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Scaled Natural Orbitals for Nuclear Radii

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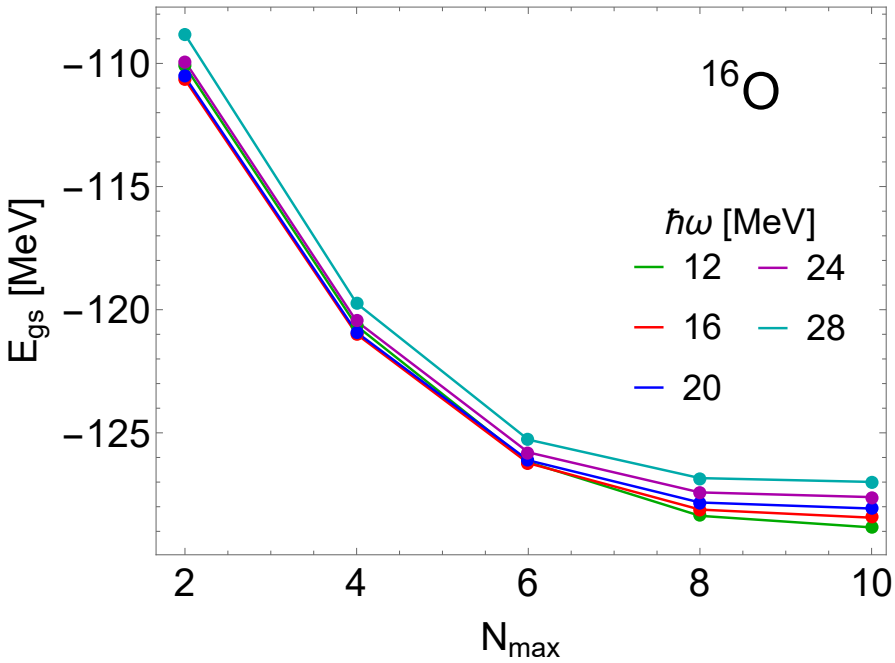
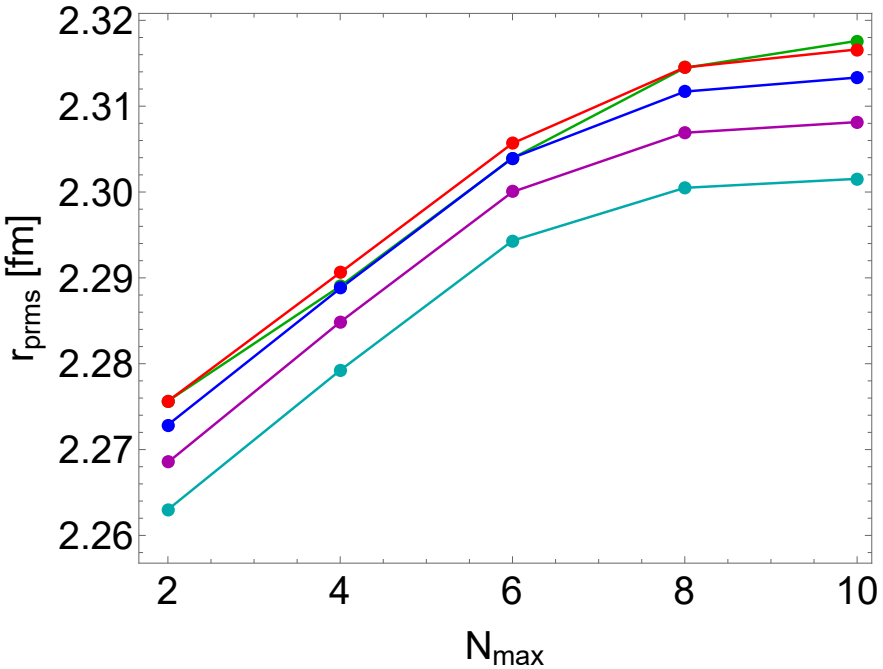
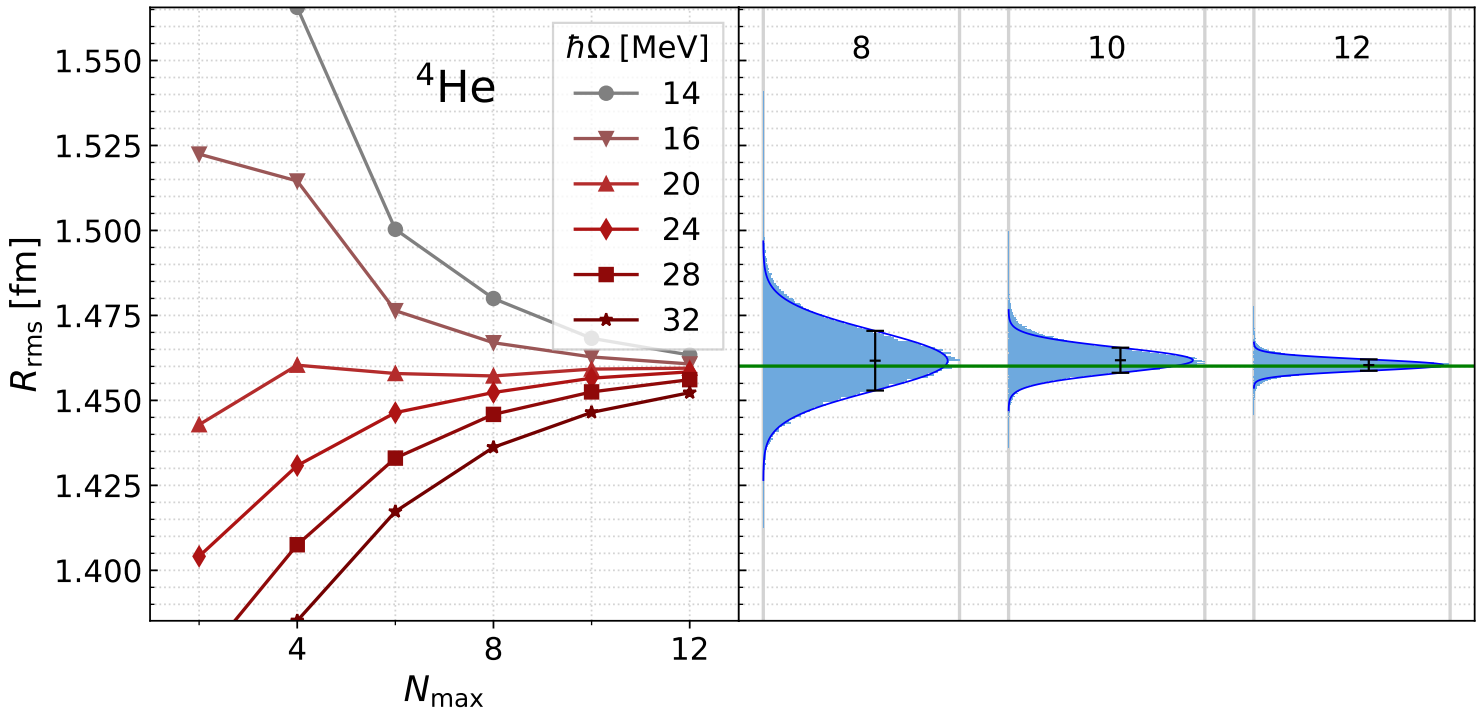
Motivation





