



Machine Learning for *Ab Initio* Nuclear Structure Calculations

Tobias Wolfgruber

Progress in *Ab Initio* Nuclear Theory
TRIUMF 2023

No-Core Shell Model

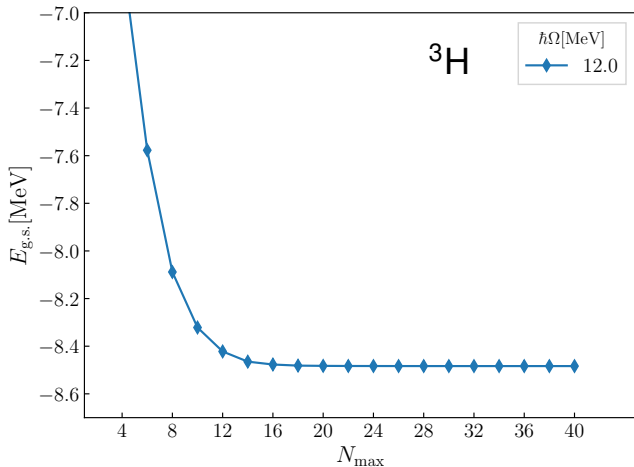


- ▶ stationary Schrödinger equation as matrix eigenvalue problem
- ▶ Slater determinants $|\phi_i\rangle$ constructed from HO basis
→ dependency on HO frequency $\hbar\Omega$
- ▶ truncate model space by number of excitation quanta N_{\max}
w.r.t. the lowest-energy Slater determinant

No-Core Shell Model

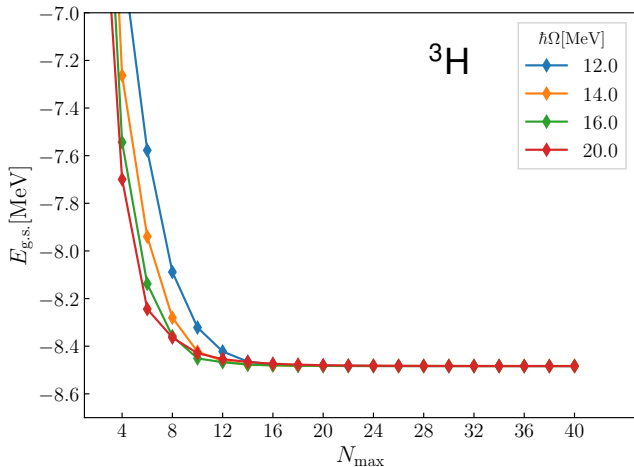
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- ▶ Slater determinants $|\phi_i\rangle$ constructed from HO basis
→ dependency on HO frequency $\hbar\Omega$
- ▶ truncate model space by number of excitation quanta N_{\max}
w.r.t. the lowest-energy Slater determinant
- ▶ **convergence controlled by two parameters**

Convergence Behavior



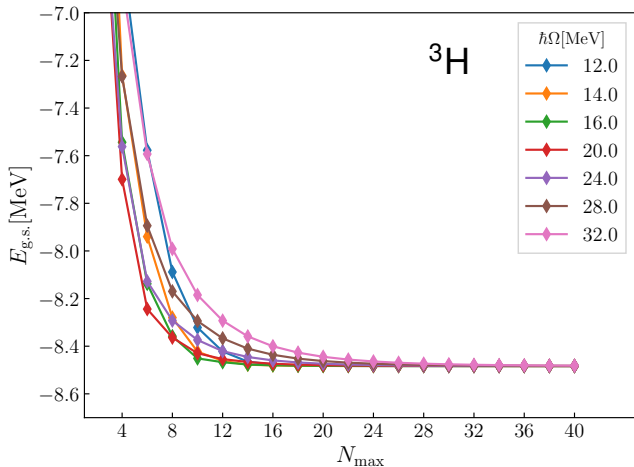
▶ monotonously
decreasing with
 N_{\max}

