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Precision Calculation of Nuclear Observables with the NCSM

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General Context

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- Aim: Solve time-independent nuclear Schrödinger equation $\hat{H}\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle$
- Hamiltonian $\widehat{H}$: Consistent NN + 3N interactions from chiral EFT
- Employ systematically improvable method with quantifiable uncertainties
- Light nuclei: up to $A \approx 20$

No-Core Shell Model (NCSM)

- Schrödinger equation as matrix eigenvalue problem

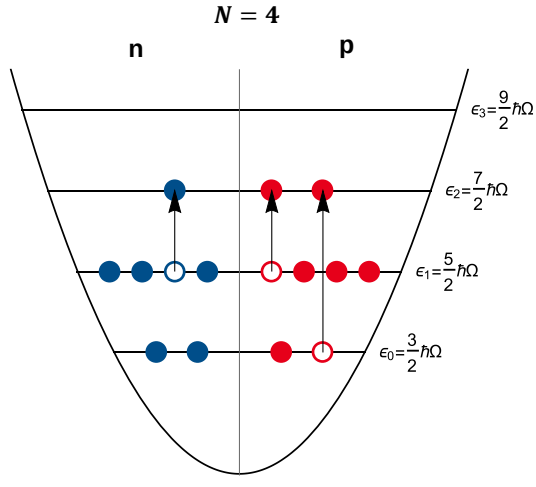
$$\sum_j \langle \Phi_i | \hat{H} | \Phi_j \rangle \langle \Phi_j | \Psi_n \rangle = E_n \langle \Phi_i | \Psi_n \rangle \quad \forall i$$

- Expansion in harmonic oscillator (HO) Slater determinants $|\Phi_i\rangle$ with frequency $\hbar\Omega$ of single-particle states

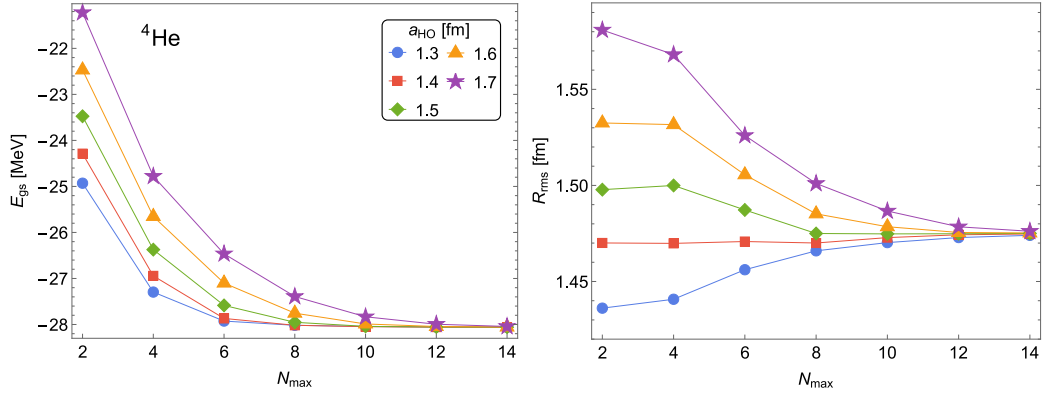
$$a_{\mathrm{HO}} = \sqrt{\frac{\hbar}{m\Omega}}$$

- Truncation to finite model space via $E_* - E_0 \leq N_{\max}\hbar\Omega$

- Recover full Hilbert space for $N_{\max} \to \infty$



No-Core Shell Model (NCSM)



- Convergence dependent on a_{HO}
- Requires calculations for multiple a_{HO} to determine best converging sequence

Natural Orbitals (NATs)

