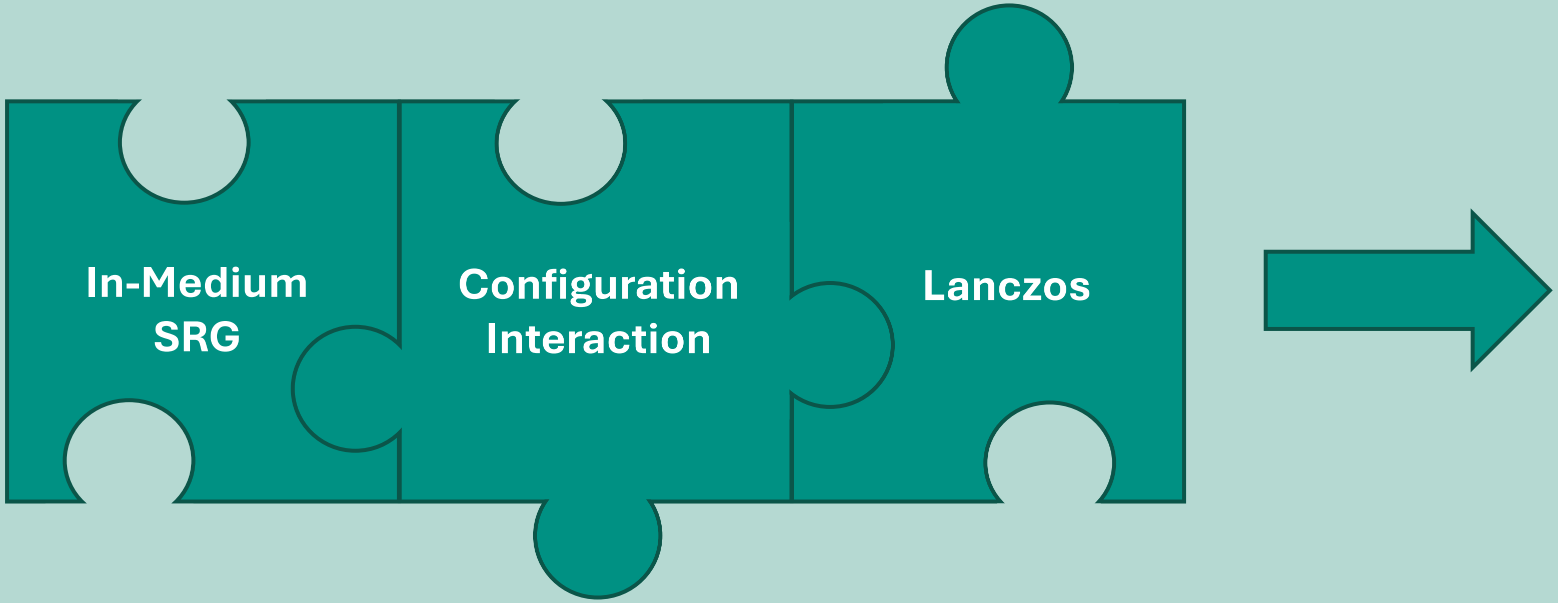
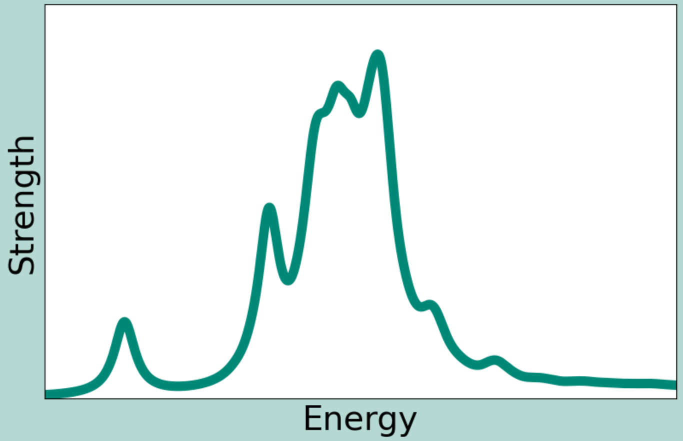
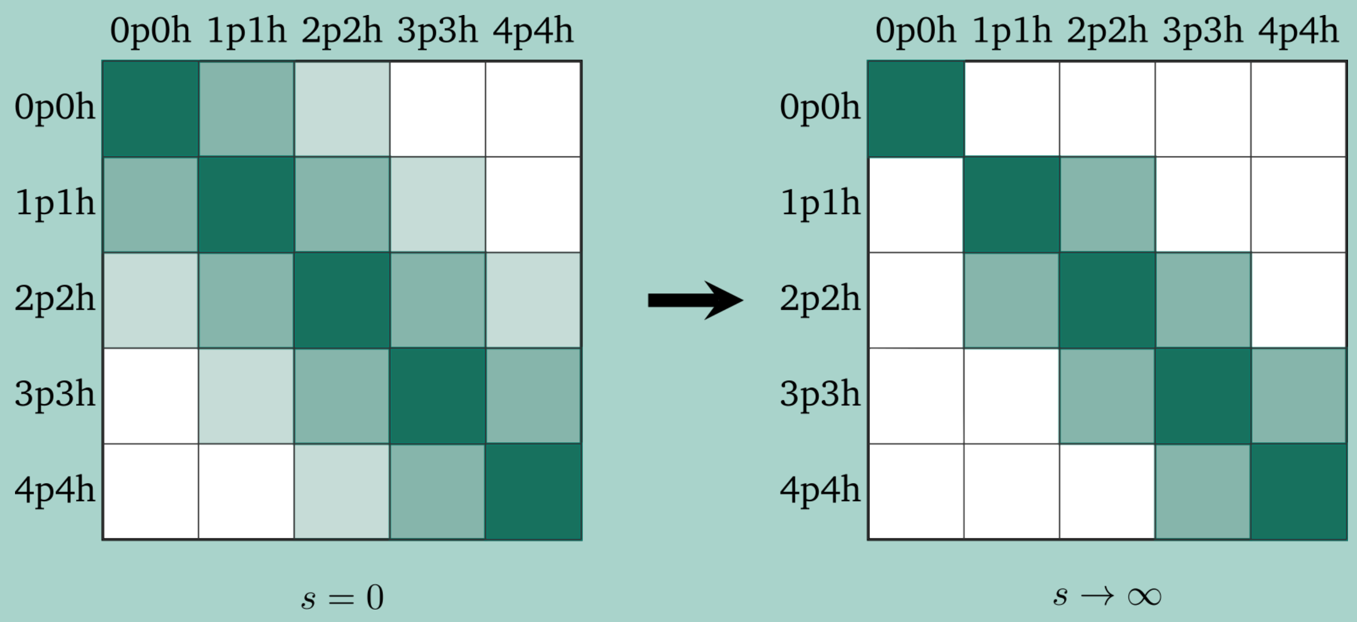
Collective Excitations in Open-Shell Nuclei:
In-Medium CI with Lanczos Strength-Function Method