Convergence Behavior



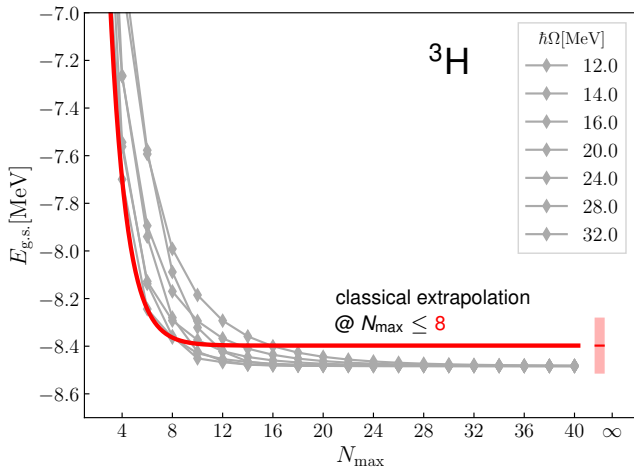
- ▶ monotonously decreasing with N_{\max}
- ▶ different rates of convergence for different HO frequencies

Convergence Behavior



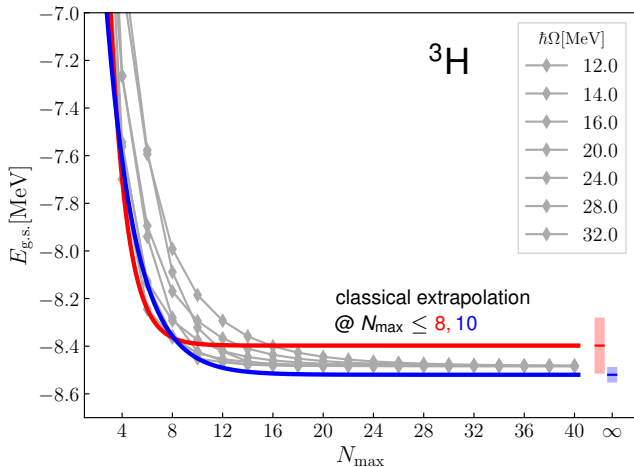
- ▶ monotonously decreasing with N_{\max}
- ▶ different rates of convergence for different HO frequencies
- ▶ all sequences share the same limit

Convergence Behavior



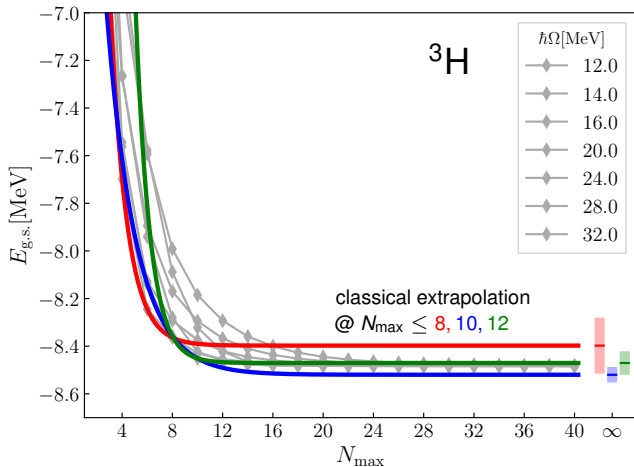
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Convergence Behavior



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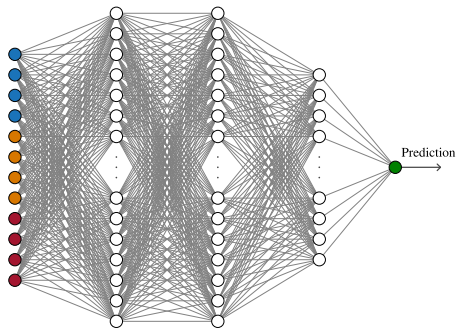
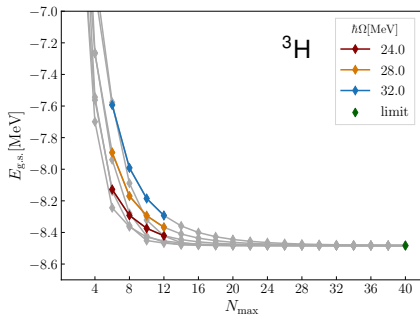
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Machine Learning Approach

