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Scaled Natural Orbitals for Radii and E2 Observables in the NCSM

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Motivation

nuclear wave
function

$$|\Psi\rangle$$
$$\propto e^{-r}$$
$$r \gg 0$$

expanded in

$$|\Phi\rangle$$

constructed from

$$|\phi\rangle$$

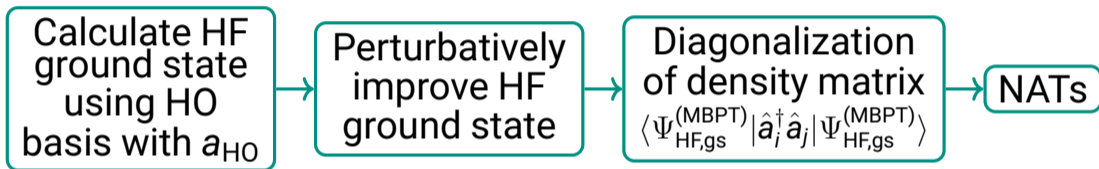
$$\propto e^{-r^2}$$
$$r \gg 0$$

many-body HO
states

single-particle
HO states

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

Natural Orbitals (NATs)



Natural Orbitals (NATs)

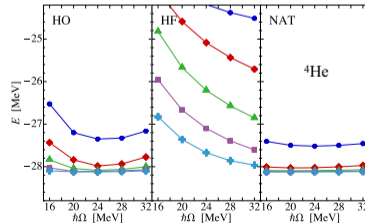
Calculate HF
ground state
using HO
basis with a_{HO}

Perturbatively
improve HF
ground state

Diagonalization
of density matrix
 $\langle \Psi_{\text{HF,gs}}^{(\text{MBPT})} | \hat{a}_i^\dagger \hat{a}_j | \Psi_{\text{HF,gs}}^{(\text{MBPT})} \rangle$

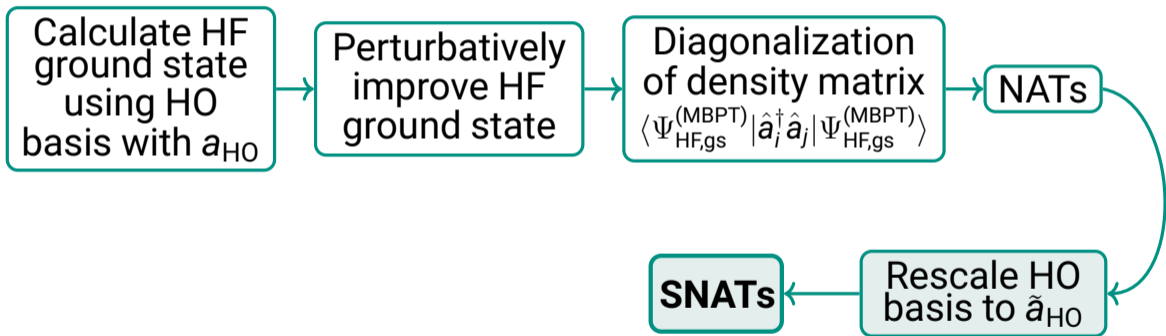
NATs

NATs independent of a_{HO}

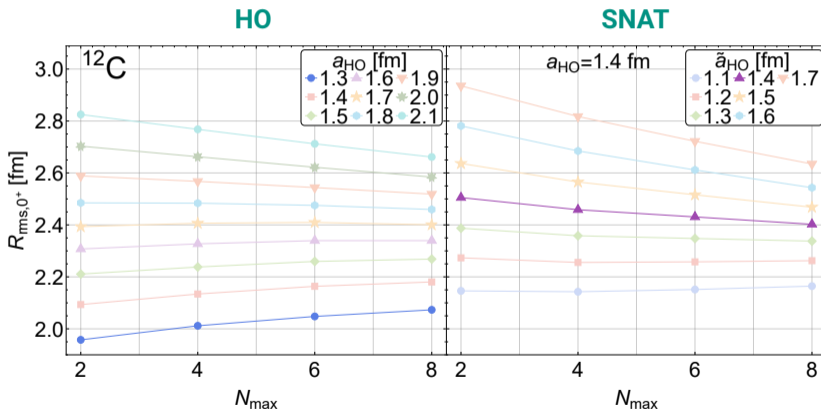


Tichai et. al.,
Phys. Rev. C 99 (2019)

Scaled Natural Orbitals (SNATs)