Michelle Müller





In-Medium Similarity Renormalization Group



- to describe giant resonances, we first need a reliable ground state on which excitations are built
- IM-SRG: powerful method to describe ground-state observables
- goal: decouple reference state from its particle-hole excitations
- multi-reference IM-SRG to describe open-shell nuclei

(In-Medium) Configuration Interaction

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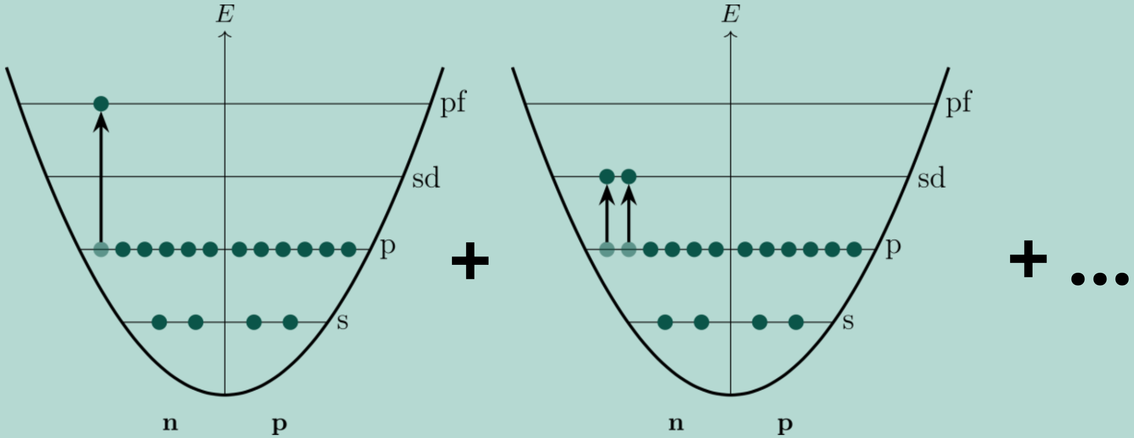
- expansion of Hamiltonian eigenstates in basis of *A*-body Slater determinants
- Slater determinants are built from single-particle states in harmonic oscillator, Hartree Fock or natural orbital basis
- inserting expansion into Schrödinger equation leads to matrix eigenvalue problem

  → can be solved numerically in a truncated model space

- **IM-CI:** employ IM-SRG evolved matrix elements in CI calculations

$$\begin{pmatrix} \langle\phi_1|\hat{H}|\phi_1\rangle & \langle\phi_1|\hat{H}|\phi_2\rangle & \cdots \\ \langle\phi_2|\hat{H}|\phi_1\rangle & \langle\phi_2|\hat{H}|\phi_2\rangle & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \langle\phi_1|\psi_n\rangle \\ \langle\phi_2|\psi_n\rangle \\ \vdots \end{pmatrix} = E_n \begin{pmatrix} \langle\phi_1|\psi_n\rangle \\ \langle\phi_2|\psi_n\rangle \\ \vdots \end{pmatrix}$$