- ▶ previous applications: capture $f(N_{\max}, \hbar\Omega)$
- ▶ now: directly predict converged value from available calculations
 - ▶ include information of multiple frequencies

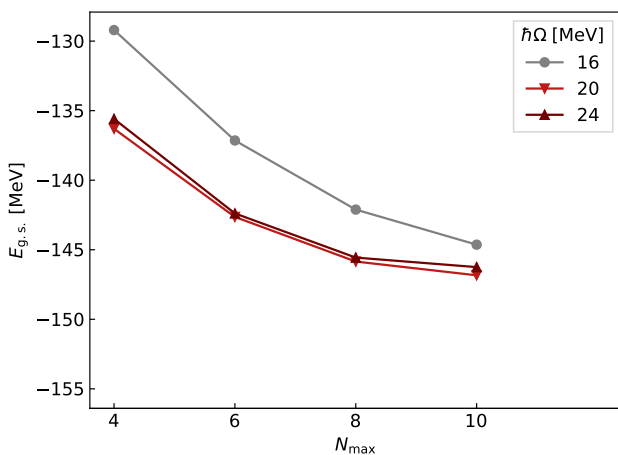
Negoita et al. PR C 99, 054308 (2019)

Jiang et al. PR C 100, 054326 (2019)



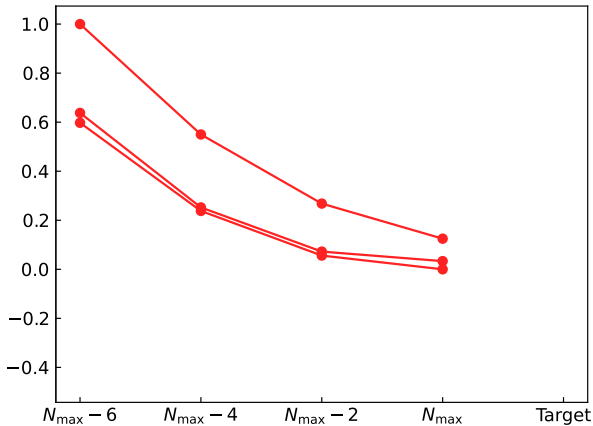
Knöll, TW et al. PLB 839, 137781 (2023)

^{16}O Prediction



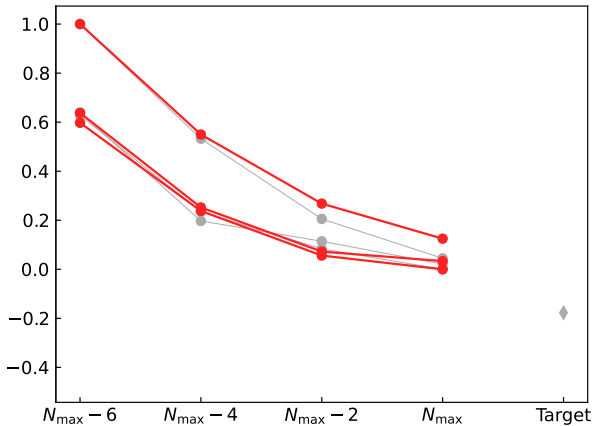
▶ ^{16}O sequence

^{16}O Prediction



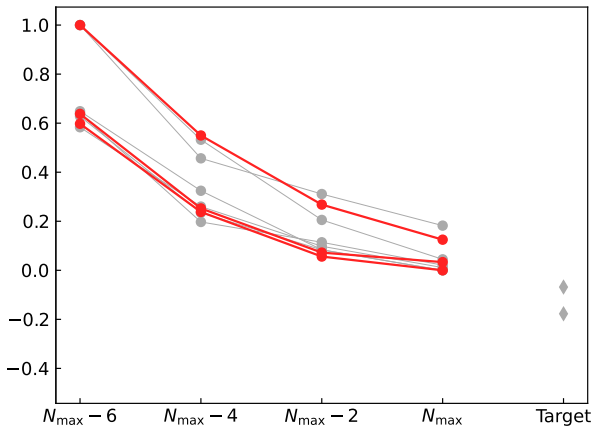
- ▶ ^{16}O sequence sample
- ▶ no N_{\max} or $\hbar\Omega$ information
- ▶ New: MINMAX norm
→ rescale to $[0, 1]$