- Natural orbitals are great tool in all kinds of many-body methods
- Convergence almost independent of underlying HO basis frequency

Motivation



Courtesy of Tobias Wolfgruber

- Generate radius sequences converging from above as evaluation data for artificial neural networks (ANNs)

Natural Orbitals (NATs)

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Scaled Natural Orbitals (SNATs)

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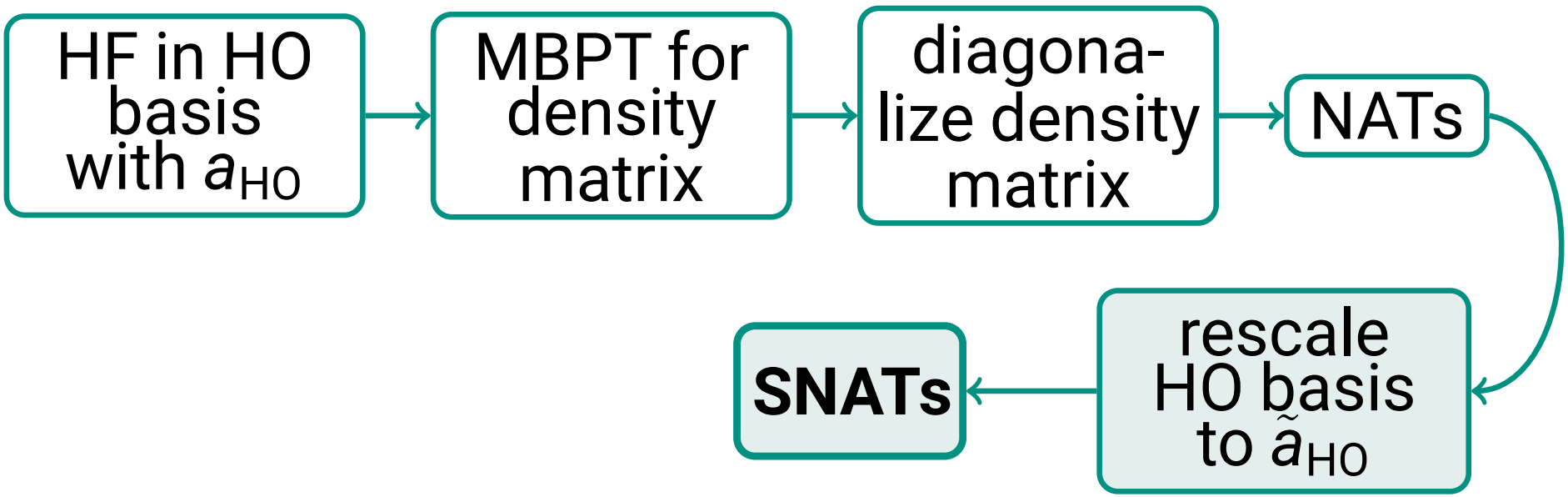
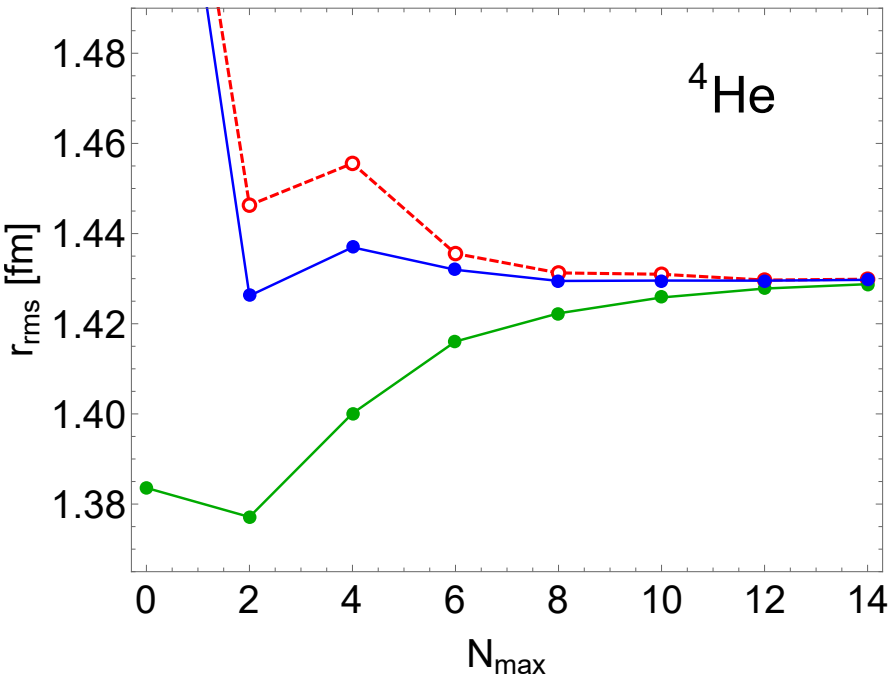
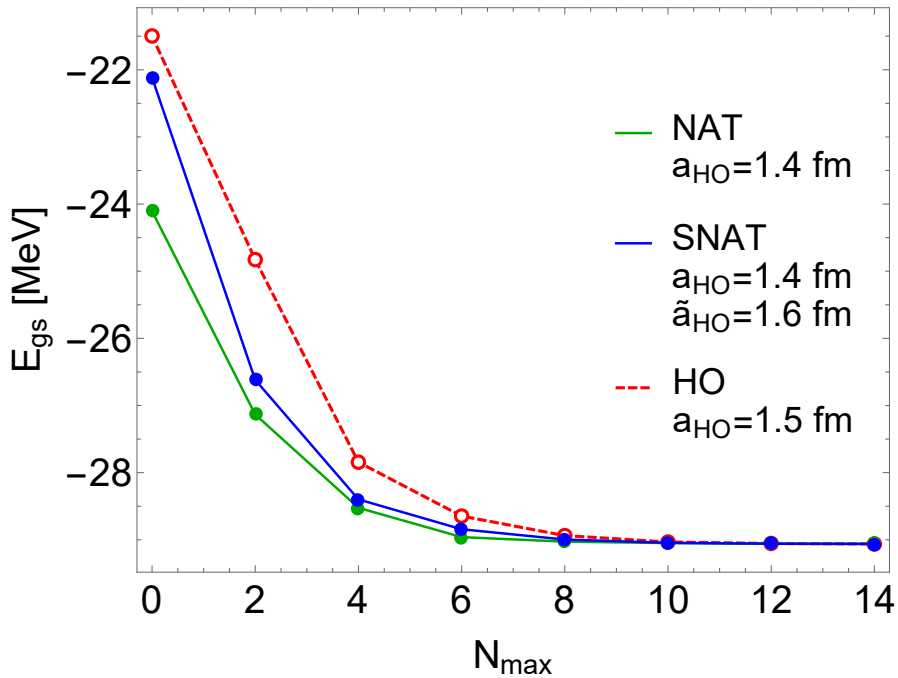