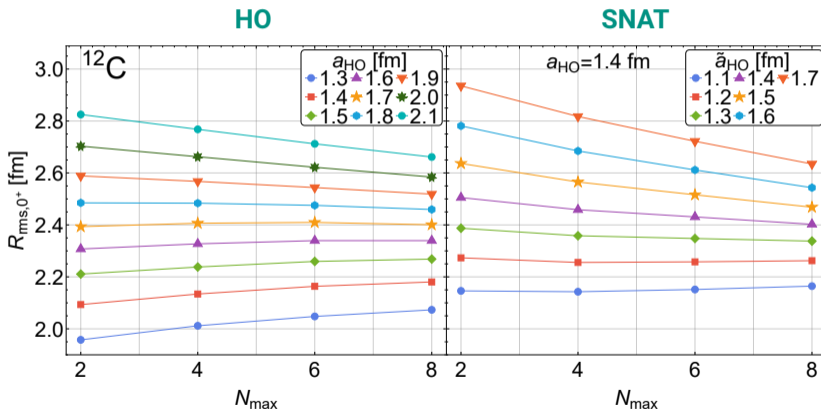
^{12}C - Rms Radius



Starting points for length parameter variation:

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

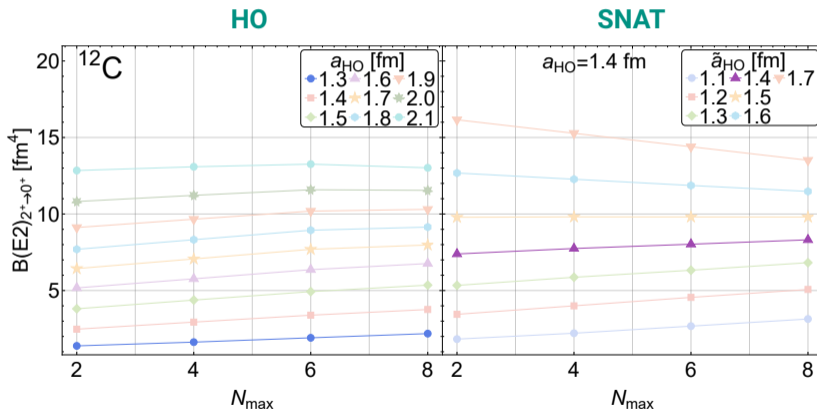
^{12}C - Rms Radius



Optimal sequences:

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

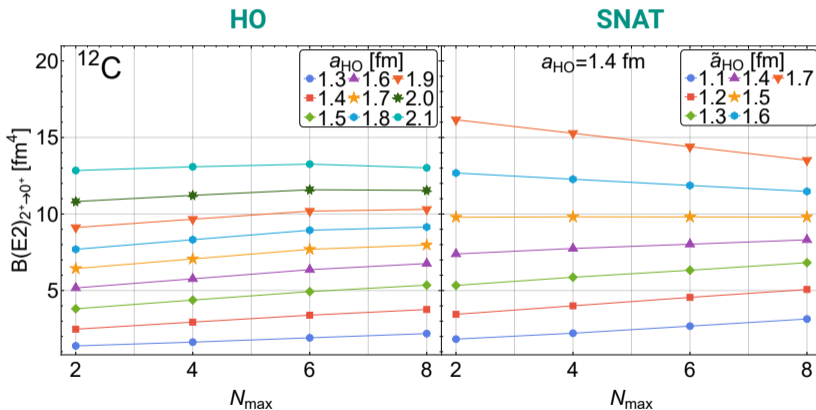
^{12}C - E2 Transition Strength



Starting points for length parameter variation:

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

^{12}C - E2 Transition Strength



Optimal sequences:

- HO:
 $a_{\text{HO}} \approx 2.1 \text{ fm}$
- SNAT:
 $\tilde{a}_{\text{HO}} = 1.5 \text{ fm}$,
- ▶ Finding optimal sequence requires less variation for SNATs