^{16}O Prediction



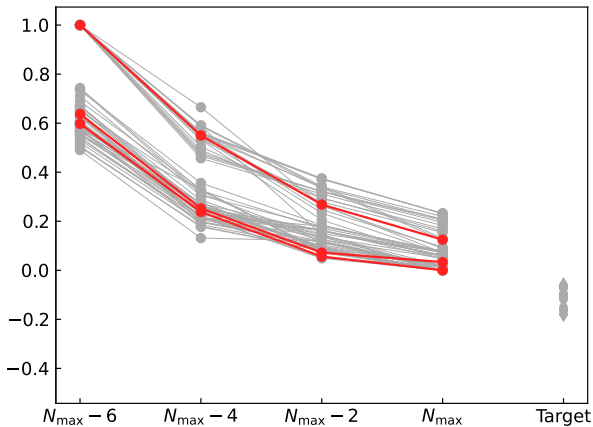
- ▶ ^{16}O sequence sample
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→ rescale to [0, 1]
- ▶ very similar to ^2H training samples

^{16}O Prediction



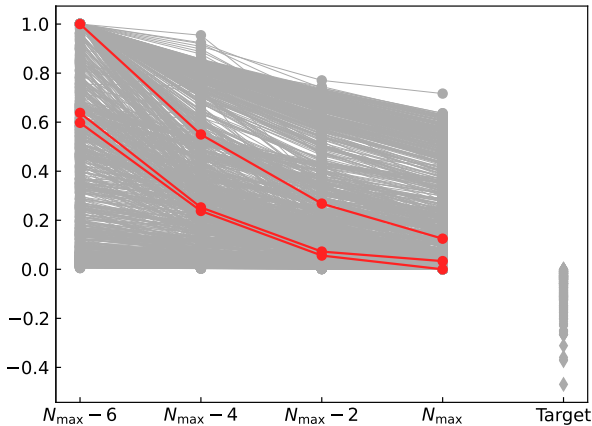
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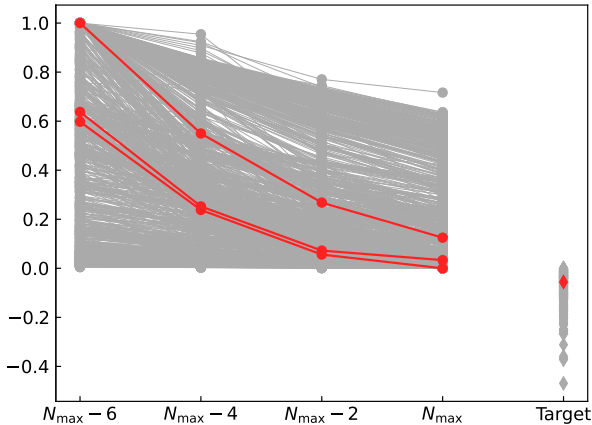
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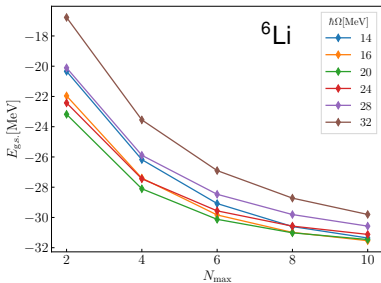


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- ▶ total of 340 200 samples across ^2H , ^3H , and ^4He

