Scaled Natural Orbitals for Radii and E2 Observables in the NCSM

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Motivation

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nuclear wave function		many-body HO states		single-particle HO states
$\lvert\Psi\rangle$	expanded in $\longrightarrow$	$\lvert\Phi\rangle$	constructed from $\longrightarrow$	$\lvert\phi\rangle$
$\underset{r \gg 0}{\propto} e^{-r}$				$\underset{r \gg 0}{\propto} e^{-r^2}$

- Long-range sensitive observables profit from optimization of single-particle basis

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Natural Orbitals (NATs)

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1. Calculate HF ground state using HO basis with a_{HO} →
2. Perturbatively improve HF ground state →
3. Diagonalization of density matrix $\langle \Psi^{(\mathrm{MBPT})}_{\mathrm{HF,gs}} | \hat{a}^{\dagger}_{i} \hat{a}_{j} | \Psi^{(\mathrm{MBPT})}_{\mathrm{HF,gs}} \rangle$ →
4. NATs

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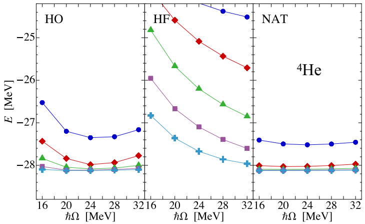
Natural Orbitals (NATs)

Calculate HF ground state using HO basis with a_{HO} → Perturbatively improve HF ground state → Diagonalization of density matrix $\langle \Psi^{(\mathrm{MBPT})}_{\mathrm{HF,gs}} | \hat{a}^\dagger_i \hat{a}_j | \Psi^{(\mathrm{MBPT})}_{\mathrm{HF,gs}} \rangle$ → NATs

NATs independent of a_{HO}



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

Scaled Natural Orbitals (SNATs)

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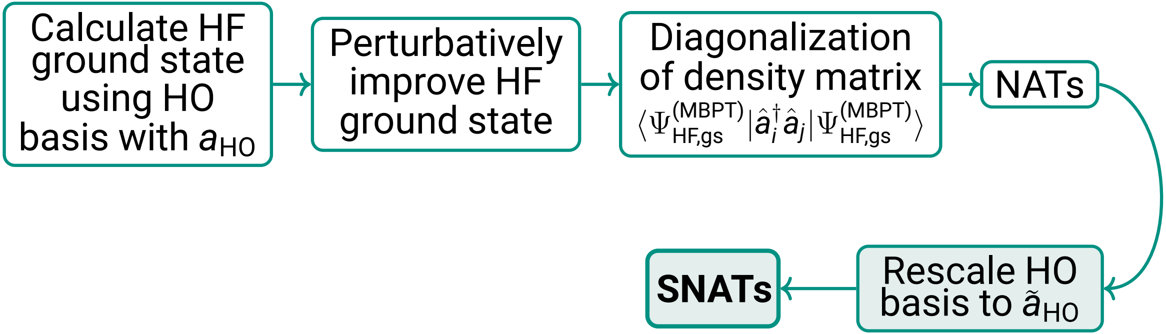

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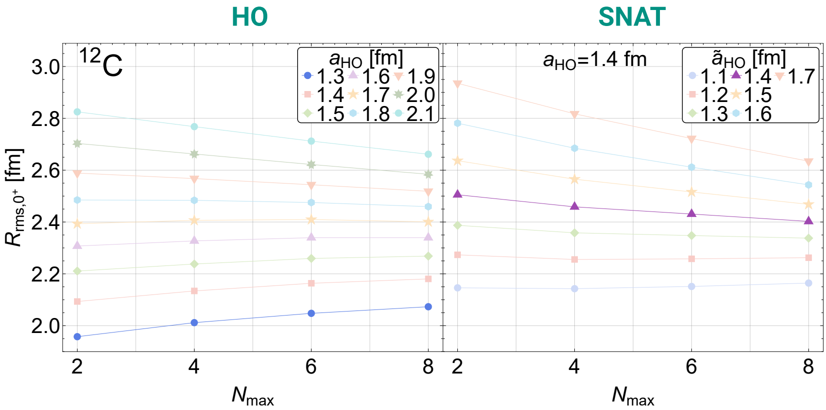
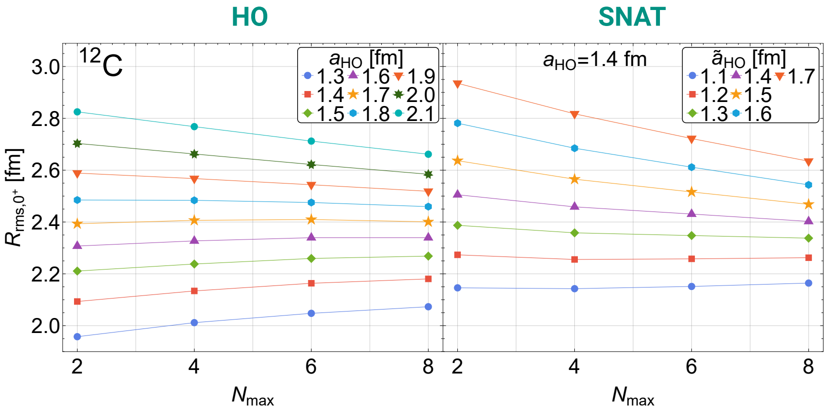
^{12}C - Rms Radius