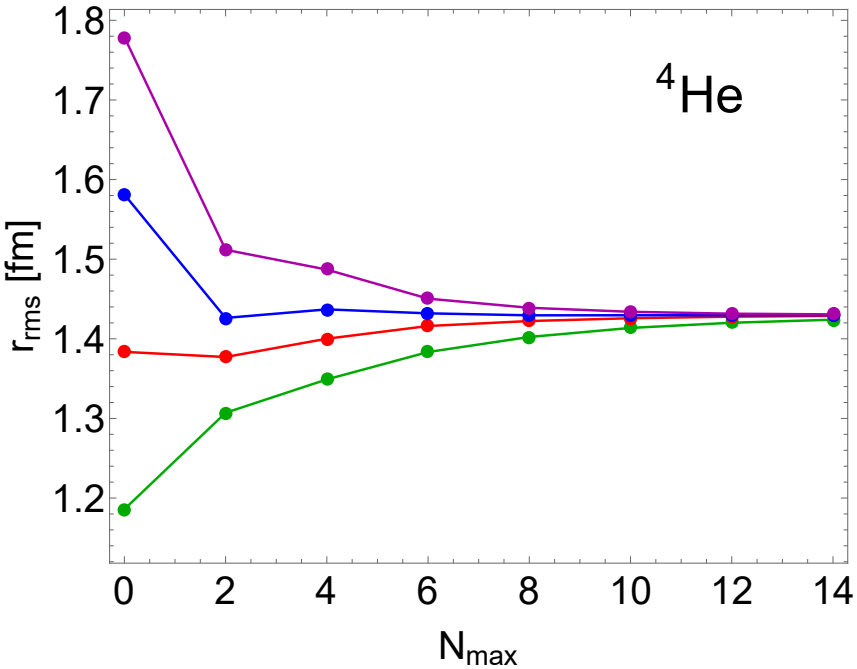
Optimal Convergence

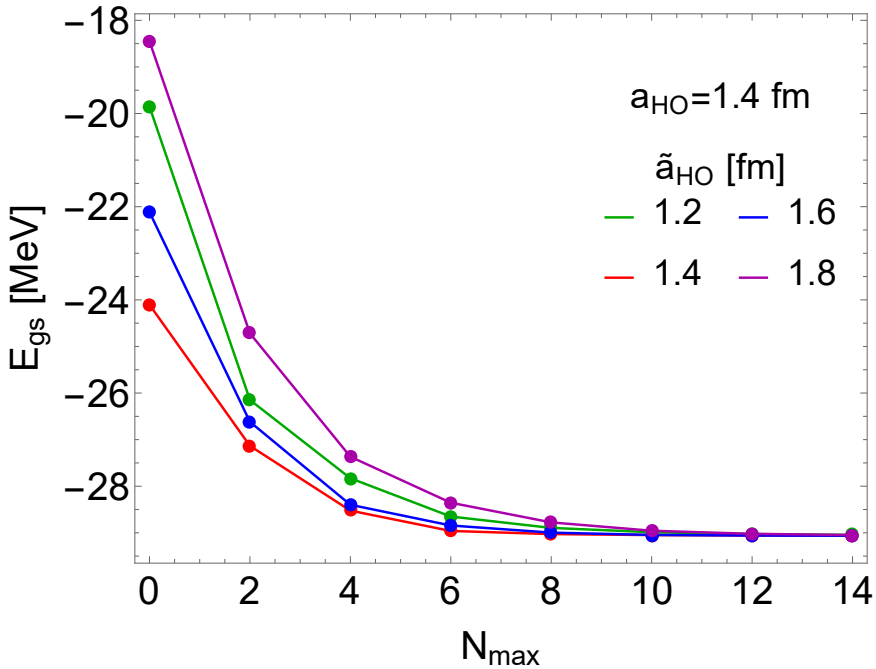




- Easy to dial-in optimal radius convergence with SNATs
- No significant loss in convergence rate for energy

Convergence From Above





- Generate radius sequences converging from above & below
- Next step: Application as evaluation data for ANNs

Scaled Natural Orbitals for Nuclear Radii

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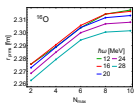
Lisa Wagner and Robert Roth

Motivation

- Natural orbitals (NATs) [1]: Improved energy convergence over standard HO NCSM
- But: Radii still differ significantly from converged results for small model spaces
- Change in HO frequency cannot influence this unlike in HO calculations



Aim

(1) Introduce parameter in NAT construction that allows shifting of radius sequences towards optimal curve

(2) Generate radius sequences converging from above as evaluation data for artificial neural networks (ANNs) [2]

Natural Orbitals

- Hartree-Fock (HF) calculation from single Slater determinant (SD) $|\phi_{\mathrm{HF}}\rangle \propto |\varphi_1 \dots \varphi_A\rangle$ as reference state
- Minimization of nucleonic Hamiltonian expectation value in reference state under preservation of normalization of single particle orbitals $|\varphi_i\rangle$ $\delta\left[\langle\phi_{\mathrm{HF}}|H|\phi_{\mathrm{HF}}\rangle - \sum_i \epsilon_i\left(\langle\varphi_i|\varphi_i\rangle - 1\right)\right] = 0$ yields HF equations
- Solve HF equations self-consistently to obtain HF basis of single SDs
- Construct one-body density matrix from perturbatively improved HF ground state
- Diagonalization of density matrix gives natural orbitals