^{16}O Prediction

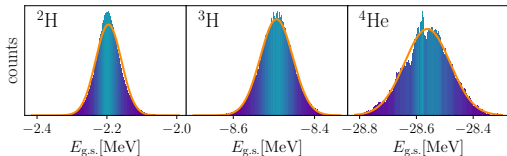


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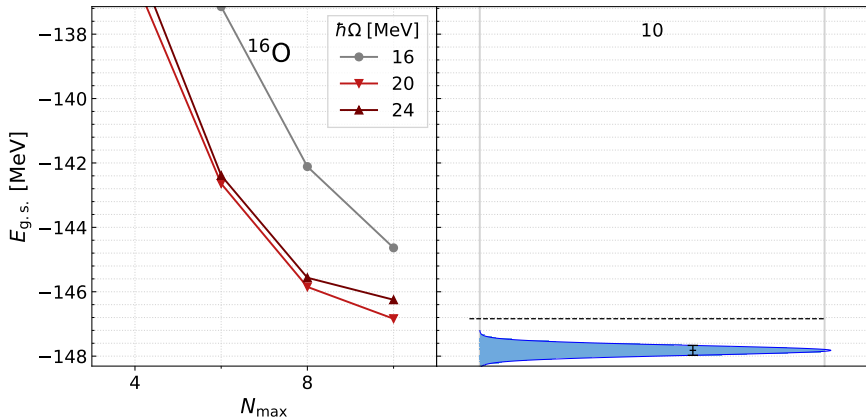


- ▶ apply 1000 ANN
- ▶ prediction and uncertainty from Gaussian fit

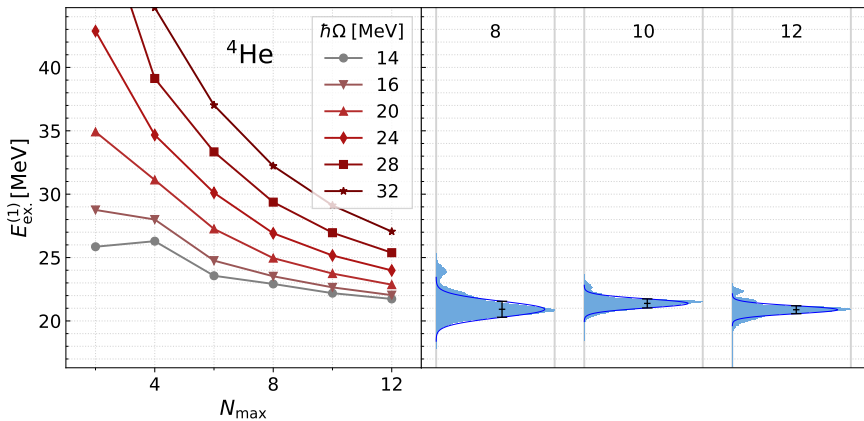
- ▶ different family of interactions
Maris et al. PR C 103, 054001 (2021)
- ▶ construction of evaluation samples analogously to training samples
- ▶ different predictions from one ANN
- ▶ turn to statistical approach



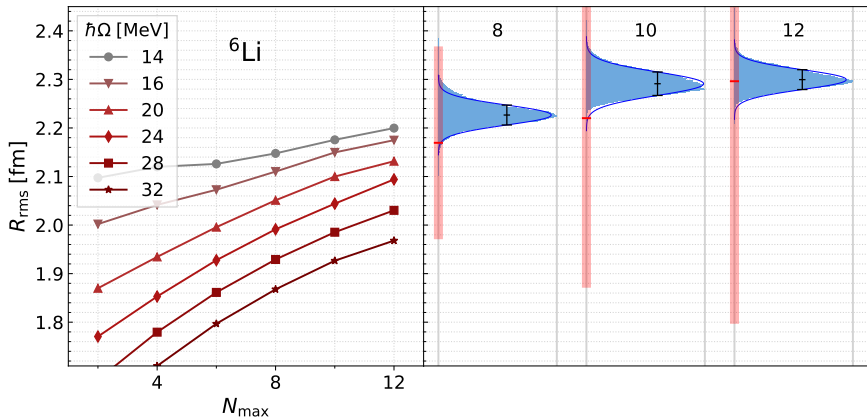
^{16}O Ground-State Energy



^4He Excitation Energy



${}^6\text{Li}$ Radius



Thank you for your attention!