Model-Space Truncations: N_{max}



$$N_{\mathrm{max}} = 2$$

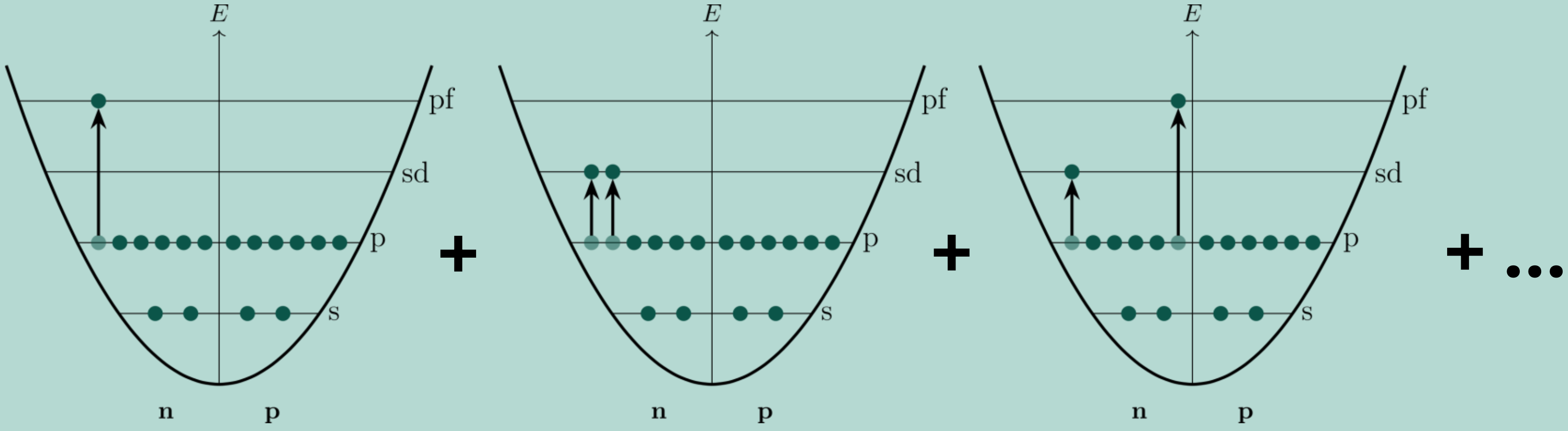
N_{max}

- truncation based on total number of excitation quanta

T_{max}

- truncation based on particle-hole level

Model-Space Truncations: T_{max}



$$T_{\text{max}} = 2$$

N_{max}

- truncation based on total number of excitation quanta

T_{max}

- truncation based on particle-hole level

Importance Truncation

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- model-space dimensions increase significantly with larger values of T_{max} and N_{max}

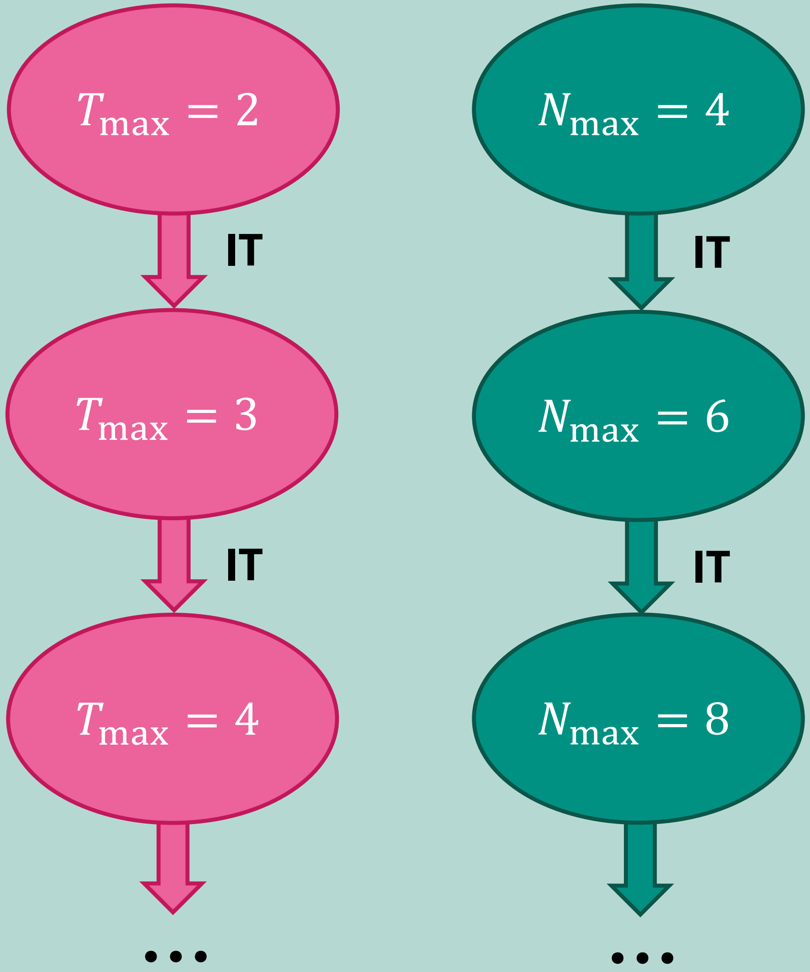
  $\rightarrow$ additional truncation is required