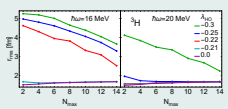
External Constraint

- Modify intrinsic one-body Hamiltonian of HF calculation by adding external potential
- Keep Hamiltonian for NAT calculation unaltered
- Prefactor λ of external potential allows for adjustment of strength
  → Parameter for alteration of radius sequence

HO Potential

- External potential: $\lambda_{\mathrm{HO}} \cdot r^2$
- Matrix elements in single-particle HO basis [3]:

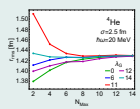
$$\langle nl|r^2|n'l'\rangle = \begin{cases} a_{\mathrm{HO}}^2(l+2n+1.5), & n=n' \\ -a_{\mathrm{HO}}^2\sqrt{n(l+n+0.5)}, & n=n'-1 \\ -a_{\mathrm{HO}}^2\sqrt{(l+n+1.5)(n+1)}, & n=n'+1 \end{cases}$$



Problem:
- Sudden, frequency dependent jumps in radius sequence for small changes in λ_{HO}
- Extreme fine tuning necessary
  → Impractical

Gaussian Potential

- External potential: $\lambda_G \cdot e^{-r^2/2\sigma^2}$
- Numerical calculation of matrix elements in single-particle HO basis



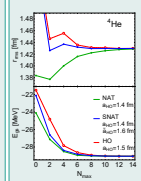
Problem:
- No simple correspondence between λ_G and radius sequence
- Finding λ_G for optimal radius convergence becomes trial-and-error based
  → Impractical

Outlook

- Apply SNATs to heavier nuclei
- Feed multiple convergence sequences into ANNs as evaluation data to improve radius prediction of heavier nuclei
- Explore applicability to other observables, e.g. electric quadrupole moment

Scaled Natural Orbitals (SNATs)

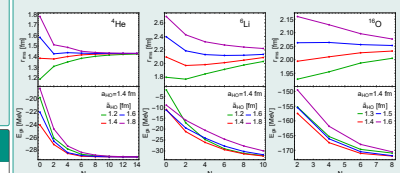
- Calculate NAT expansion coefficients for specific HO oscillator length a_{HO}
- Use these coefficients to expand in HO basis with secondary, larger $\tilde{a}_{\mathrm{HO}}$
  → Stretch NAT basis



- Optimal radius convergence easily achievable with SNATs
- No loss in energy convergence speed compared to HO results with similar radius sequence

Advantage over HO:
- HO basis first requires nucleus-dependent optimization of a_{HO}
- NATs frequency independent, so a_{HO} can be picked freely without optimization
- Choose $\tilde{a}_{\mathrm{HO}}$ larger by a fixed amount relative to a_{HO} depending on deviation from converged value for small model space sizes

Rms radii and ground state energies calculated with non-local chiral NN interaction at N^{3}LO with cutoff parameter $\Lambda = 500$ MeV and SRG evolution with flow parameter $\alpha = 0.08\,\mathrm{fm}^4$.



- SNATs allow for reliable creation of radius convergence sequences from above across different nuclei
  → Applicable for generation of ANN evaluation data

References

[1] A. Tichai, J. Müller, K. Vobig, and R. Roth, Phys. Rev. C **99** (2019).
[2] M. Knöll, T. Wolfgruber, M. L. Agel, C. Wenz, and R. Roth, Phys. Lett. B **839**, 137781 (2023).
[3] D. J. Rowe, J. Phys. A: Math. Gen. **38**, 10181 (2005).

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Further information on my poster

Thank you for your attention!

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