► thanks to my group and collaborators

P. Falk, K. Katzenmeier, **M. Knöll**, L. Mertes,
J. Müller, **R. Roth**, L. Wagner, C. Wenz



Machine Learning for Ab Initio Nuclear Structure Calculations



Tobias Wolflgruber, Marco Knoll & Robert Roth

Motivation	No-Core Shell Model	Methodology and Network Topology
<p>Only only fewer resources to compute ground state for full droplet, use ML procedure, more for development to reduce the cost and improve the accuracy of many-body methods in nuclear structure theory, like the no-core shell model (NCSM) [1]. ML methods are used to approximate NCSM, which has already been used to predict ground state physics [2, 3]. ML methods are used to approximate NCSM, which has already been used to predict ground state physics [2, 3]. ML methods are used to approximate NCSM, which has already been used to predict ground state physics [2, 3].</p>	<p>no-core many-body Schrödinger equation to solve the nuclear structure problem</p> $\sum_{\alpha} \langle \Psi \hat{H} \alpha \rangle \langle \alpha \Psi \rangle = E_0 \langle \Psi \Psi \rangle$ <p>State determinants $\alpha\rangle$ are constructed from 182 basis → dependency on 182 frequency for model space truncated via total number of basis spinors N_{spin} convergence controlled by N_{spin} basis for $N_{spin} \rightarrow \infty$ independent of Ω energies systematically decreasing with N_{spin} other observables: static or resonance or non-ergodic pattern</p>	<p>fully connected feed-forward neural network</p> <ul style="list-style-type: none"> apply trained NNs to arbitrary nuclei accessible in the NCSM evaluate all predictions consistently to extract converged value and uncertainty <p>layer sizes: 12, 48, 96, 24, 1</p>
<p>ground state energy results</p> <ul style="list-style-type: none"> ground state energy calculated only within a shell shell much better than classical extrapolation [2] to avoid shell gaps observed state split and less state dependent results with NCSM nuclear structure theory 	<p>calculating excitation energies, use NCSM to extract ground state energies</p> <p>apply NNs to ground and excited state absolute energies separately</p> <p>validate different ML and compare for all NNs and parameters in whole distribution</p>	<p>Training Data, Training & Statistical Evaluation</p> <ul style="list-style-type: none"> train on few body data (^2He, ^3He, and ^4He) for which the converged value can be easily obtained via shell-NCSM calculations use calculations of 76 different observables (binding energy, static radii, and SFC) for 7 different 182 frequency (12-24 MeV) the generator a total of 182 20 energy training samples generally full fit to the results in a range of observable quantities which differ in 182 frequency for the case of intermediate N_{spin} values only the network fits the information about the machine, interaction, NCSM or the specific 182 frequency or N_{spin} values apply NNs to extrapolate to each training sample to extract all values of observables via the neural NN prevent overfitting and overfitting due to divergence present in the ground state energy values applying the networks in heavier nuclei statistical approach with 1000 NNs and Gaussian fit to extract prediction and uncertainty
<p>Radius Results</p> <ul style="list-style-type: none"> radii are a lot more challenging than ground or excited state energies → no statistical principle to restrict convergence behavior need at least one more N_{spin} step than energies for reasonably good results generally more stable and precise than classical extrapolation technique 	<p>Conclusion</p> <ul style="list-style-type: none"> data from lighter systems up to ^4He allow to train NNs used for general state in heavier system generally independent classical energy methods especially in smaller nuclei space universal approach network topology works well for the ground and excited state energies, radii and mass more observations only case more generalizable and precise of radius, interaction, ... 	<p>Outlook</p> <ul style="list-style-type: none"> generate state independent training data using artificially modified ground or state ray parameters generate more training quality and improve any existing NNs make observables available in few-body systems that are not present in realistic potential, e.g. observables more transitions, ... expand to more observables Further optimize network topology

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