- idea: use first-order correction in MCPT to define importance measure

$$\kappa_j^{(n)} = -\frac{\langle \Phi_j | \hat{H} | \Psi_{\mathrm{ref}}^{(n)} \rangle}{\Delta\varepsilon_j} \longleftarrow$$

reference state determined by preceding (IT-)CI

- only include states with $|\kappa_j^{(n)}| \geq \kappa_{\mathrm{min}}$ for a fixed value of κ_{min}
- model spaces are built iteratively



IM-CI with Lanczos Strength-Function Method

- idea: construct orthonormal basis $V_p = (\vec{v}_1, \vec{v}_2, ..., \vec{v}_p)$ in which Hamiltonian becomes tridiagonal

- clever choice of **pivot vector**

electric multipole operator

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

- diagonalization of tridiagonal matrix yields approximate Hamiltonian eigenpairs

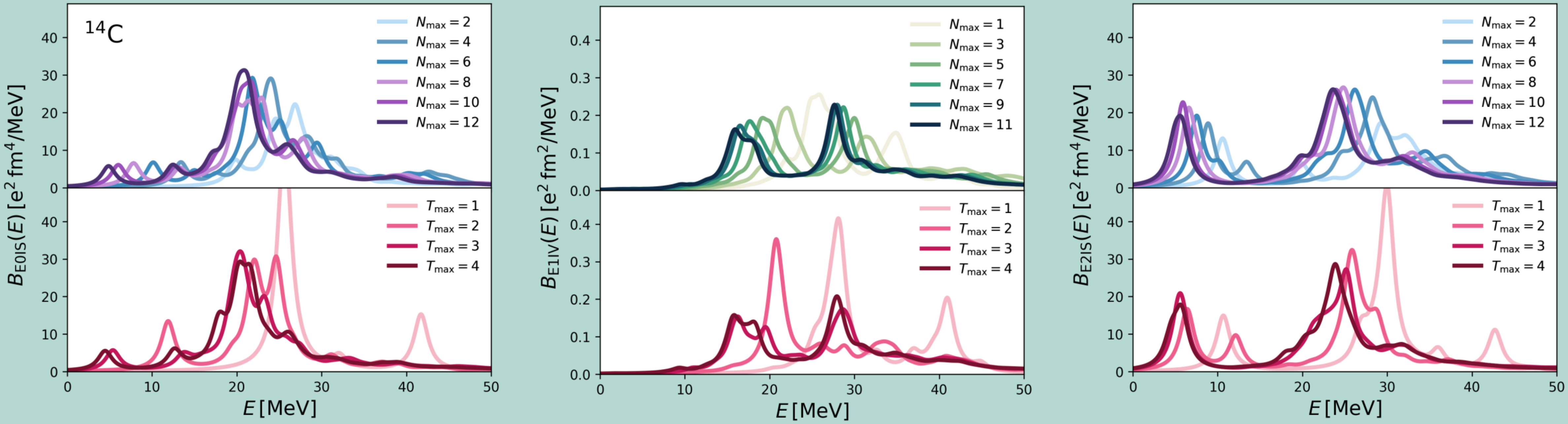
$$|\Phi_n\rangle = \sum_{j=1}^{p} C_j^{(n)}|v_j\rangle$$

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

$$C_1^{(n)} = \langle\Phi_n|v_1\rangle = \frac{1}{\sqrt{S}} \langle\Phi_n|\hat{T}_{\mathrm{E}\lambda}|\Psi_0\rangle \longleftarrow$$