Scaled Natural Orbitals for Radii and E2 Observables in the NCSM



Lisa Wagner and Robert Roth

Motivation	Natural Orbitals (NATs)
<ul style="list-style-type: none"> NCSM [1]: Expansion of nuclear wave function with exponential fall-off to harmonic oscillator (HO) basis with Gaussian long-range behavior Star ideal for radii and central electromagnetic observables that are sensitive to long-range part of nuclear wave function Derive more physical basis from natural orbitals with controllable length parameter for the scaling of converging sequences This paper: Comparison between HO and this new basis for ^{12}C and ^{16}O for radii, quadrupole moments and E2 transition strength 	<p>Harmon-Boltz (HB) [4]:</p> <ul style="list-style-type: none"> Single HO Slater determinant (SD) $\Phi\rangle = \dots, n_x, \dots\rangle$ as reference state Minimization of energy expectation value $\langle \Phi \hat{H} \Phi \rangle = \sum_{i=1}^N \langle \Phi \hat{H} \Phi \rangle - \epsilon_i = 0$ HF equations Self-consistent solution of HF equations \rightarrow HF basis <p>Natural Orbitals [2]:</p> <ul style="list-style-type: none"> One-body density matrix from perturbatively improved HF ground state SD Diagonalization of density matrix \rightarrow NATs Independence of HO length η_{HO}
<p>^{12}C</p> <ul style="list-style-type: none"> Non-local NN+3N interaction derived from chiral effective field theory at N²LO with cutoff $\Lambda = 500\text{ MeV}$ [2]; SRG evolved with flow parameter $\omega = 0.68\text{ fm}^{-1}$ Results for r_{rms} obtained via extrapolation of impure truncated (IT) NCSM calculations [2] Most likely reason for cheap bond in quadrupole moment sequences 	<p>Scaled Natural Orbitals (SNATs)</p> <ul style="list-style-type: none"> Calculate NATs with specific oscillator length ω_{HO} of underlying HO basis Rescale HO basis to different ω_{HO} $ \Phi^{(SNAT)}\rangle = \sum_{i=1}^N \Phi_i(\eta_{HO})\rangle \langle \Phi_i(\eta_{HO}) \hat{H} \Phi_i(\eta_{HO}) \rangle$ <ul style="list-style-type: none"> Modification of single-particle wave functions only depends on relation between ω_{HO} and ω_{NAT}, not initial choice of ω_{HO} $\omega_{HO} = \omega_{NAT}$ standard NATs, $\omega_{HO} > \omega_{NAT}$ stretched, $\omega_{HO} < \omega_{NAT}$ compressed
<p>^{16}O</p> <ul style="list-style-type: none"> Non-local NN+3N interaction derived from chiral effective field theory at N²LO with cutoff $\Lambda = 500\text{ MeV}$ [2]; SRG evolved with flow parameter $\omega = 0.68\text{ fm}^{-1}$ 	<p>^{16}O</p> <ul style="list-style-type: none"> Non-local NN+3N interaction derived from chiral effective field theory at N²LO with cutoff $\Lambda = 500\text{ MeV}$ [2]; SRG evolved with flow parameter $\omega = 0.68\text{ fm}^{-1}$
<p>HO</p> <p>SNAT</p>	<p>HO</p> <p>SNAT</p>
<ul style="list-style-type: none"> No clear starting point for ω_{HO} Initial guess necessary ω_{HO} for optimal energy convergence (here: $\omega_{HO} = 1.2\text{ fm}^{-1}$ for easy bond case that converges for other observables) 	<ul style="list-style-type: none"> Quadrupole moment: Zig-zag pattern makes finding optimal sequence and predicting a value very difficult BE2: Starting from $\omega_{HO} = 1.5\text{ fm}^{-1}$ (optimal energy convergence) large variation necessary
<ul style="list-style-type: none"> Clear correlation between radii and electric quadrupole moment for both HO and SNAT for $r_{\text{rms}} = 8$ results (filled markers) Correlation becomes less systematic for smaller bond 	<p>Conclusion</p> <ul style="list-style-type: none"> Stable $\omega_{HO} = \omega_{NAT}$ for SNATs consistently good starting point across various observables and nuclei From them, only slight variation in ω_{HO} required to optimize convergence for larger Stable $\omega_{HO} = \omega_{NAT}$ for SNATs consistently good starting point across various observables and nuclei Inference to optimal ω_{HO} for other observables rather large SNATs facilitate optimization of converging sequences for radii & E2 observables



More details on my poster

Thank you for your attention!

References: [1] S. K. Boger, P. Mariani et al., Phys. Rev. Lett. 108, 082501 (2012); [2] T. Taniuchi, A. Taniuchi et al., Phys. Lett. B 688 (2010); [3] S. Roth, Phys. Rev. C 76 (2007); [4] A. Bohr and B. L. Nielsen, Nuclear Structure in Single-Particle Motion (Benjamin, 1968); [5] A. Taniuchi, J. Phys. G: Nucl. Part. Phys. 36 (2009).