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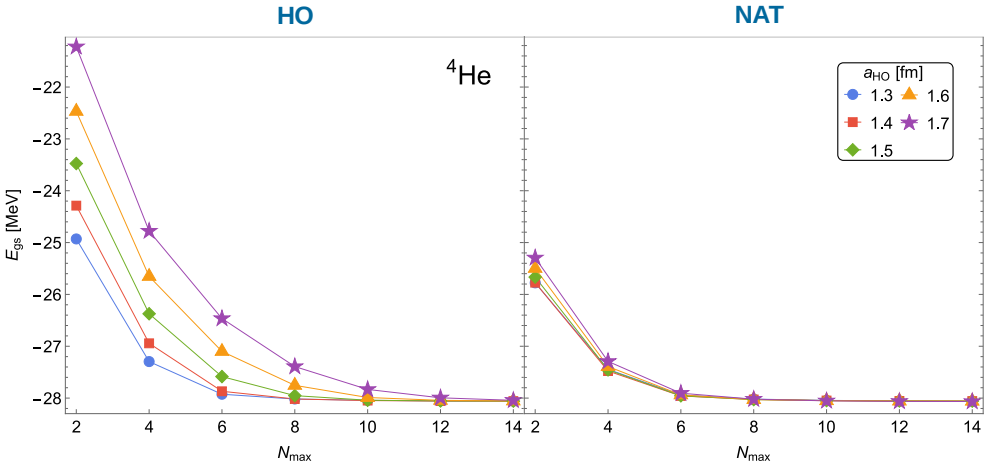
- Problem:
  - Long-range behavior of nuclear wave function is exponential $|\Psi\rangle \propto e^{-r}$
  - Single-particle HO wave functions have Gaussian fall-off: $|\phi\rangle \propto e^{-r^2}$

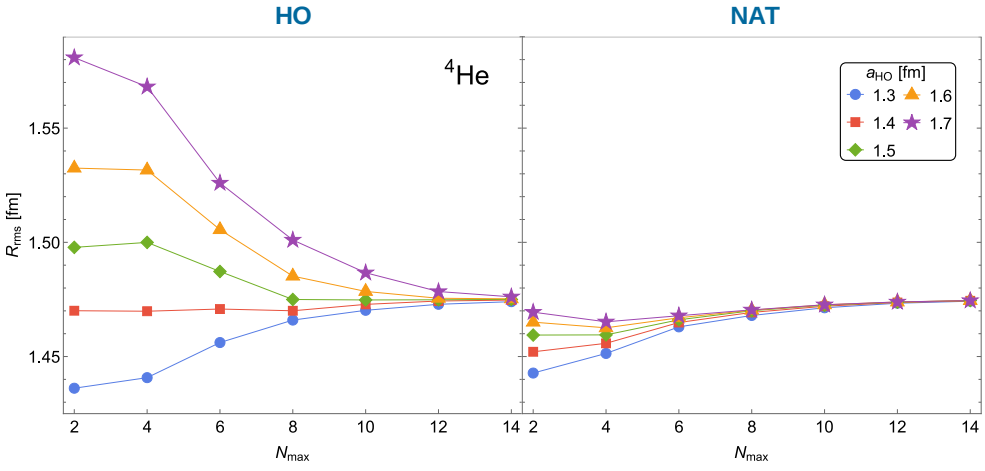
- Aim: Physically more reasonable single-particle basis & improved convergence

Natural Orbitals (NATs)



NATs almost independent of a_{HO}

Natural Orbitals (NATs)



HO:
Adjustment via a_{HO} possible to better assess converged value

Scaled Natural Orbitals (SNATs)

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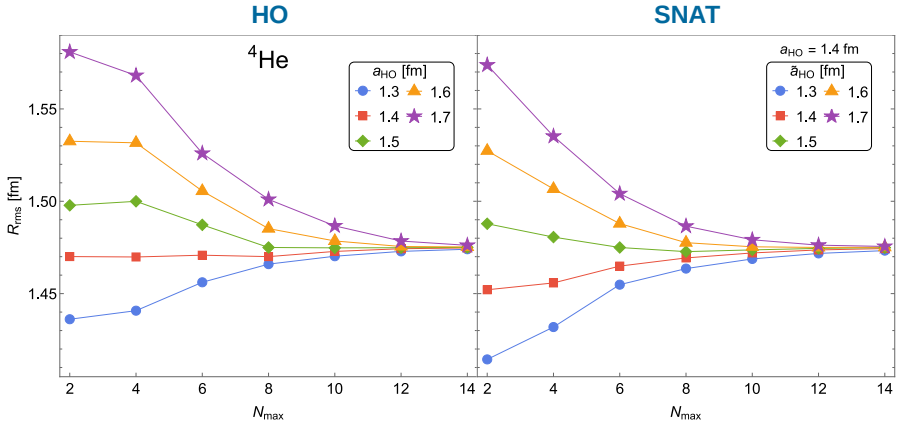
More physical long-range behavior of NATs