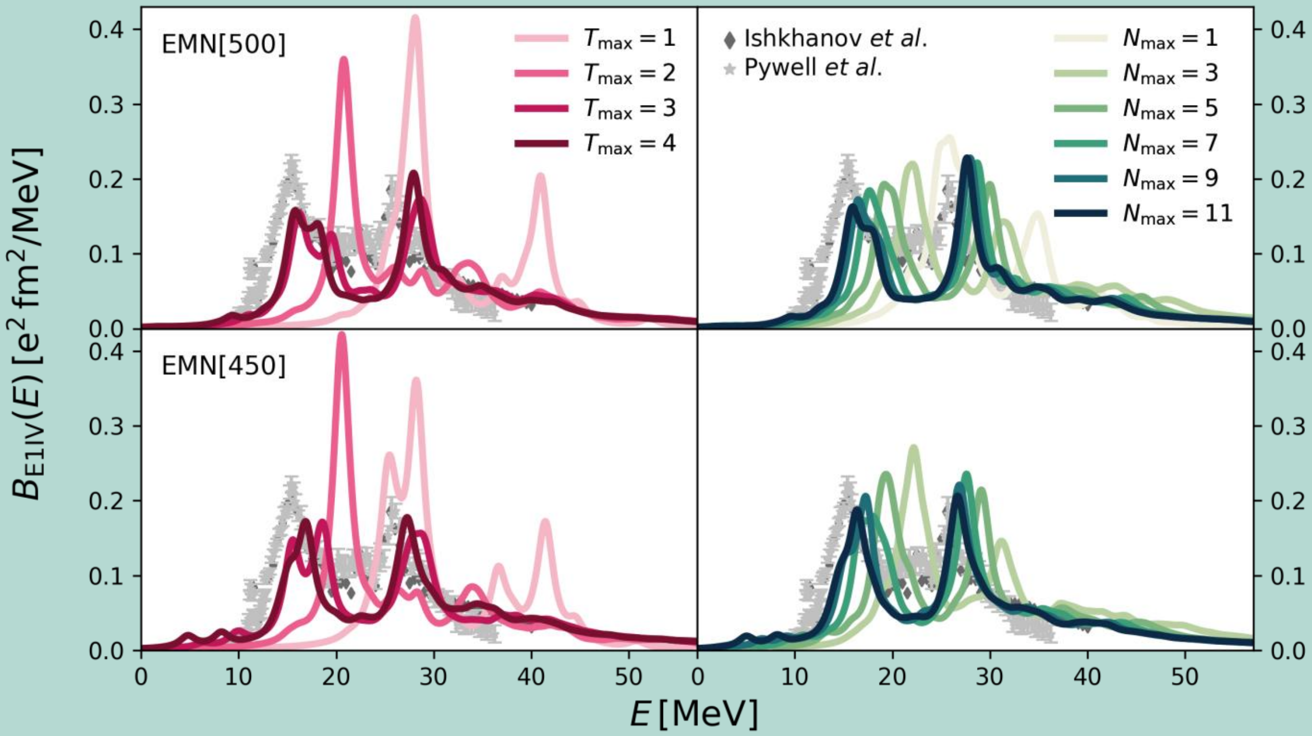
ground state determined by preceding IM-CI

$N_{\max}$ vs. $T_{\max}$ Convergence



- $N_{\max}$ convergence more stable than $T_{\max}$ convergence
- $N_{\max}$ computationally more efficient ($T_{\max} = 4$: 25000 CPU hours; $N_{\max} = 12$: 5000 CPU hours)
- consistent: results converge to closely matching strength distributions for both truncations