Starting points for length parameter variation:

- HO:
  a_{HO} of optimal energy convergence,
  here: $a_{HO} = 1.3$ fm
- SNAT:
  Normal NATs:
  $\tilde{a}_{HO} = a_{HO} = 1.4$ fm

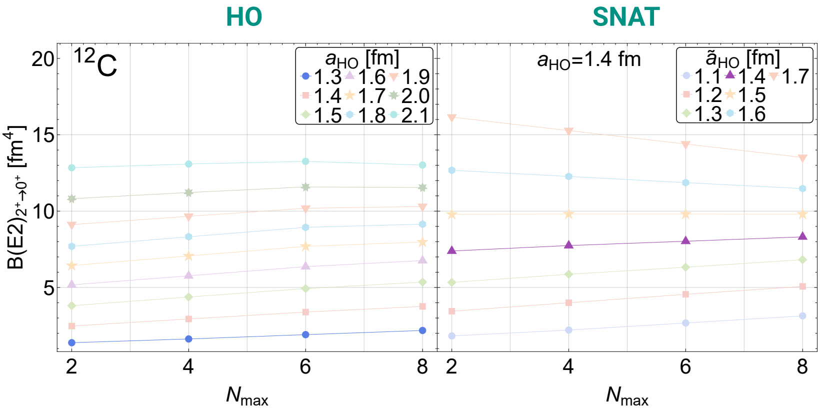
^{12}C - Rms Radius



Optimal sequences:

- HO:
  $a_{\mathrm{HO}} = 1.7\,\mathrm{fm}$
- SNAT:
  $\tilde{a}_{\mathrm{HO}} = 1.2\,\mathrm{fm}$,
  closer to starting value than HO

^{12}C - E2 Transition Strength



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  a_{HO} of optimal energy convergence,
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^{12}C - E2 Transition Strength

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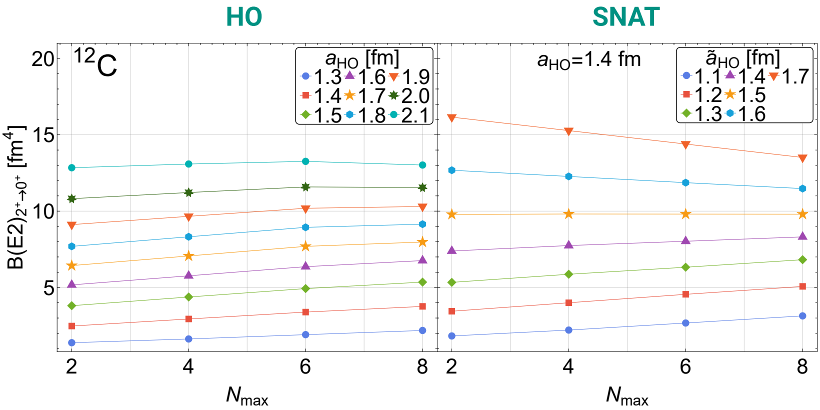

Optimal sequences:

- HO: $a_{HO} \approx 2.1\,\mathrm{fm}$
- SNAT: $\tilde{a}_{HO} = 1.5\,\mathrm{fm}$,

▶ Finding optimal sequence requires less variation for SNATs

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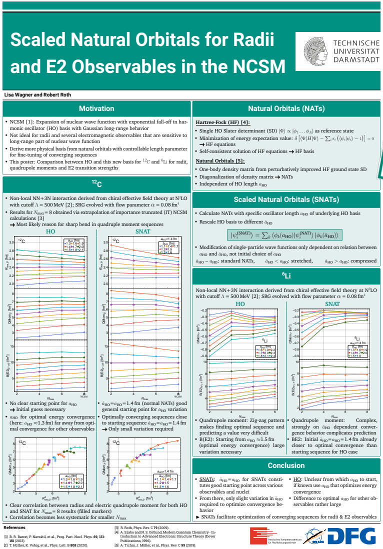

More details on my poster

Thank you for your attention!

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