Controllable length parameter like in HO basis

Scaled Natural Orbitals

by stretching/ compressing NATs



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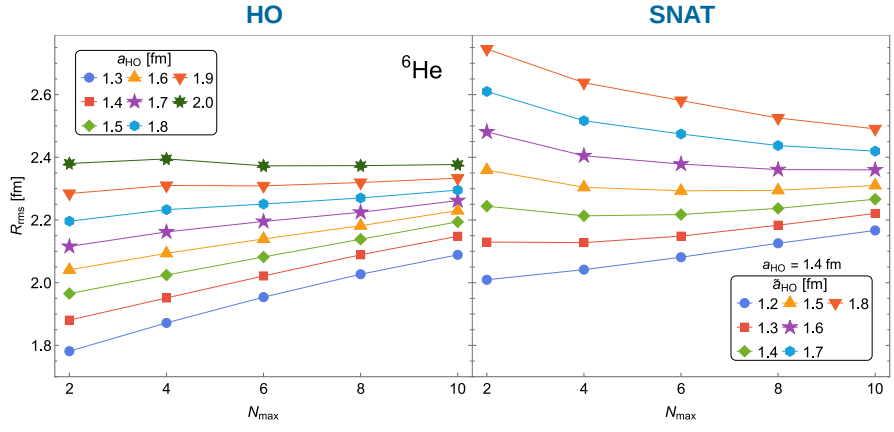
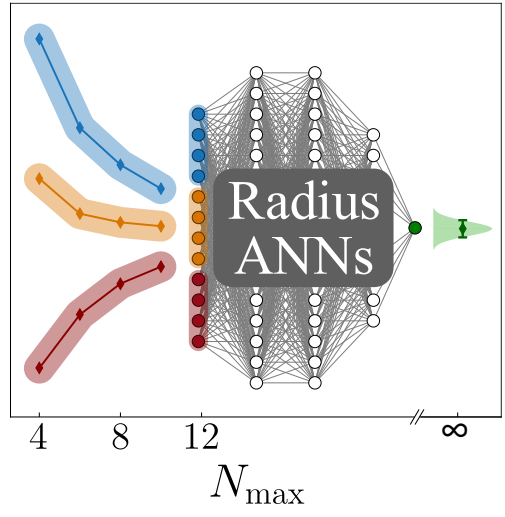


SNATs: Facilitate extraction of radius value

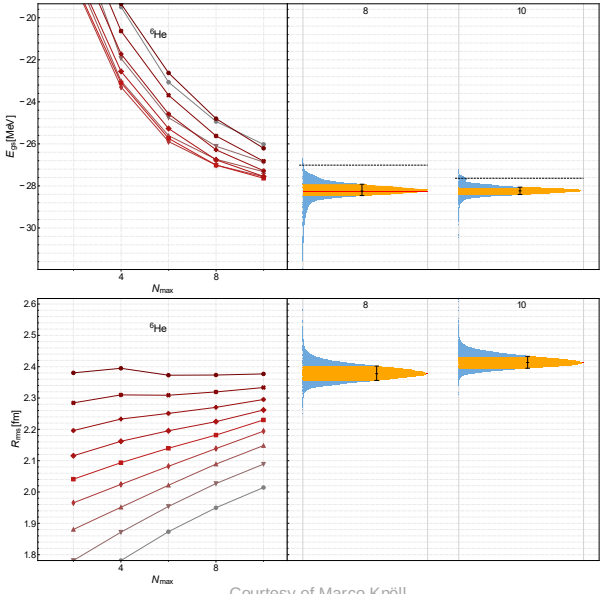
Artificial Neural Networks (ANNs)

- Idea: Capture convergence pattern via artificial neural networks (ANNs)
- Trained on very light nuclei
- Application to heavier nuclei which cannot be fully converged
- Input: Data points 4 consecutive $N_{\max}$ and 3 sequences
- Output: Prediction of converged value
- Sampling & evaluation via multiple ANNs → statistical uncertainty estimate



Courtesy of Tobias Wolfgruber

Artificial Neural Networks (ANNs)



Courtesy of Marco Knöll

- Final prediction: Most likely value
- Uncertainty interval contains 68% of values
- Predictions consistent within uncertainty intervals

Conclusion

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- Two ways to increase precision for extracting a value from NCSM calculations:

1. Optimization of single particle basis for more physical long-range behavior & controlling sequences via length parameter
2. ANNs to predict converged value with uncertainties from not fully converged sequences

Thank you for your attention!

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