Isovector Dipole Strength Distributions for ^{14}C

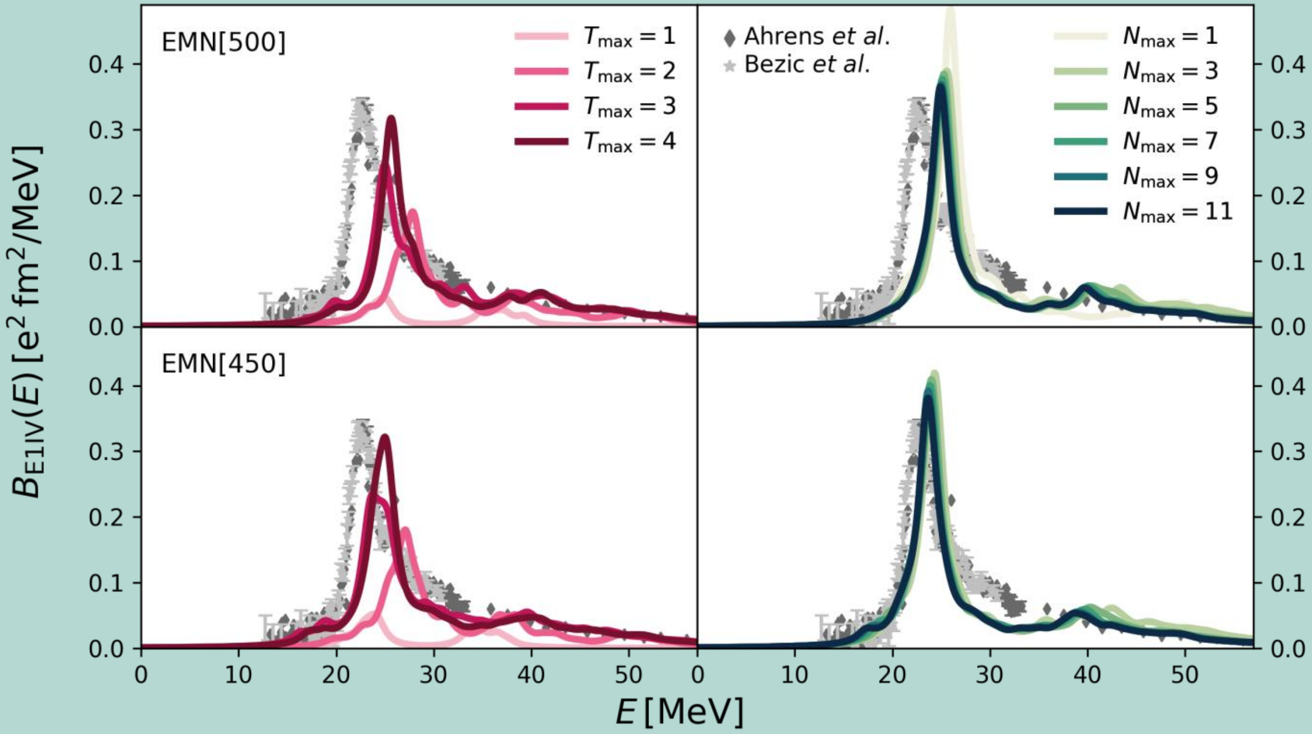


- chiral NN+3N interactions at two cutoffs

NN: Entem, Machleidt, Nosyk, Phys. Rev. C 96, 024002 (2017)
3N: Hüther, Vobig, Hebeler, Machleidt, Roth, Phys. Lett. B 808, 135651 (2020)

- double-peak structure reproduced by both chiral interactions
- EMN[500]: strengths shifted towards higher energies compared to experimental data
- EMN[450]: strengths shifted closer to data

Isovector Dipole Strength Distributions for $^{12}\mathrm{C}$



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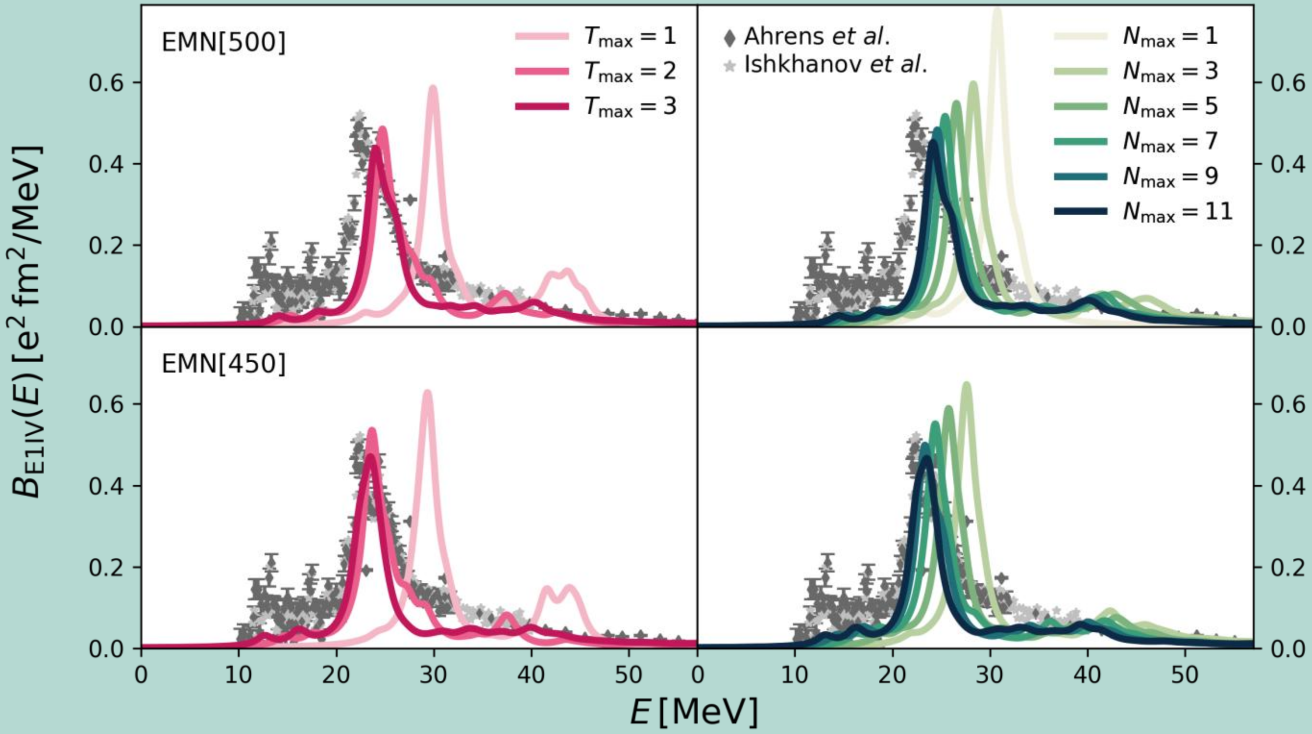
- EMN[450]: strengths shifted closer to data

