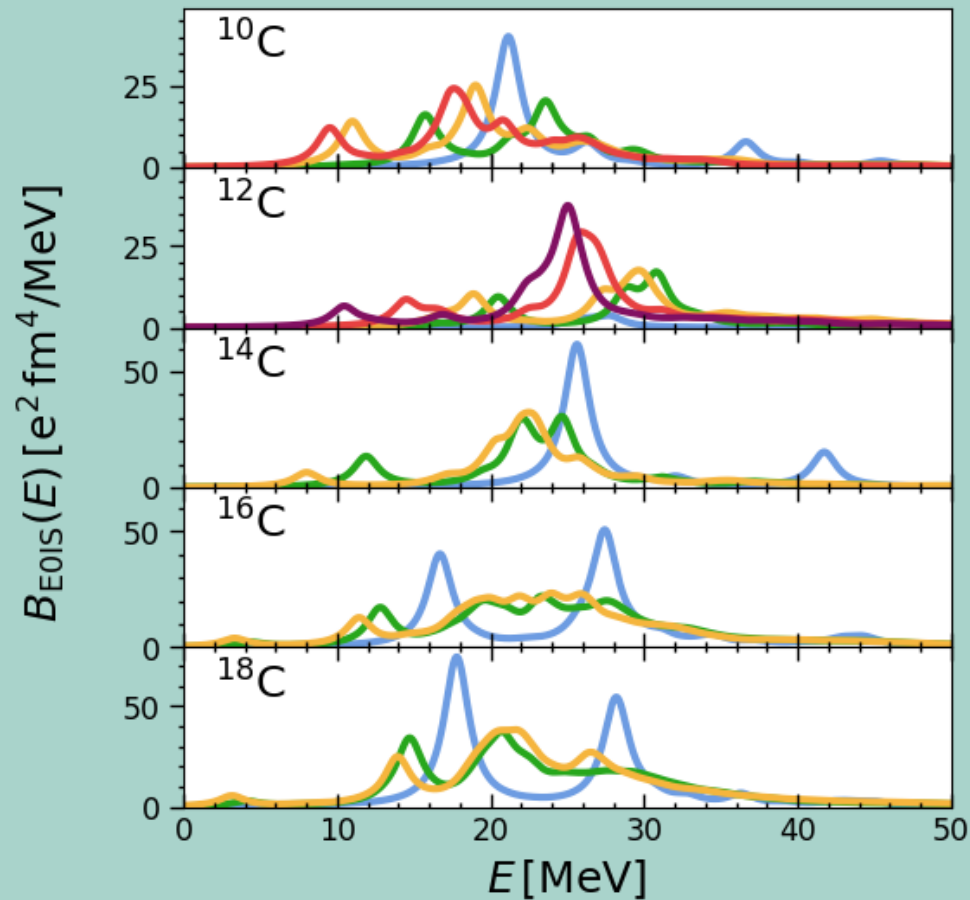


Oxygen Isotopes – E0IS and E2IS



- IM-CI(1p1h)
- IM-CI(2p2h)
- IM-CI(3p3h)
- IM-CI(4p4h)

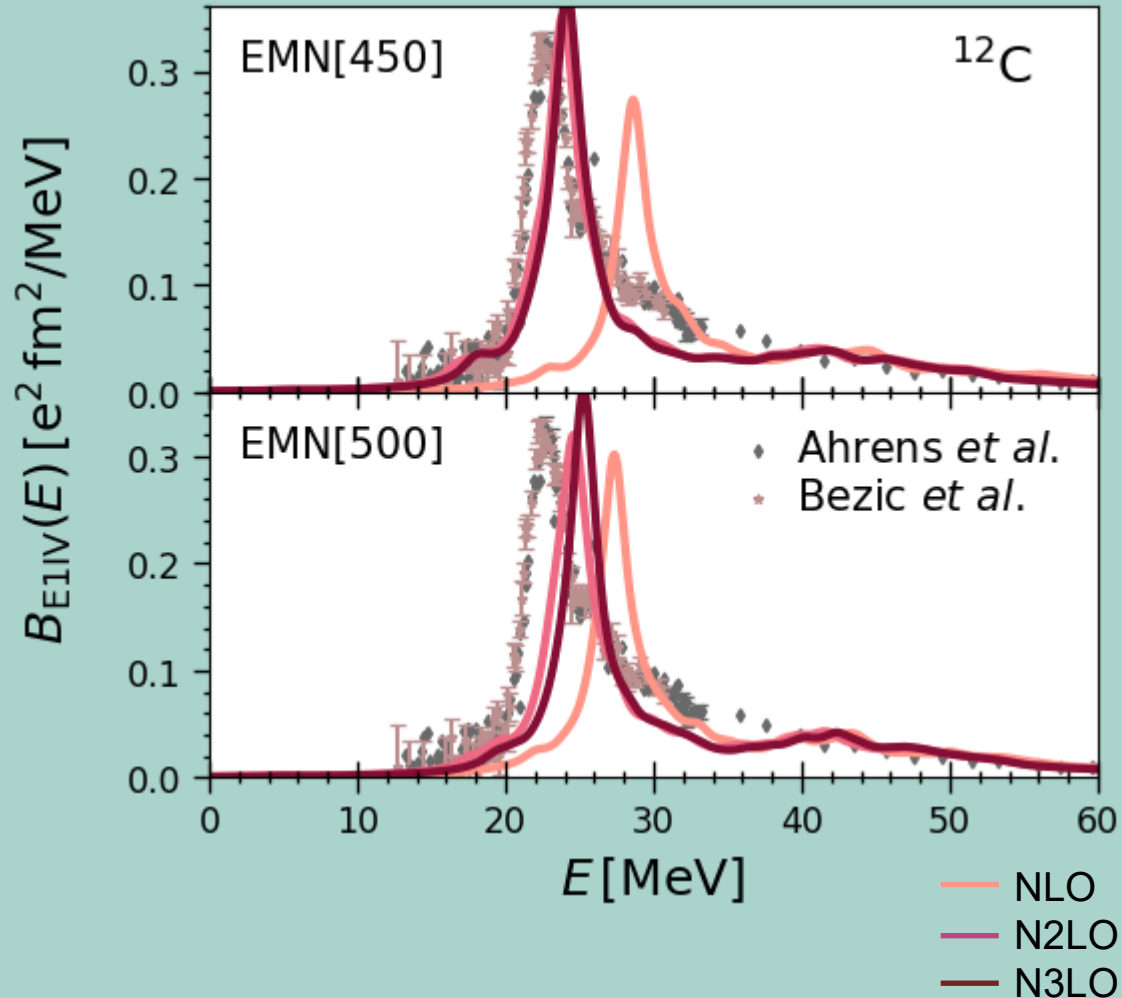
Carbon Isotopes – E0IS and E2IS



- IM-CI(1p1h)
- IM-CI(2p2h)
- IM-CI(3p3h)
- IM-CI(4p4h)
- IM-CI(5p5h)

Impact of Interaction Cutoffs

^{12}C



- chiral NN+3N interactions at two different cutoffs
 NN: Entem, Machleidt, Nosyk, Phys. Rev. C 96, 024002 (2017)
 3N: Hüther, Vobig, Hebeler, Machleidt, Roth, Phys. Lett. B 808, 135651 (2020)
- comparing different chiral orders at 4p4h truncation (reminder: ^{12}C is not converged at this truncation)
- N2LO and N3LO yield similar strength distributions
- EMN[450] at N3LO close to experimental data