Isovector Dipole Strength Distributions for ^{16}O



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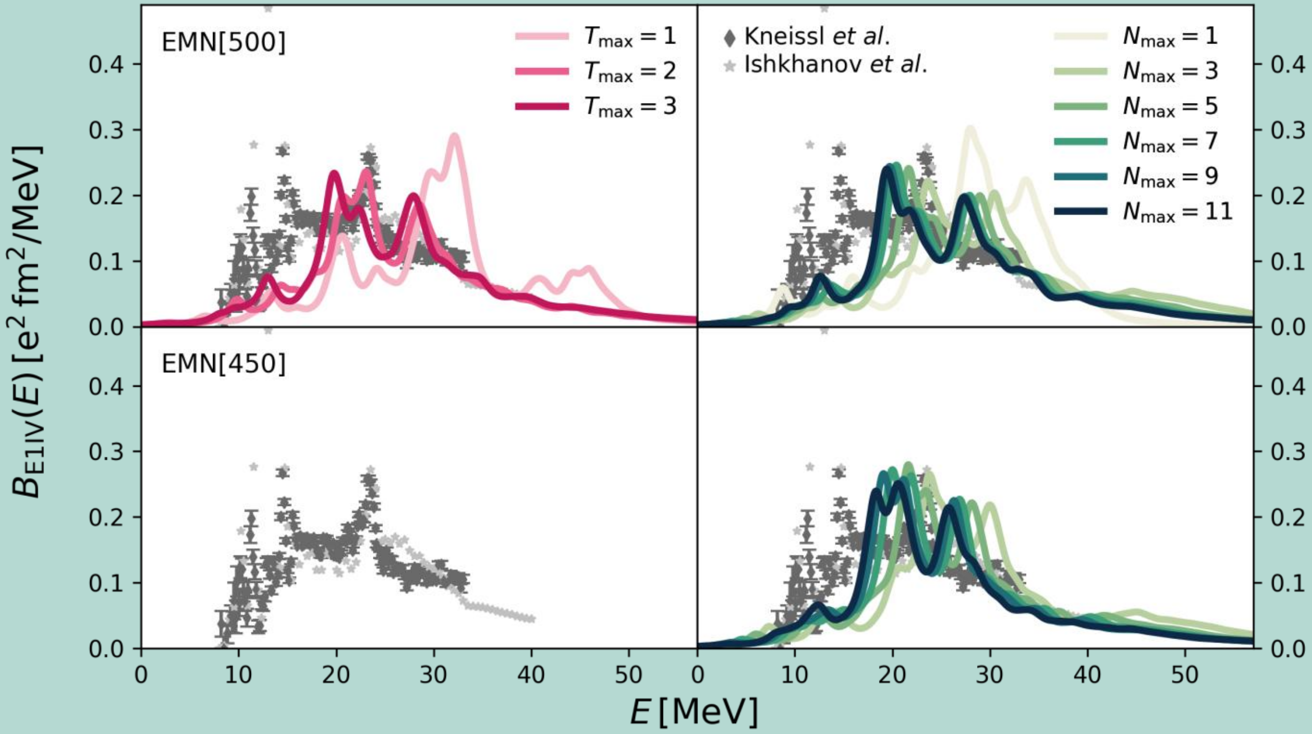
- EMN[500]: strengths shifted towards higher energies compared to experimental data

- EMN[450]: main peak matches well with data

Isovector Dipole Strength Distributions for ^{18}O



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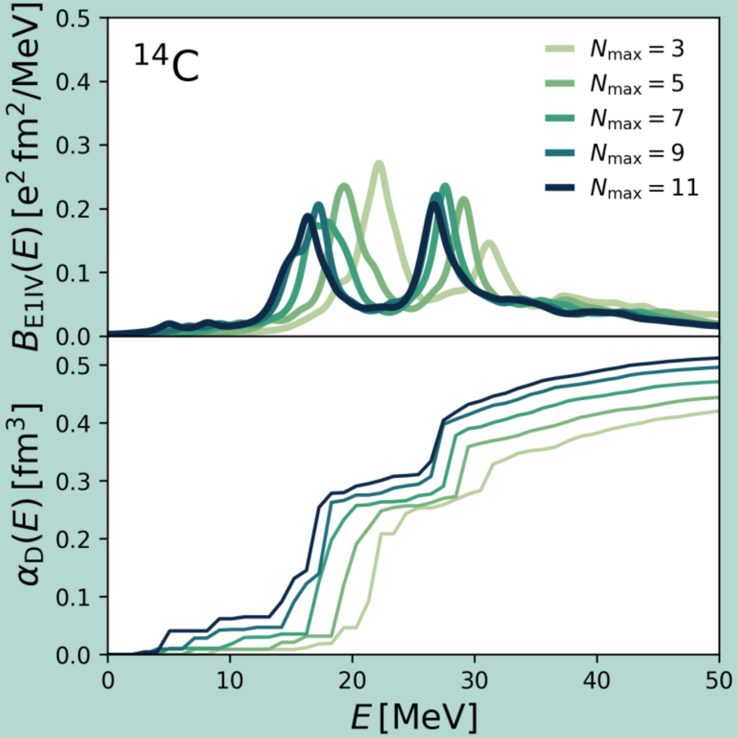
- smeared-out structure of strength distribution, more challenging to compare to experiment
- EMN[500]: strengths shifted towards higher energies compared to experimental data
- EMN[450]: strengths shifted closer to data

Dipole Polarizabilities: Running Sum



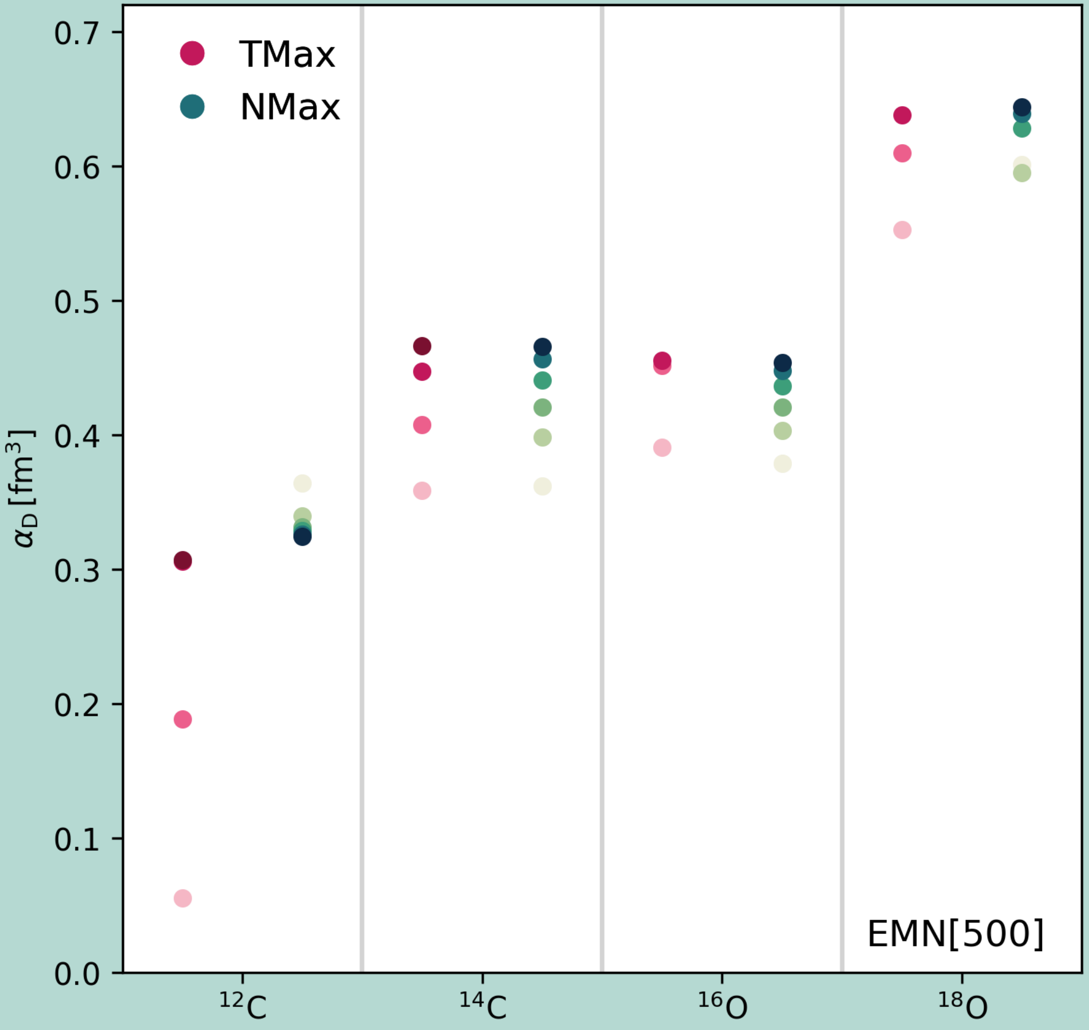
- dipole polarizabilities can directly be obtained from isovector dipole strengths

$$\alpha_{\mathrm{D}}(E) = \frac{8\pi}{9} e^2 \sum_{E_i \leq E} \frac{B_{\mathrm{E1IV}}(E_i)}{E_i}$$

- strength numerator: main contributions for polarizability at peaks of strength distribution
- energy denominator: polarizability increases predominantly at lower energies

→ major role of energy shifts of strength distributions for larger model spaces

Dipole Polarizabilities: Convergence



$$\alpha_{\mathrm{D}}(E) = \frac{8\pi}{9} e^2 \sum_{E_i \leq E} \frac{B_{\mathrm{E1IV}}(E_i)}{E_i}$$

- polarizabilities mostly converge from below

  → reason: strength distributions shifted to lower energies for increasing truncations

- $N_{\max}$ and $T_{\max}$ provide consistent results for converged polarizabilities

Conclusion and Outlook

Take-Home Messages

- IM-CI allows exploration of transition strengths and polarizabilities in open-shell nuclei
- N_{max} truncation is more efficient than T_{max} truncation
- truncation schemes provide identical results at convergence
- EMN[450] yields strength distributions consistent with experimental data

Future Plans

- further explore oxygen and carbon isotopic chains: strengths and polarizabilities
- develop energy-based truncation scheme

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Thank you for your attention!